

Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2021 – 01:17 pm BST

PDB ID	:	7A0K
Title	:	Crystal structure of the entire ectodomain from the Physcomitrella patens
		receptor kinase CR4
Authors	:	Hothorn, M.; Okuda, S.
Deposited on	:	2020-08-09
Resolution	:	2.70 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	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive	Similar resolution
	$(\# \mathbf{Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122(2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069(2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	383	% 91%	6% ·
1	В	383	89%	6% 5%
1	С	383	91%	• 5%
1	D	383	90%	5% •
1	Е	383	<mark>6%</mark> 91%	5% •



Mol	Chain	Length	Quality of chain		
1	F	383	88%	7%	5%
1	G	383	91%	•	5%
1	Н	383	89%	•	7%
2	Ι	2	100%		
2	К	2	50% 50%		
2	М	2	100%		
2	О	2	50% 50%		
2	Q	2	100%		
2	S	2	50% 50%		
2	Т	2	100%		
2	U	2	100%		
3	J	2	100%		
3	Ν	2	100%		
3	Р	2	50% 50%		
3	R	2	100%		
4	L	3	100%		

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	Н	502	-	-	-	Х
7	EDO	А	503	-	-	-	Х
7	EDO	A	504	-	-	-	Х



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 21072 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		At	oms			ZeroOcc	AltConf	Trace
1	Δ	260	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	A	309	2610	1639	434	505	32	0	0	0
1	В	363	Total	С	Ν	Ο	S	0	0	0
	D	303	2582	1618	431	501	32	0	0	0
1	C	363	Total	С	Ν	Ο	S	0	0	0
		303	2559	1604	429	494	32	0	0	0
1	П	367	Total	С	Ν	0	S	0	0	0
		307	2576	1616	433	495	32	0	0	0
1	F	367	Total	С	Ν	Ο	S	0	0	0
		307	2570	1611	429	498	32	0	0	0
1	Б	262	Total	С	Ν	Ο	S	0	0	0
	Г	303	2542	1595	422	493	32	0	0	0
1	C	364	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	G	304	2540	1589	423	496	32	0	0	0
1	ц	358	Total	С	Ν	0	S	0	0	0
L 1		358	2435	1525	410	469	31			U

• Molecule 1 is a protein called Predicted protein.

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	406	LEU	-	expression tag	UNP A9RKG8
А	407	GLU	-	expression tag	UNP A9RKG8
А	408	ASN	-	expression tag	UNP A9RKG8
А	409	LEU	-	expression tag	UNP A9RKG8
A	410	TYR	-	expression tag	UNP A9RKG8
А	411	PHE	-	expression tag	UNP A9RKG8
А	412	GLN	-	expression tag	UNP A9RKG8
В	406	LEU	-	expression tag	UNP A9RKG8
В	407	GLU	-	expression tag	UNP A9RKG8
В	408	ASN	-	expression tag	UNP A9RKG8
В	409	LEU	-	expression tag	UNP A9RKG8
В	410	TYR	-	expression tag	UNP A9RKG8
В	411	PHE	-	expression tag	UNP A9RKG8



Chain	Residue	Modelled	Actual	Comment	Reference
В	412	GLN	-	expression tag	UNP A9RKG8
С	406	LEU	-	expression tag	UNP A9RKG8
С	407	GLU	-	expression tag	UNP A9RKG8
С	408	ASN	-	expression tag	UNP A9RKG8
С	409	LEU	-	expression tag	UNP A9RKG8
С	410	TYR	-	expression tag	UNP A9RKG8
С	411	PHE	-	expression tag	UNP A9RKG8
С	412	GLN	-	expression tag	UNP A9RKG8
D	406	LEU	-	expression tag	UNP A9RKG8
D	407	GLU	-	expression tag	UNP A9RKG8
D	408	ASN	-	expression tag	UNP A9RKG8
D	409	LEU	-	expression tag	UNP A9RKG8
D	410	TYR	-	expression tag	UNP A9RKG8
D	411	PHE	-	expression tag	UNP A9RKG8
D	412	GLN	-	expression tag	UNP A9RKG8
E	406	LEU	-	expression tag	UNP A9RKG8
E	407	GLU	-	expression tag	UNP A9RKG8
Е	408	ASN	-	expression tag	UNP A9RKG8
Е	409	LEU	-	expression tag	UNP A9RKG8
E	410	TYR	-	expression tag	UNP A9RKG8
Е	411	PHE	-	expression tag	UNP A9RKG8
E	412	GLN	-	expression tag	UNP A9RKG8
F	406	LEU	-	expression tag	UNP A9RKG8
F	407	GLU	-	expression tag	UNP A9RKG8
F	408	ASN	-	expression tag	UNP A9RKG8
F	409	LEU	-	expression tag	UNP A9RKG8
F	410	TYR	-	expression tag	UNP A9RKG8
F	411	PHE	-	expression tag	UNP A9RKG8
F	412	GLN	-	expression tag	UNP A9RKG8
G	406	LEU	-	expression tag	UNP A9RKG8
G	407	GLU	-	expression tag	UNP A9RKG8
G	408	ASN	-	expression tag	UNP A9RKG8
G	409	LEU	-	expression tag	UNP A9RKG8
G	410	TYR	-	expression tag	UNP A9RKG8
G	411	PHE	-	expression tag	UNP A9RKG8
G	412	GLN	-	expression tag	UNP A9RKG8
Н	406	LEU	-	expression tag	UNP A9RKG8
H	407	GLU	-	expression tag	UNP A9RKG8
H	408	ASN	-	expression tag	UNP A9RKG8
H	409	LEU	-	expression tag	UNP A9RKG8
H	410	TYR	-	expression tag	UNP A9RKG8
Н	411	PHE	-	expression tag	UNP A9RKG8



