

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

### Oct 25, 2023 – 07:25 PM EDT

PDB ID	:	3D4G
Title	:	ZP-N domain of mammalian sperm receptor ZP3 (crystal form II)
Authors	:	Jovine, L.; Monne, M.
Deposited on	:	2008-05-14
Resolution	:	2.30  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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
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 2.30 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	$\begin{array}{c} {\rm Whole \ archive} \\ (\#{\rm Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575(2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	481	2% 90%	7%	
		101	4%	, , , ,	
1	В	481	88%	10%	•
1	$\mathbf{C}$	481	89%	9%	•
1	D	481	91%	7%	•
		101	3%	770	-
1	Е	481	91%	7%	•



Mol	Chain	Length	Quality	of chain	
1	F	481	<u>4%</u> 90%	8%	·
1	G	481	5% 90%	8%	•
1	Н	481	5%	9%	
2	Ι	2	10	0%	-
2	J	2	50%	50%	-
2	К	2	50%	50%	-
2	L	2	50%	50%	
2	М	2	50%	50%	-
2	Ν	2	50%	50%	-
2	О	2	50%	50%	-
2	Р	2	50%	50%	-



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# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 31230 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 Maltose-binding periplasmic protein, LINKER, Zona pellucida protein 3.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
1	Δ	471	Total	С	Ν	0	$\mathbf{S}$	0	0	0
1	A	471	3637	2325	605	696	11	0	0	0
1	Р	471	Total	С	Ν	0	S	0	0	0
1	D	471	3637	2325	605	696	11	0	0	0
1	C	471	Total	С	Ν	0	S	0	0	0
1		471	3637	2325	605	696	11	0	0	0
1	П	460	Total	С	Ν	0	S	0	0	0
1		409	3621	2316	603	691	11	0	0	0
1	F	479	Total	С	Ν	0	S	0	0	0
1	Ľ	412	3645	2331	606	697	11	0	0	0
1	Б	479	Total	С	Ν	0	S	0	0	0
	Г	412	3645	2331	606	697	11	0	0	0
1	C	479	Total	С	Ν	0	S	0	0	0
1	G	412	3645	2331	606	697	11	0	0	0
1	ц	460	Total	С	Ν	0	S	0	0	0
	п	409	3621	2316	603	691	11	0	0	U

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MET	-	initiating methionine	UNP POAEX9
А	3	THR	ILE	engineered mutation	UNP P0AEX9
А	360	ALA	GLU	engineered mutation	UNP P0AEX9
А	363	ALA	LYS	engineered mutation	UNP P0AEX9
А	364	ALA	ASP	engineered mutation	UNP P0AEX9
А	368	ASN	ARG	engineered mutation	UNP P0AEX9
А	474	LEU	-	expression tag	UNP P10761
А	475	GLU	-	expression tag	UNP P10761
А	476	HIS	-	expression tag	UNP P10761
A	477	HIS	-	expression tag	UNP P10761
А	478	HIS	-	expression tag	UNP P10761
А	479	HIS	-	expression tag	UNP P10761



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Chain	Residue	Modelled	Actual	Comment	Reference
А	480	HIS	-	expression tag	UNP P10761
A	481	HIS	-	expression tag	UNP P10761
В	1	MET	-	initiating methionine	UNP POAEX9
В	3	THR	ILE	engineered mutation	UNP POAEX9
В	360	ALA	GLU	engineered mutation	UNP POAEX9
В	363	ALA	LYS	engineered mutation	UNP POAEX9
В	364	ALA	ASP	engineered mutation	UNP POAEX9
В	368	ASN	ARG	engineered mutation	UNP POAEX9
В	474	LEU	-	expression tag	UNP P10761
В	475	GLU	-	expression tag	UNP P10761
В	476	HIS	-	expression tag	UNP P10761
В	477	HIS	-	expression tag	UNP P10761
В	478	HIS	-	expression tag	UNP P10761
В	479	HIS	-	expression tag	UNP P10761
В	480	HIS	-	expression tag	UNP P10761
В	481	HIS	-	expression tag	UNP P10761
С	1	MET	-	initiating methionine	UNP POAEX9
С	3	THR	ILE	engineered mutation	UNP POAEX9
С	360	ALA	GLU	engineered mutation	UNP POAEX9
С	363	ALA	LYS	engineered mutation	UNP POAEX9
С	364	ALA	ASP	engineered mutation	UNP POAEX9
С	368	ASN	ARG	engineered mutation	UNP POAEX9
С	474	LEU	-	expression tag	UNP P10761
С	475	GLU	-	expression tag	UNP P10761
С	476	HIS	-	expression tag	UNP P10761
С	477	HIS	-	expression tag	UNP P10761
С	478	HIS	-	expression tag	UNP P10761
С	479	HIS	-	expression tag	UNP P10761
С	480	HIS	-	expression tag	UNP P10761
С	481	HIS	-	expression tag	UNP P10761
D	1	MET	-	initiating methionine	UNP P0AEX9
D	3	THR	ILE	engineered mutation	UNP P0AEX9
D	360	ALA	GLU	engineered mutation	UNP P0AEX9
D	363	ALA	LYS	engineered mutation	UNP P0AEX9
D	364	ALA	ASP	engineered mutation	UNP POAEX9
D	368	ASN	ARG	engineered mutation	UNP POAEX9
D	474	LEU	_	expression tag	UNP P10761
D	475	GLU	-	expression tag	UNP P10761
D	476	HIS	_	expression tag	UNP P10761
D	477	HIS	-	expression tag	UNP P10761
D	478	HIS	-	expression tag	UNP P10761
D	479	HIS	-	expression tag	UNP P10761



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Chain	Residue	Modelled	Actual	Comment	Reference
D	480	HIS	-	expression tag	UNP P10761
D	481	HIS	-	expression tag	UNP P10761
Е	1	MET	-	initiating methionine	UNP P0AEX9
Е	3	THR	ILE	engineered mutation	UNP POAEX9
Е	360	ALA	GLU	engineered mutation	UNP POAEX9
Е	363	ALA	LYS	engineered mutation	UNP P0AEX9
Е	364	ALA	ASP	engineered mutation	UNP P0AEX9
Е	368	ASN	ARG	engineered mutation	UNP P0AEX9
Е	474	LEU	-	expression tag	UNP P10761
Е	475	GLU	-	expression tag	UNP P10761
Е	476	HIS	-	expression tag	UNP P10761
Е	477	HIS	-	expression tag	UNP P10761
Е	478	HIS	-	expression tag	UNP P10761
Е	479	HIS	-	expression tag	UNP P10761
Е	480	HIS	-	expression tag	UNP P10761
Е	481	HIS	-	expression tag	UNP P10761
F	1	MET	-	initiating methionine	UNP P0AEX9
F	3	THR	ILE	engineered mutation	UNP POAEX9
F	360	ALA	GLU	engineered mutation	UNP P0AEX9
F	363	ALA	LYS	engineered mutation	UNP POAEX9
F	364	ALA	ASP	engineered mutation	UNP POAEX9
F	368	ASN	ARG	engineered mutation	UNP POAEX9
F	474	LEU	-	expression tag	UNP P10761
F	475	GLU	-	expression tag	UNP P10761
F	476	HIS	-	expression tag	UNP P10761
F	477	HIS	-	expression tag	UNP P10761
F	478	HIS	-	expression tag	UNP P10761
F	479	HIS	-	expression tag	UNP P10761
F	480	HIS	-	expression tag	UNP P10761
F	481	HIS	-	expression tag	UNP P10761
G	1	MET	-	initiating methionine	UNP P0AEX9
G	3	THR	ILE	engineered mutation	UNP P0AEX9
G	360	ALA	GLU	engineered mutation	UNP P0AEX9
G	363	ALA	LYS	engineered mutation	UNP P0AEX9
G	364	ALA	ASP	engineered mutation	UNP P0AEX9
G	368	ASN	ARG	engineered mutation	UNP P0AEX9
G	474	LEU	-	expression tag	UNP P10761
G	475	GLU	-	expression tag	UNP P10761
G	476	HIS	-	expression tag	UNP P10761
G	477	HIS	-	expression tag	UNP P10761
G	478	HIS	-	expression tag	UNP P10761
G	479	HIS	-	expression tag	UNP P10761