Chain	Residue	Modelled	Actual	Comment	Reference
Η	412	GLN	-	expression tag	UNP A9RKG8

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2 I	I	2	Total	С	Ν	Ο	0	0	0
	_	24	14	1	9	Ŭ	0		
2	K	2	Total	\mathbf{C}	Ν	Ο	0	Ο	Ο
	11		24	14	1	9	0	0	0
0	М	2	Total	С	Ν	Ο	0	0	0
	111	Δ	24	14	1	9	0		
0	0	2	Total	С	Ν	Ο	0	0	0
	0		24	14	1	9		0	
0	0	2	Total	С	Ν	Ο	0	0	0
	Q		24	14	1	9			
0	c	0	Total	С	Ν	Ο	0	0	0
	G	Δ	24	14	1	9	0	0	0
0	т	2	Total	С	Ν	Ο	0	0	0
	1	Δ	24	14	1	9	0	0	0
0	T	2	Total	С	Ν	Ο	0	0	0
2	U		24	14	1	9	U		U

• 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	J	2	Total C N O 28 16 2 10	0	0	0
3	Ν	2	Total C N O 28 16 2 10	0	0	0
3	Р	2	Total C N O 28 16 2 10	0	0	0



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
3	R	2	Total 28	C 16	N 2	O 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
4	L	3	Total (39 2	C N 22 2	O 15	0	0	0

• Molecule 5 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
5	А	1	Total 9	С 4	O 5	0	0

• Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	Λ	1	Total	С	Ν	0	0	0	
0	А	L	14	8	1	5	0	0	
6	В	1	Total	С	Ν	Ο	0	0	
0	D	T	14	8	1	5	0	0	
6	С	1	Total	С	Ν	Ο	0	0	
0	U	I	14	8	1	5	0	0	
6	П	1	Total	С	Ν	Ο	0	0	
0	D	T	14	8	1	5	0	0	
6	E	1	Total	С	Ν	Ο	0	0	
0	Ľ	L	14	8	1	5	0		
6	F	1	Total	С	Ν	Ο	0	0	
0	T	, I	14	8	1	5	0	0	
6	G	1	Total	С	Ν	Ο	0	0	
0	u	, I	14	8	1	5	0	0	
6	G	1	Total	С	Ν	Ο	0	0	
0	u	I.	14	8	1	5	0	0	
6	н	1	Total	С	Ν	Ο	0	0	
	11	1	14	8	1	5	0	U	
6	н	1	Total	С	N	0	0	0	
	11		14	8	1	5			

• Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





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

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	32	$\begin{array}{cc} \text{Total} & \text{O} \\ 32 & 32 \end{array}$	0	0
8	В	42	$\begin{array}{cc} \text{Total} & \text{O} \\ 42 & 42 \end{array}$	0	0
8	С	10	Total O 10 10	0	0
8	D	9	Total O 9 9	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	Ε	14	Total O 14 14	0	0
8	F	4	Total O 4 4	0	0
8	G	14	Total O 14 14	0	0
8	Н	9	Total O 9 9	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: Predicted protein





• Molecule 2:	2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-	glucopyranose
Chain I:	100%	_
NAG1 FUC2		
• Molecule 2:	2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-	glucopyranose
Chain K:	50% 50%	_
NAG 1 FUC2		
• Molecule 2:	2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-	glucopyranose
Chain M:	100%	
NAG1 FUC2		
• Molecule 2:	2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-	glucopyranose
Chain O:	50% 50%	
FUC2		
• Molecule 2:	2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-	glucopyranose
Chain Q:	100%	
NAG1 FUC2		
• Molecule 2:	2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-	glucopyranose
Chain S:	50% 50%	
INAG 1 FUC2		
• Molecule 2:	2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-	glucopyranose
Chain T:	100%	
NAG1 FUC2		
• Molecule 2:	: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-	glucopyranose
Chain U:	100%	_
	WORLDWIDE PROTEIN DATA BANK	

NAG1 FUC2

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

Chain J:		100%			
NAG1 NAG2					
• Molecule 3: opyranose	2-acetamido-2-deoxy-	beta-D-glucopyr	anose- $(1-4)$ -2-ace	tamido-2-deoxy-be	ta-D-gluc
Chain N:		100%			
NAG1 NAG2					
• Molecule 3: opyranose	2-acetamido-2-deoxy-	beta-D-glucopyr	anose-(1-4)-2-ace	etamido-2-deoxy-be	ta-D-gluc
Chain P:	50%		50%		
NAG1 NAG2					
• Molecule 3: opyranose	2-acetamido-2-deoxy-	beta-D-glucopyr	anose-(1-4)-2-ace	etamido-2-deoxy-be	ta-D-gluc
Chain R:		100%			
NAG1 NAG2					
• Molecule 4: etamido-2-de	beta-D-mannopyranos oxy-beta-D-glucopyran	se-(1-4)-2-acetan ose	nido-2-deoxy-beta	a-D-glucopyranose-	(1-4)-2-ac

Chain L: 100%

NAG1 NAG2 BMA3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	88.58Å 183.96Å 98.17Å	Depositor
a, b, c, α , β , γ	90.00° 96.05° 90.00°	Depositor
$\mathbf{Bosolution} \left(\overset{\circ}{\mathbf{A}} \right)$	45.87 - 2.70	Depositor
Resolution (A)	47.18 - 2.70	EDS
$\% { m Data \ completeness}$	99.9(45.87-2.70)	Depositor
(in resolution range $)$	90.2(47.18-2.70)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) > 1$	$0.68 (at 2.69 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
D D .	0.216 , 0.246	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.216 , 0.247	DCC
R_{free} test set	4283 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	61.2	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.30 , 46.0	EDS
L-test for $twinning^2$	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21072	wwPDB-VP
Average B, all atoms $(Å^2)$	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.95% 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.