**D** 

Chain	Residue	Modelled	Actual	Comment	Reference
G	480	HIS	-	expression tag	UNP P10761
G	481	HIS	-	expression tag	UNP P10761
Н	1	MET	-	initiating methionine	UNP P0AEX9
Н	3	THR	ILE	engineered mutation	UNP POAEX9
Н	360	ALA	GLU	engineered mutation	UNP P0AEX9
Н	363	ALA	LYS	engineered mutation	UNP POAEX9
Н	364	ALA	ASP	engineered mutation	UNP POAEX9
Н	368	ASN	ARG	engineered mutation	UNP POAEX9
Н	474	LEU	-	expression tag	UNP P10761
Н	475	GLU	-	expression tag	UNP P10761
Н	476	HIS	-	expression tag	UNP P10761
Н	477	HIS	-	expression tag	UNP P10761
Н	478	HIS	-	expression tag	UNP P10761
Н	479	HIS	-	expression tag	UNP P10761
Н	480	HIS	-	expression tag	UNP P10761
H	481	HIS	-	expression tag	UNP P10761

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• Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	T	2	Total C O	0	0	0
2	L	2	23 12 11	0	0	0
2	T	9	Total C O	0	0	0
2	0	2	23 12 11	0	0	0
9	K	9	Total C O	0	0	0
	Γ	2	23 12 11	0	0	0
0	т	2	Total C O	0	0	0
		2	23 12 11	0		
0	М	M	Total C O	0	0	0
	111	2	23 12 11			
0	N	2	Total C O	0	0	0
	IN	2	23 12 11	0		
0	0	2	Total C O	0	0	0
		2	23 12 11	0	0	0
9	P	0	Total C O	0	0	0
	T	2	23 12 11	0	0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	3	Total Ca 3 3	0	0
3	В	3	Total Ca 3 3	0	0
3	С	3	Total Ca 3 3	0	0
3	D	3	Total Ca 3 3	0	0
3	Е	3	Total Ca 3 3	0	0
3	F	3	Total Ca 3 3	0	0
3	G	3	Total Ca 3 3	0	0
3	Н	3	Total Ca 3 3	0	0

### • Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	288	Total         O           288         288	0	0
4	В	205	Total         O           205         205	0	0
4	С	291	Total         O           291         291	0	0
4	D	205	Total         O           205         205	0	0
4	Е	282	Total         O           282         282	0	0
4	F	272	Total O 272 272	0	0
4	G	195	Total O 195 195	0	0
4	Н	196	Total O 196 196	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: Maltose-binding periplasmic protein, LINKER, Zona pellucida protein 3



Chain D:



7%

91%



C469 R470 LEU LEU HIS HIS	HIS HIS HIS		
• Molecule 2:	alpha-D-glucopyranose-(1-4)	-alpha-D-glucopyranose	
Chain I:	1009	6	
GLC1 GLC2			
• Molecule 2:	alpha-D-glucopyranose-(1-4)	-alpha-D-glucopyranose	
Chain J:	50%	50%	
GLC1 GLC2			
• Molecule 2:	alpha-D-glucopyranose-(1-4)	-alpha-D-glucopyranose	
Chain K:	50%	50%	
di Ci Ci Ci Ci Ci			
• Molecule 2:	alpha-D-glucopyranose-(1-4)	-alpha-D-glucopyranose	
Chain L:	50%	50%	
Chain L: <mark>물</mark> 물	50%	50%	
Chain L: 탈탈 • Molecule 2:	50% alpha-D-glucopyranose-(1-4)	50% -alpha-D-glucopyranose	
Chain L:	50% alpha-D-glucopyranose-(1-4) 50%	50% -alpha-D-glucopyranose 50%	
Chain L:	50% alpha-D-glucopyranose-(1-4) 50%	50% -alpha-D-glucopyranose 50%	
Chain L:	50% alpha-D-glucopyranose-(1-4) 50% alpha-D-glucopyranose-(1-4)	50% -alpha-D-glucopyranose 50% -alpha-D-glucopyranose	
Chain L:	50% alpha-D-glucopyranose-(1-4) 50% 50%	50% -alpha-D-glucopyranose -alpha-D-glucopyranose	
Chain L:	50% alpha-D-glucopyranose-(1-4) 50% so%	50% -alpha-D-glucopyranose -alpha-D-glucopyranose	
Chain L: Molecule 2: Chain M: Chain N: Chain N:	50% alpha-D-glucopyranose-(1-4) 50% so% alpha-D-glucopyranose-(1-4)	50% -alpha-D-glucopyranose -alpha-D-glucopyranose 50% -alpha-D-glucopyranose	
Chain L: Molecule 2: Chain M: Chain M: Chain N: Chain N: Chain N: Chain N:	50% alpha-D-glucopyranose-(1-4) 50% alpha-D-glucopyranose-(1-4) 50%	50% -alpha-D-glucopyranose -alpha-D-glucopyranose 50% -alpha-D-glucopyranose	



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

50%

Chain P:

50%

GLC1 GLC2



# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1	Depositor	
Cell constants	91.05Å 91.96Å 140.48Å	Deperitor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$89.99^{\circ}$ $90.18^{\circ}$ $89.98^{\circ}$	Depositor	
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	50.00 - 2.30	Depositor	
Resolution (A)	47.64 - 2.30	EDS	
% Data completeness	95.5(50.00-2.30)	Depositor	
(in resolution range)	94.6(47.64-2.30)	EDS	
R <sub>merge</sub>	(Not available)	Depositor	
R <sub>sym</sub>	0.05	Depositor	
$< I/\sigma(I) > 1$	$1.70 (at 2.29 \text{\AA})$	Xtriage	
Refinement program	REFMAC 5.3.0038	Depositor	
D D	0.201 , $0.227$	Depositor	
$\pi, \pi_{free}$	0.205 , $0.232$	DCC	
$R_{free}$ test set	2139 reflections $(1.11\%)$	wwPDB-VP	
Wilson B-factor $(Å^2)$	43.9	Xtriage	
Anisotropy	0.185	Xtriage	
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 50.0	EDS	
L-test for twinning <sup>2</sup>	$<  L  > = 0.49, < L^2 > = 0.33$	Xtriage	
	0.000 for -k,h,l		
	0.000 for k,-h,l		
	0.448 for h,-k,-l		
Estimated twinning fraction	0.459 for -h,k,-l	Xtriage	
	0.447 for -h,-k,l		
	0.000 for -k,-h,-l		
	0.002 for k,h,-l		
$F_o, F_c$ correlation	0.96	EDS	
Total number of atoms	31230	wwPDB-VP	
Average B, all atoms $(Å^2)$	62.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 57.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2121e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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: GLC, CA

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	Mol Chain		Bond lengths		angles
IVIOI	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.37	0/3719	0.49	0/5055
1	В	0.35	0/3719	0.49	0/5055
1	С	0.36	0/3719	0.49	0/5055
1	D	0.35	0/3703	0.48	0/5033
1	Ε	0.37	0/3727	0.49	0/5066
1	F	0.36	0/3727	0.49	0/5066
1	G	0.35	0/3727	0.48	0/5066
1	Н	0.34	0/3703	0.48	0/5033
All	All	0.36	0/29744	0.49	0/40429

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	2
1	F	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	3	THR	Peptide
1	А	458	LEU	Peptide
1	F	452	VAL	Peptide



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Mol	Chain	$\operatorname{Res}$	Type	Group
1	F	457	ILE	Peptide