 $^{^1 {\}rm Intensities}$ 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, NAG, EDO, FUC, MLT

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
IVIOI	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.25	0/2678	0.45	0/3662
1	В	0.26	0/2649	0.48	0/3620
1	С	0.25	0/2624	0.46	0/3588
1	D	0.25	0/2642	0.46	0/3616
1	Е	0.26	0/2636	0.47	0/3608
1	F	0.25	0/2608	0.45	0/3569
1	G	0.26	0/2605	0.46	0/3566
1	Н	0.25	0/2498	0.46	0/3427
All	All	0.25	0/20940	0.46	0/28656

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	2610	0	2431	16	0
1	В	2582	0	2408	15	0
1	С	2559	0	2358	6	0
1	D	2576	0	2385	13	0
1	Е	2570	0	2371	9	0



|--|

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2542	0	2330	20	0
1	G	2540	0	2318	8	0
1	Н	2435	0	2145	9	0
2	Ι	24	0	22	0	0
2	K	24	0	22	0	0
2	М	24	0	22	0	0
2	0	24	0	22	1	0
2	Q	24	0	22	0	0
2	S	24	0	22	0	0
2	Т	24	0	22	0	0
2	U	24	0	22	0	0
3	J	28	0	25	0	0
3	Ν	28	0	25	0	0
3	Р	28	0	25	1	0
3	R	28	0	25	0	0
4	L	39	0	34	0	0
5	А	9	0	4	0	0
6	А	14	0	13	0	0
6	В	14	0	13	0	0
6	С	14	0	13	1	0
6	D	14	0	13	0	0
6	Е	14	0	13	0	0
6	F	14	0	13	1	0
6	G	28	0	26	1	0
6	Н	28	0	26	0	0
7	А	12	0	18	4	0
7	В	12	0	18	0	0
7	С	4	0	6	0	0
7	G	4	0	6	0	0
8	А	32	0	0	0	0
8	В	42	0	0	0	0
8	С	10	0	0	0	0
8	D	9	0	0	0	0
8	Е	14	0	0	0	0
8	F	4	0	0	1	0
8	G	14	0	0	0	0
8	Н	9	0	0	0	0
All	All	21072	0	19238	86	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 2.