## 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	3637	0	3610	26	0
1	В	3637	0	3610	35	0
1	С	3637	0	3610	30	0
1	D	3621	0	3597	21	0
1	Е	3645	0	3621	23	0
1	F	3645	0	3621	26	0
1	G	3645	0	3621	25	0
1	Н	3621	0	3597	29	0
2	Ι	23	0	21	0	0
2	J	23	0	21	0	0
2	Κ	23	0	21	0	0
2	L	23	0	21	0	0
2	М	23	0	21	0	0
2	Ν	23	0	21	1	0
2	0	23	0	21	0	0
2	Р	23	0	21	0	0
3	А	3	0	0	0	0
3	В	3	0	0	0	0
3	С	3	0	0	0	0
3	D	3	0	0	0	0
3	Ε	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	Н	3	0	0	0	0
4	А	288	0	0	2	0
4	В	205	0	0	2	0
4	С	291	0	0	2	0
4	D	205	0	0	2	0
4	Е	282	0	0	2	0
4	F	272	0	0	2	0
4	G	195	0	0	2	0
4	Н	196	0	0	1	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31230	0	29055	204	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 4.

All (204) 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:D:32:THR:HG22	1:D:34:ILE:HD13	1.47	0.97	
1:B:32:THR:HG22	1:B:34:ILE:HD13	1.49	0.95	
1:H:32:THR:HG22	1:H:34:ILE:HD13	1.48	0.94	
1:E:32:THR:HG22	1:E:34:ILE:HD13	1.48	0.93	
1:A:32:THR:HG22	1:A:34:ILE:HD13	1.50	0.92	
1:C:32:THR:HG22	1:C:34:ILE:HD13	1.50	0.92	
1:G:32:THR:HG22	1:G:34:ILE:HD13	1.50	0.90	
1:F:32:THR:HG22	1:F:34:ILE:HD13	1.53	0.89	
1:F:152:LEU:HD11	1:F:205:MET:HE3	1.56	0.86	
1:G:152:LEU:HD11	1:G:205:MET:HE3	1.58	0.85	
1:D:152:LEU:HD11	1:D:205:MET:HE3	1.59	0.84	
1:C:152:LEU:HD11	1:C:205:MET:HE3	1.61	0.82	
1:B:152:LEU:HD11	1:B:205:MET:HE3	1.64	0.79	
1:E:152:LEU:HD11	1:E:205:MET:HE3	1.66	0.77	
1:A:152:LEU:HD11	1:A:205:MET:HE3	1.67	0.75	
1:A:457:ILE:HG22	1:A:458:LEU:HG	1.68	0.75	
1:H:152:LEU:HD11	1:H:205:MET:HE3	1.72	0.70	
1:E:3:THR:HG23	1:E:57:GLY:O	1.96	0.66	
1:B:457:ILE:HG22	1:B:458:LEU:HD13	1.80	0.64	
1:B:457:ILE:HG22	1:B:458:LEU:CD1	2.28	0.63	
1:G:436:LYS:NZ	4:G:578:HOH:O	2.30	0.62	
1:H:436:LYS:NZ	4:H:1824:HOH:O	2.33	0.62	
1:E:459:ARG:HG2	1:E:460:THR:N	2.14	0.62	
1:B:436:LYS:NZ	4:B:571:HOH:O	2.33	0.62	
1:C:458:LEU:HD13	1:D:111:VAL:HG21	1.82	0.60	
1:F:48:PHE:CG	1:F:61:ILE:HD12	2.37	0.60	
1:C:349:ILE:HD13	1:C:470:ARG:NH2	2.17	0.59	
1:F:436:LYS:NZ	4:F:575:HOH:O	2.35	0.58	