All (86) 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)	
1:F:200:GLU:OE2	1:F:216:GLN:NE2	2.24	0.70	
1:A:135:ALA:HB1	1:B:382:SER:HB2	1.75	0.69	
1:B:226:ARG:HG2	2:O:2:FUC:H62	1.81	0.62	
1:F:332:LEU:HB2	1:F:357:ILE:CD1	2.29	0.62	
1:F:241:THR:HG23	1:F:255:LYS:HA	1.85	0.59	
1:A:332:LEU:HB2	1:A:357:ILE:HD13	1.85	0.58	
1:D:110:VAL:O	1:F:74:ARG:NH2	2.36	0.57	
1:A:241:THR:HG23	1:A:255:LYS:HA	1.86	0.56	
1:B:332:LEU:HB2	1:B:357:ILE:HD13	1.88	0.55	
1:D:91:SER:O	1:D:95:ARG:HD3	2.07	0.55	
1:H:241:THR:HG23	1:H:255:LYS:HA	1.88	0.55	
1:H:332:LEU:HB2	1:H:357:ILE:HD13	1.87	0.55	
1:B:322:SER:HB2	1:F:53:ASP:HB2	1.89	0.54	
1:E:241:THR:HG23	1:E:255:LYS:HA	1.89	0.54	
1:G:241:THR:HG23	1:G:255:LYS:HA	1.89	0.54	
1:D:241:THR:HG23	1:D:255:LYS:HA	1.91	0.53	
1:G:332:LEU:HB2	1:G:357:ILE:HD13	1.89	0.53	
1:A:139:ALA:HB2	1:B:388:CYS:H	1.73	0.52	
1:A:38:VAL:O	7:A:504:EDO:O1	2.20	0.52	
1:D:375:SER:OG	1:H:56:ASN:ND2	2.42	0.52	
1:F:231:GLN:NE2	1:F:335:GLU:O	2.42	0.52	
1:F:231:GLN:HE22	1:F:335:GLU:C	2.12	0.52	
1:C:241:THR:HG23	1:C:255:LYS:HA	1.92	0.52	
1:B:37:ALA:HA	1:B:283:VAL:HG21	1.92	0.52	
1:F:221:THR:HB	1:F:234:VAL:HG21	1.91	0.51	
1:B:91:SER:O	1:B:95:ARG:HA	2.11	0.51	
1:E:332:LEU:HB2	1:E:357:ILE:HD13	1.91	0.51	
1:A:248:PHE:H	7:A:503:EDO:H21	1.75	0.51	
1:F:332:LEU:HB2	1:F:357:ILE:HD11	1.92	0.50	
1:D:179:THR:HG21	3:P:1:NAG:H82	1.95	0.49	
1:F:216:GLN:NE2	1:F:217:ASN:HB2	2.28	0.49	
1:F:37:ALA:HA	1:F:283:VAL:HG21	1.94	0.49	
1:A:107:GLU:OE2	1:E:74:ARG:NH1	2.45	0.49	
1:F:240:PHE:HZ	1:F:261:LEU:HD23	1.78	0.48	
1:E:298:LEU:HD22	1:E:299:PRO:HD2	1.96	0.48	
1:B:241:THR:HG23	1:B:255:LYS:HA	1.96	0.48	
1:H:97:PRO:O	1:H:110:VAL:HG22	2.14	0.48	
1:C:358:ASN:OD1	6:C:501:NAG:N2	2.47	0.47	
1:H:208:GLY:HA3	1:H:247:LYS:HA	1.97	0.47	
1:A:139:ALA:HB2	1:B:386:SER:O	2.16	0.46	
1:F:332:LEU:HB2	1:F:357:ILE:HD13	1.97	0.46	
1:H:189:SER:HB2	1:H:191:VAL:HG13	1.98	0.46	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:248:PHE:H	7:A:503:EDO:C2	2.29	0.45	
1:G:72:PRO:HA	1:G:73:PRO:HD3	1.88	0.45	
1:C:189:SER:HB2	1:C:191:VAL:HG13	2.00	0.44	
6:F:501:NAG:H82	8:F:603:HOH:O	2.17	0.44	
1:A:37:ALA:HA	1:A:283:VAL:HG21	2.00	0.44	
1:G:319:MET:HB2	6:G:502:NAG:H81	1.98	0.44	
1:A:82:GLY:N	7:A:504:EDO:O2	2.51	0.44	
1:A:189:SER:HB2	1:A:191:VAL:HG13	1.98	0.43	
1:B:216:GLN:NE2	1:B:217:ASN:HB2	2.33	0.43	
1:E:117:HIS:HB2	1:E:133:GLN:CD	2.38	0.43	
1:C:37:ALA:HA	1:C:283:VAL:HG21	2.00	0.43	
1:D:77:LEU:HD23	1:D:91:SER:HA	2.00	0.43	
1:B:200:GLU:HB2	1:B:216:GLN:HG2	2.01	0.43	
1:D:376:THR:HB	1:H:92:MET:SD	2.58	0.43	
1:G:37:ALA:HA	1:G:283:VAL:HG21	2.01	0.43	
1:H:91:SER:O	1:H:95:ARG:HA	2.18	0.43	
1:A:91:SER:O	1:A:95:ARG:HA	2.19	0.43	
1:B:149:TYR:OH	1:D:312:PRO:HB2	2.19	0.43	
1:A:161:LEU:HG	1:A:175:ALA:HA	2.01	0.42	
1:B:77:LEU:HD23	1:B:91:SER:HA	2.01	0.42	
1:C:178:PHE:HB2	1:C:200:GLU:HB3	2.01	0.42	
1:E:37:ALA:HA	1:E:283:VAL:HG21	2.01	0.42	
1:A:95:ARG:HG2	1:A:118:TYR:O	2.20	0.42	
1:F:38:VAL:HG22	1:F:283:VAL:HG22	2.02	0.42	
1:F:357:ILE:HD12	1:F:357:ILE:N	2.35	0.42	
1:B:189:SER:HB2	1:B:191:VAL:HG13	2.02	0.42	
1:F:77:LEU:HD23	1:F:91:SER:HA	2.02	0.41	
1:F:240:PHE:CZ	1:F:261:LEU:HD23	2.54	0.41	
1:H:333:SER:OG	1:H:336:VAL:HG12	2.20	0.41	
1:D:332:LEU:HG	1:D:336:VAL:HG13	2.03	0.41	
1:B:152:THR:HB	1:D:346:THR:HG23	2.03	0.41	
1:E:38:VAL:HG22	1:E:283:VAL:HG22	2.02	0.41	
1:F:189:SER:HB2	1:F:191:VAL:HG13	2.01	0.41	
1:G:53:ASP:N	1:G:53:ASP:OD1	2.54	0.41	
1:A:53:ASP:N	1:A:53:ASP:OD1	2.54	0.41	
1:D:161:LEU:HG	1:D:175:ALA:HA	2.03	0.41	
1:E:142:PRO:HB2	1:E:154:SER:HB3	2.03	0.41	
1:C:53:ASP:OD1	1:C:53:ASP:N	2.54	0.41	
1:D:53:ASP:OD1	1:D:53:ASP:N	2.54	0.40	
1:D:189:SER:HB2	1:D:191:VAL:HG13	2.02	0.40	
1:G:189:SER:HB2	1:G:191:VAL:HG13	2.02	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:ASP:N	1:E:53:ASP:OD1	2.54	0.40
1:F:60:CYS:HB2	1:F:68:VAL:HA	2.03	0.40
1:F:261:LEU:HD21	1:G:135:ALA:HB2	2.04	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	entiles
1	А	365/383~(95%)	350~(96%)	14 (4%)	1 (0%)	41	66
1	В	357/383~(93%)	348~(98%)	8 (2%)	1 (0%)	41	66
1	С	355/383~(93%)	338 (95%)	16 (4%)	1 (0%)	41	66
1	D	363/383~(95%)	352 (97%)	10 (3%)	1 (0%)	41	66
1	Е	363/383~(95%)	346~(95%)	17 (5%)	0	100	100
1	F	359/383~(94%)	345~(96%)	13~(4%)	1 (0%)	41	66
1	G	360/383~(94%)	344 (96%)	15 (4%)	1 (0%)	41	66
1	Н	352/383~(92%)	339 (96%)	13 (4%)	0	100	100
All	All	2874/3064~(94%)	2762 (96%)	106 (4%)	6 (0%)	47	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	156	ILE
1	В	156	ILE
1	С	156	ILE
1	D	156	ILE
1	F	156	ILE
1	G	156	ILE