1:F:349:ILE:HD13	1:F:470:ARG:NH2	2.18	0.57	
1:F:416:THR:HG22	1:H:73:GLN:CD	2.23	0.57	
1:B:73:GLN:CD	1:C:416:THR:HG22	2.26	0.56	
1:A:349:ILE:HD13	1:A:470:ARG:NH2	2.21	0.56	
1:G:349:ILE:HD13	1:G:470:ARG:NH2	2.20	0.56	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:D:436:LYS:NZ	4:D:576:HOH:O	2.38	0.56	
1:H:349:ILE:HD13	1:H:470:ARG:NH2	2.21	0.55	
1:B:416:THR:HG22	1:C:73:GLN:CD	2.26	0.55	
1:G:7:LYS:HA	1:G:34:ILE:HG23	1.90	0.54	
1:C:378:GLU:O	1:H:426:HIS:NE2	2.41	0.53	
1:G:152:LEU:HD21	1:G:205:MET:HE1	1.90	0.53	
1:B:69:GLY:HA3	1:B:333:ASN:O	2.09	0.53	
1:B:90:LEU:HD12	1:B:95:TRP:CZ2	2.43	0.53	
1:H:457:ILE:N	1:H:457:ILE:HD12	2.23	0.53	
1:G:385:VAL:HG21	1:G:445:LEU:HD21	1.91	0.53	
1:A:48:PHE:CG	1:A:61:ILE:HD12	2.44	0.53	
1:D:349:ILE:HD13	1:D:470:ARG:NH2	2.24	0.52	
1:F:196:LEU:HD11	1:F:205:MET:HE1	1.91	0.52	
1:D:7:LYS:HA	1:D:34:ILE:HG23	1.91	0.52	
1:F:73:GLN:CD	1:H:416:THR:HG22	2.29	0.52	
1:B:7:LYS:HA	1:B:34:ILE:HG23	1.92	0.52	
1:A:69:GLY:HA3	1:A:333:ASN:O	2.10	0.52	
1:D:137:ASP:HA	1:D:147:ALA:HB2	1.92	0.52	
1:A:93:PHE:CD1	1:B:457:ILE:HG23	2.44	0.51	
1:D:69:GLY:HA3	1:D:333:ASN:O	2.10	0.51	
1:E:349:ILE:HD13	1:E:470:ARG:NH2	2.26	0.51	
1:A:436:LYS:NZ	4:A:574:HOH:O	2.43	0.51	
1:C:69:GLY:HA3	1:C:333:ASN:O	2.10	0.51	
1:H:7:LYS:HA	1:H:34:ILE:HG23	1.93	0.51	
1:B:457:ILE:HG22	1:B:458:LEU:N	2.26	0.51	
1:G:137:ASP:HA	1:G:147:ALA:HB2	1.92	0.51	
1:F:100:TYR:HB3	1:F:105:ILE:HD13	1.93	0.51	
1:F:457:ILE:HG22	1:F:458:LEU:HB2	1.93	0.51	
1:G:69:GLY:HA3	1:G:333:ASN:O	2.10	0.51	
1:B:349:ILE:HD13	1:B:470:ARG:NH2	2.25	0.50	
1:D:90:LEU:HD12	1:D:95:TRP:CZ2	2.46	0.50	
1:E:69:GLY:HA3	1:E:333:ASN:O	2.12	0.50	
1:F:69:GLY:HA3	1:F:333:ASN:O	2.12	0.50	
1:B:137:ASP:HA	1:B:147:ALA:HB2	1.94	0.49	
1:H:385:VAL:HG21	1:H:445:LEU:HD21	1.95	0.49	
1:B:381:LEU:HD13	1:B:469:CYS:SG	2.53	0.49	
1:E:48:PHE:CG	1:E:61:ILE:HD12	2.47	0.49	
1:B:182:VAL:HG12	1:B:184:VAL:HG13	1.95	0.49	
1:C:7:LYS:HA	1:C:34:ILE:HG23	1.95	0.49	
1:E:7:LYS:HA	1:E:34:ILE:HG23	1.94	0.49	
1:F:7:LYS:HA	1:F:34:ILE:HG23	1.94	0.49	