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	278/301~(92%)	277~(100%)	1 (0%)	91	97
1	В	278/301~(92%)	276~(99%)	2 (1%)	84	94
1	С	269/301~(89%)	266~(99%)	3~(1%)	73	90
1	D	270/301~(90%)	267~(99%)	3~(1%)	73	90
1	Ε	270/301~(90%)	265~(98%)	5(2%)	57	82
1	F	265/301~(88%)	263~(99%)	2(1%)	81	93
1	G	265/301~(88%)	262~(99%)	3~(1%)	73	90
1	Н	237/301~(79%)	236 (100%)	1 (0%)	91	97
All	All	2132/2408 (88%)	2112 (99%)	20 (1%)	78	92

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	379	ARG
1	В	194	THR
1	В	379	ARG
1	С	347	LEU
1	С	379	ARG
1	С	401	PRO
1	D	194	THR
1	D	376	THR
1	D	379	ARG
1	Е	107	GLU
1	Е	194	THR
1	Е	200	GLU
1	Е	298	LEU
1	Е	379	ARG
1	F	200	GLU
1	F	379	ARG
1	G	133	GLN
1	G	194	THR
1	G	379	ARG



Mol	Chain	\mathbf{Res}	Type
1	Н	379	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	133	GLN
1	С	301	GLN
1	F	231	GLN
1	F	354	ASN
1	Н	56	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)

27 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Tuno		Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain		Dec Link	Bo	Bond lengths		Bond angles		
	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2										
2	NAG	Ι	1	2,1	14, 14, 15	0.48	0	$17,\!19,\!21$	0.42	0										
2	FUC	Ι	2	2	10, 10, 11	0.65	0	$14,\!14,\!16$	0.75	0										
3	NAG	J	1	3,1	14,14,15	0.25	0	17,19,21	0.44	0										
3	NAG	J	2	3	14, 14, 15	0.28	0	17,19,21	0.37	0										
2	NAG	K	1	2,1	14, 14, 15	0.51	0	$17,\!19,\!21$	0.46	0										
2	FUC	K	2	2	10, 10, 11	0.90	1 (10%)	14,14,16	1.03	1 (7%)										
4	NAG	L	1	4,1	14,14,15	0.23	0	17,19,21	0.39	0										



Mal	Tune	Chain	Res	Tink	Bo	Bond lengths			Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	NAG	L	2	4	14,14,15	0.20	0	17,19,21	0.46	0	
4	BMA	L	3	4	11,11,12	0.80	0	$15,\!15,\!17$	0.89	0	
2	NAG	М	1	2,1	14,14,15	0.56	0	17,19,21	0.47	0	
2	FUC	М	2	2	10, 10, 11	0.81	0	$14,\!14,\!16$	0.85	0	
3	NAG	N	1	3,1	14,14,15	0.21	0	$17,\!19,\!21$	0.35	0	
3	NAG	N	2	3	14,14,15	0.22	0	17,19,21	0.43	0	
2	NAG	0	1	2,1	14, 14, 15	0.36	0	$17,\!19,\!21$	0.44	0	
2	FUC	0	2	2	10, 10, 11	0.80	0	$14,\!14,\!16$	0.73	0	
3	NAG	Р	1	3,1	14,14,15	0.38	0	17,19,21	0.44	0	
3	NAG	Р	2	3	14,14,15	0.26	0	$17,\!19,\!21$	0.57	0	
2	NAG	Q	1	2,1	14,14,15	0.59	0	17,19,21	0.49	0	
2	FUC	Q	2	2	10, 10, 11	0.67	0	$14,\!14,\!16$	0.79	0	
3	NAG	R	1	3,1	14, 14, 15	0.21	0	$17,\!19,\!21$	0.38	0	
3	NAG	R	2	3	14, 14, 15	0.23	0	$17,\!19,\!21$	0.50	0	
2	NAG	S	1	2,1	14, 14, 15	0.61	0	$17,\!19,\!21$	0.52	0	
2	FUC	S	2	2	10, 10, 11	1.77	1 (10%)	$14,\!14,\!16$	2.15	7 (50%)	
2	NAG	Т	1	2,1	14,14,15	0.69	1 (7%)	$17,\!19,\!21$	0.51	0	
2	FUC	Т	2	2	10, 10, 11	0.66	0	14,14,16	0.92	1 (7%)	
2	NAG	U	1	2,1	14, 14, 15	0.36	0	$17,\!19,\!21$	0.41	0	
2	FUC	U	2	2	10, 10, 11	0.61	0	$14,\!14,\!16$	0.79	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
2	NAG	Ι	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	Ι	2	2	-	-	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	K	2	2	-	-	0/1/1/1
4	NAG	L	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	BMA	L	3	4	-	2/2/19/22	0/1/1/1
2	NAG	М	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	М	2	2	-	-	0/1/1/1
3	NAG	N	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1



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Mol	Type	Chain	\mathbf{Res}	Link	Chirals	Torsions	Rings
2	NAG	Ο	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	Ο	2	2	-	-	0/1/1/1
3	NAG	Р	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Р	2	3	-	4/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	Q	2	2	-	-	0/1/1/1
3	NAG	R	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
2	NAG	S	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	S	2	2	-	-	0/1/1/1
2	NAG	Т	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	Т	2	2	-	-	0/1/1/1
2	NAG	U	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	U	2	2	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	S	2	FUC	O5-C5	4.03	1.52	1.43
2	Т	1	NAG	C1-C2	2.26	1.55	1.52
2	Κ	2	FUC	C1-C2	2.23	1.57	1.52

All (´9`) bond	angle	outliers	are	listed	below:
\	, <u> </u>	,	~	OGUIDID	or c	110000	0010111

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	S	2	FUC	C1-O5-C5	3.94	121.71	112.78
2	S	2	FUC	O5-C5-C4	3.58	115.95	109.52
2	S	2	FUC	O3-C3-C4	-2.93	103.58	110.35
2	S	2	FUC	C6-C5-C4	-2.79	107.91	113.07
2	Κ	2	FUC	C1-C2-C3	2.66	112.94	109.67
2	S	2	FUC	C2-C3-C4	-2.38	106.77	110.89
2	S	2	FUC	O2-C2-C1	2.26	113.78	109.15
2	Т	2	FUC	C1-O5-C5	2.13	117.59	112.78
2	S	2	FUC	C1-C2-C3	-2.06	107.13	109.67

There are no chirality outliers.

All (32) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	М	1	NAG	O5-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	Т	1	NAG	O5-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
3	Р	2	NAG	O5-C5-C6-O6
2	0	1	NAG	C4-C5-C6-O6
2	U	1	NAG	C4-C5-C6-O6
2	Ι	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	0	1	NAG	O5-C5-C6-O6
4	L	3	BMA	O5-C5-C6-O6
2	М	1	NAG	C4-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
2	Т	1	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	Ι	1	NAG	C4-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
3	Р	2	NAG	C4-C5-C6-O6
4	L	3	BMA	C4-C5-C6-O6
3	Р	1	NAG	O5-C5-C6-O6
3	Р	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	Ν	2	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	Р	2	NAG	C3-C2-N2-C7
3	Р	2	NAG	C1-C2-N2-C7
3	R	1	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Р	1	NAG	1	0
2	0	2	FUC	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)

19 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	Tune	Chain	Dog	Link	Bo	ond leng	ths	Bond angles		
	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	А	502	1	14, 14, 15	0.56	0	17,19,21	0.46	0
7	EDO	А	503	-	$3,\!3,\!3$	0.45	0	2,2,2	0.22	0
7	EDO	А	504	-	$3,\!3,\!3$	0.41	0	2,2,2	0.09	0
6	NAG	E	501	1	$14,\!14,\!15$	0.28	0	17,19,21	0.45	0
7	EDO	В	501	-	$3,\!3,\!3$	0.46	0	2,2,2	0.30	0
6	NAG	F	501	1	14,14,15	0.40	0	17,19,21	0.72	1(5%)
6	NAG	H	501	1	14, 14, 15	0.27	0	17,19,21	0.44	0
7	EDO	B	502	-	3,3,3	0.44	0	2,2,2	0.40	0
7	EDO	G	503	-	3, 3, 3	0.44	0	2,2,2	0.32	0



Mal	Tune	Chain	Dog	Tink	Bo	ond leng	\mathbf{ths}	Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
6	NAG	Н	502	1	14, 14, 15	0.27	0	17,19,21	0.40	0
5	MLT	А	501	-	2,8,8	0.50	0	$3,\!10,\!10$	0.91	0
7	EDO	A	505	-	$3,\!3,\!3$	0.46	0	2,2,2	0.33	0
7	EDO	В	504	-	$3,\!3,\!3$	0.47	0	2,2,2	0.28	0
6	NAG	C	501	1	14, 14, 15	0.34	0	17,19,21	0.43	0
7	EDO	C	502	-	$3,\!3,\!3$	0.44	0	2,2,2	0.38	0
6	NAG	D	501	1	14,14,15	0.50	0	17,19,21	0.67	1(5%)
6	NAG	В	503	1	14,14,15	0.47	0	17,19,21	0.47	0
6	NAG	G	501	1	14, 14, 15	0.27	0	17,19,21	0.46	0
6	NAG	G	502	1	14,14,15	0.56	0	17,19,21	0.49	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	\mathbf{Res}	Link	Chirals	Torsions	Rings
6	NAG	А	502	1	-	2/6/23/26	0/1/1/1
7	EDO	А	503	-	-	0/1/1/1	-
7	EDO	А	504	-	-	0/1/1/1	-
6	NAG	Е	501	1	-	0/6/23/26	0/1/1/1
7	EDO	В	501	-	-	0/1/1/1	-
6	NAG	F	501	1	-	0/6/23/26	0/1/1/1
6	NAG	Н	501	1	-	1/6/23/26	0/1/1/1
7	EDO	В	502	-	-	1/1/1/1	-
7	EDO	G	503	-	-	0/1/1/1	-
6	NAG	Н	502	1	-	0/6/23/26	0/1/1/1
5	MLT	А	501	-	-	0/2/8/8	-
7	EDO	А	505	-	-	0/1/1/1	-
7	EDO	В	504	-	-	0/1/1/1	-
6	NAG	С	501	1	-	1/6/23/26	0/1/1/1
7	EDO	С	502	-	-	1/1/1/1	-
6	NAG	D	501	1	-	0/6/23/26	0/1/1/1
6	NAG	B	503	1	-	0/6/23/26	0/1/1/1
6	NAG	G	501	1	-	0/6/23/26	0/1/1/1
6	NAG	G	502	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
6	F	501	NAG	C1-O5-C5	2.53	115.61	112.19
6	D	501	NAG	C1-O5-C5	2.43	115.49	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
6	А	502	NAG	O5-C5-C6-O6
6	А	502	NAG	C4-C5-C6-O6
6	С	501	NAG	O5-C5-C6-O6
6	Н	501	NAG	O5-C5-C6-O6
7	В	502	EDO	O1-C1-C2-O2
7	С	502	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	А	503	EDO	2	0
7	А	504	EDO	2	0
6	F	501	NAG	1	0
6	С	501	NAG	1	0
6	G	502	NAG	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	$Q{<}0.9$
1	А	369/383~(96%)	0.01	2 (0%) 91 92	41, 63, 114, 172	0
1	В	363/383~(94%)	0.06	7 (1%) 66 69	40, 61, 110, 158	0
1	С	363/383~(94%)	0.31	21 (5%) 23 22	48, 83, 143, 172	0
1	D	367/383~(95%)	0.30	18 (4%) 29 28	56, 94, 140, 199	0
1	Ε	367/383~(95%)	0.40	24 (6%) 18 17	60, 93, 147, 197	0
1	F	363/383~(94%)	0.38	19 (5%) 27 25	59, 92, 143, 198	0
1	G	364/383~(95%)	0.31	21 (5%) 23 22	62, 94, 135, 204	0
1	Η	358/383~(93%)	0.64	45 (12%) 3 3	62, 109, 164, 188	0
All	All	2914/3064~(95%)	0.30	157 (5%) 25 24	40, 87, 145, 204	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	391	ASN	8.0
1	F	158	ALA	7.3
1	Η	391	ASN	7.0
1	Е	391	ASN	6.1
1	С	401	PRO	6.0
1	Н	172	GLY	5.9
1	С	228	LEU	5.7
1	С	294	LEU	5.3
1	Н	143	ALA	5.1
1	G	390	HIS	4.8
1	Е	297	SER	4.4
1	F	391	ASN	4.2
1	Н	390	HIS	4.2
1	F	390	HIS	4.2
1	D	390	HIS	4.0
1	В	314	GLY	4.0



7	A	0	Κ

Mol	Chain	Res	Type	RSRZ
1	F	175	ALA	4.0
1	F	161	LEU	3.9
1	Н	208	GLY	3.8
1	Н	281	ALA	3.8
1	С	265	PHE	3.7
1	Е	291	GLY	3.7
1	С	226	ARG	3.6
1	G	240	PHE	3.6
1	Е	390	HIS	3.6
1	Н	175	ALA	3.6
1	D	112	ALA	3.5
1	G	172	GLY	3.5
1	F	198	GLY	3.4
1	Н	293	PRO	3.4
1	H	158	ALA	3.4
1	D	51	ARG	3.4
1	G	292	LEU	3.4
1	Н	173	LEU	3.4
1	Н	299	PRO	3.3
1	Е	155	PHE	3.3
1	А	390	HIS	3.3
1	D	297	SER	3.3
1	F	215	LEU	3.3
1	G	75	LEU	3.2
1	Н	223	CYS	3.2
1	Н	274	PRO	3.2
1	D	161	LEU	3.2
1	С	296	PRO	3.2
1	Е	267	LEU	3.1
1	Н	275	THR	3.1
1	H	162	SER	3.1
1	D	275	THR	3.1
1	D	281	ALA	3.1
1	Е	300	GLN	3.1
1	С	301	GLN	3.0
1	С	399	TYR	3.0
1	Н	139	ALA	2.9
1	H	222	PHE	2.9
1	D	268	PRO	2.9
1	Е	274	PRO	2.9
1	G	342	ALA	2.9
1	Е	139	ALA	2.8



Mol	Chain	Res	Type	RSRZ
1	Е	61	PHE	2.8
1	С	272	ALA	2.8
1	С	299	PRO	2.8
1	D	216	GLN	2.7
1	Е	90	LEU	2.7
1	С	274	PRO	2.6
1	G	235	PRO	2.6
1	D	391	ASN	2.6
1	Н	34	ASN	2.6
1	Н	295	THR	2.6
1	G	393	THR	2.6
1	Н	294	LEU	2.6
1	Н	156	ILE	2.6
1	В	291	GLY	2.6
1	С	220	ARG	2.6
1	С	57	VAL	2.6
1	Н	366	GLY	2.6
1	G	392	ALA	2.5
1	С	335	GLU	2.5
1	F	238	ALA	2.5
1	F	375	SER	2.5
1	F	388	CYS	2.5
1	D	172	GLY	2.5
1	Н	159	PRO	2.5
1	G	234	VAL	2.5
1	G	291	GLY	2.5
1	Н	221	THR	2.5
1	Е	174	PHE	2.5
1	В	313	THR	2.4
1	Е	298	LEU	2.4
1	Е	217	ASN	2.4
1	Н	118	TYR	2.4
1	Е	296	PRO	2.4
1	G	112	ALA	2.4
1	Е	188	GLY	2.4
1	Н	240	PHE	2.4
1	Н	107	GLU	2.4
1	F	180	PRO	2.4
1	Е	176	ALA	2.4
1	Н	298	LEU	2.4
1	F	314	GLY	2.4
1	G	139	ALA	2.4



Mol	Chain	Res	Type	RSRZ
1	G	30	LEU	2.3
1	Н	213	GLY	2.3
1	D	181	VAL	2.3
1	F	178	PHE	2.3
1	G	161	LEU	2.3
1	G	187	THR	2.3
1	С	197	LYS	2.3
1	А	401	PRO	2.3
1	F	389	ASN	2.3
1	Н	262	CYS	2.3
1	Н	248	PHE	2.3
1	Н	97	PRO	2.3
1	С	266	THR	2.3
1	F	221	THR	2.3
1	D	292	LEU	2.2
1	Н	73	PRO	2.2
1	Н	155	PHE	2.2
1	Е	266	THR	2.2
1	С	237	GLY	2.2
1	Е	213	GLY	2.2
1	Н	218	GLY	2.2
1	G	77	LEU	2.2
1	Н	259	LEU	2.2
1	G	217	ASN	2.2
1	Н	224	TRP	2.2
1	Н	137	TYR	2.2
1	С	400	ASN	2.2
1	Н	144	VAL	2.2
1	В	316	ALA	2.2
1	G	198	GLY	2.2
1	H	176	ALA	2.2
1	Е	201	PHE	2.2
1	С	370	SER	2.1
1	F	399	TYR	2.1
1	Е	275	THR	2.1
1	В	400	ASN	2.1
1	D	113	VAL	2.1
1	В	299	PRO	2.1
1	D	238	ALA	2.1
1	F	261	LEU	2.1
1	E	204	ILE	2.1
1	F	235	PRO	2.1



Mol	Chain	Res	Type	RSRZ
1	D	282	LEU	2.1
1	D	274	PRO	2.1
1	Н	180	PRO	2.1
1	С	392	ALA	2.1
1	Н	207	GLY	2.1
1	Н	344	GLY	2.1
1	Н	277	VAL	2.0
1	F	345	ALA	2.0
1	Н	119	ALA	2.0
1	D	343	SER	2.0
1	С	231	GLN	2.0
1	Ε	160	LEU	2.0
1	E	323	LEU	2.0
1	G	282	LEU	2.0
1	В	401	PRO	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	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
3	NAG	N	2	14/15	0.73	0.28	$114,\!125,\!128,\!128$	0
3	NAG	Р	2	14/15	0.74	0.36	$130,\!138,\!139,\!140$	0
3	NAG	J	2	14/15	0.76	0.38	$105,\!112,\!117,\!121$	0
4	BMA	L	3	11/12	0.77	0.34	$120,\!125,\!132,\!134$	0
3	NAG	R	2	14/15	0.82	0.40	$118,\!126,\!131,\!131$	0
2	FUC	S	2	10/11	0.82	0.23	$108,\!119,\!123,\!127$	0
2	FUC	М	2	10/11	0.83	0.22	$110,\!112,\!114,\!118$	0
2	FUC	K	2	10/11	0.86	0.19	$87,\!94,\!96,\!99$	0
2	FUC	Q	2	10/11	0.86	0.17	$106,\!108,\!108,\!109$	0
2	FUC	U	2	10/11	0.88	0.19	$104,\!108,\!112,\!116$	0
3	NAG	Ν	1	14/15	0.89	0.16	$79,\!93,\!100,\!106$	0
2	FUC	Ι	2	10/11	0.90	0.20	$99,\!110,\!113,\!115$	0
2	NAG	T	1	14/15	0.91	0.20	72,81,88,95	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	NAG	Р	1	14/15	0.91	0.16	$84,\!103,\!108,\!120$	0
2	NAG	М	1	14/15	0.91	0.25	$61,\!66,\!89,\!100$	0
2	NAG	S	1	14/15	0.91	0.20	$64,\!74,\!91,\!100$	0
2	NAG	0	1	14/15	0.91	0.21	57,74,85,92	0
4	NAG	L	2	14/15	0.92	0.27	$97,\!112,\!116,\!121$	0
3	NAG	R	1	14/15	0.93	0.18	$69,\!89,\!102,\!107$	0
2	FUC	0	2	10/11	0.93	0.21	$87,\!94,\!99,\!100$	0
2	NAG	Q	1	14/15	0.93	0.19	$63,\!78,\!88,\!98$	0
2	NAG	K	1	14/15	0.93	0.19	53,62,72,74	0
2	NAG	U	1	14/15	0.94	0.22	$63,\!78,\!94,\!97$	0
2	FUC	Т	2	10/11	0.94	0.13	$98,\!102,\!105,\!107$	0
3	NAG	J	1	14/15	0.94	0.17	63,74,90,95	0
2	NAG	Ι	1	14/15	0.95	0.18	48,57,72,83	0
4	NAG	L	1	14/15	0.96	0.13	52,64,75,86	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	EDO	А	503	4/4	0.58	1.00	120,121,123,127	0
6	NAG	D	501	14/15	0.64	0.40	103,114,123,125	0
6	NAG	Н	502	14/15	0.70	0.44	$95,\!114,\!119,\!120$	0
7	EDO	В	504	4/4	0.75	0.24	77,79,79,82	0
7	EDO	A	504	4/4	0.76	0.71	88,90,90,90	0
6	NAG	Н	501	14/15	0.79	0.18	90,96,114,122	0
7	EDO	А	505	4/4	0.81	0.24	92,92,94,97	0
6	NAG	А	502	14/15	0.81	0.28	$76,\!91,\!103,\!108$	0
6	NAG	F	501	14/15	0.82	0.27	$94,\!100,\!129,\!134$	0
6	NAG	Е	501	14/15	0.83	0.27	96,107,115,115	0
5	MLT	А	501	9/9	0.83	0.44	96,106,114,116	0
7	EDO	В	501	4/4	0.83	0.31	71,72,76,77	0
6	NAG	G	502	14/15	0.83	0.29	101,115,119,121	0
6	NAG	С	501	14/15	0.85	0.34	92,108,118,121	0
6	NAG	В	503	14/15	0.88	0.28	91,105,118,122	0
7	EDO	G	503	4/4	0.89	0.15	70,72,78,86	0
7	EDO	С	502	4/4	0.92	0.30	71,74,74,78	0
6	NAG	G	501	14/15	0.92	0.14	65,82,88,94	0
7	EDO	В	502	4/4	0.93	0.18	52, 53, 59, 60	0

6.5 Other polymers (i)

There are no such residues in this entry.