	to ac pagem	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:230:PRO:HA	1:E:233:TRP:CE2	2.48	0.48	
1:G:90:LEU:HD12	1:G:95:TRP:CZ2	2.48	0.48	
1:D:385:VAL:HG21	1:D:445:LEU:HD21	1.96	0.48	
1:A:3:THR:O	1:A:4:GLU:HB2	2.13	0.48	
1:H:137:ASP:HA	1:H:147:ALA:HB2	1.95	0.48	
1:H:90:LEU:HD12	1:H:95:TRP:CZ2	2.48	0.48	
1:C:48:PHE:CG	1:C:61:ILE:HD12	2.49	0.47	
1:E:63:TRP:CD1	1:E:67:ARG:HG3	2.49	0.47	
1:B:426:HIS:NE2	1:F:378:GLU:O	2.47	0.47	
1:H:69:GLY:HA3	1:H:333:ASN:O	2.13	0.47	
1:A:7:LYS:HA	1:A:34:ILE:HG23	1.96	0.47	
1:F:185:ASP:HB2	4:F:678:HOH:O	2.13	0.47	
1:D:63:TRP:CD1	1:D:67:ARG:HG3	2.50	0.47	
1:F:100:TYR:CB	1:F:105:ILE:HD13	2.44	0.47	
1:A:137:ASP:HA	1:A:147:ALA:HB2	1.97	0.47	
1:A:381:LEU:HD13	1:A:469:CYS:SG	2.55	0.47	
1:D:233:TRP:HB2	1:D:299:PRO:HG2	1.97	0.47	
1:F:230:PRO:HA	1:F:233:TRP:CE2	2.50	0.47	
1:F:367:THR:HG21	1:F:463:VAL:HG11	1.97	0.47	
1:F:381:LEU:HD13	1:F:469:CYS:SG	2.55	0.47	
1:D:381:LEU:HD13	1:D:469:CYS:SG	2.56	0.46	
1:A:100:TYR:HB3	1:A:105:ILE:HD13	1.97	0.46	
1:C:230:PRO:HA	1:C:233:TRP:CE2	2.50	0.46	
1:F:261:GLY:HA2	1:F:331:MET:HE2	1.97	0.46	
1:B:230:PRO:HA	1:B:233:TRP:CE2	2.51	0.46	
1:C:436:LYS:NZ	4:C:586:HOH:O	2.48	0.46	
1:E:137:ASP:HA	1:E:147:ALA:HB2	1.97	0.46	
1:G:457:ILE:HG22	1:G:458:LEU:N	2.31	0.46	
1:D:230:PRO:HA	1:D:233:TRP:CE2	2.51	0.46	
1:B:233:TRP:HB2	1:B:299:PRO:HG2	1.98	0.46	
1:F:137:ASP:HA	1:F:147:ALA:HB2	1.98	0.46	
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.51	0.45	
1:B:385:VAL:HG21	1:B:445:LEU:HD21	1.99	0.45	
1:E:387:ARG:HA	1:E:396:VAL:HG22	1.98	0.45	
1:A:100:TYR:CB	1:A:105:ILE:HD13	2.46	0.45	
1:C:133:ILE:N	1:C:134:PRO:CD	2.79	0.45	
1:A:63:TRP:CD1	1:A:67:ARG:HG3	2.50	0.45	
1:H:100:TYR:HB3	1:H:105:ILE:HD13	1.99	0.45	
1:D:133:ILE:N	1:D:134:PRO:CD	2.80	0.45	
1:E:233:TRP:HB2	1:E:299:PRO:HG2	1.99	0.45	
1:H:182:VAL:HG12	1:H:184:VAL:HG13	1.99	0.45	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:436:LYS:NZ	4:E:1081:HOH:O	2.50	0.45
1:G:182:VAL:HG12	1:G:184:VAL:HG13	1.99	0.45
1:H:233:TRP:HB2	1:H:299:PRO:HG2	1.98	0.45
1:C:261:GLY:HA2	1:C:331:MET:HE2	1.98	0.45
1:D:48:PHE:CG	1:D:61:ILE:HD12	2.51	0.45
1:F:233:TRP:HB2	1:F:299:PRO:HG2	1.99	0.45
1:B:210:ASP:OD2	1:B:436:LYS:NZ	2.46	0.45
1:G:63:TRP:CD1	1:G:67:ARG:HG3	2.51	0.45
1:F:48:PHE:CB	1:F:61:ILE:HD12	2.46	0.44
1:A:458:LEU:O	1:A:459:ARG:C	2.55	0.44
1:B:63:TRP:CD1	1:B:67:ARG:HG3	2.52	0.44
1:G:457:ILE:HG22	1:G:458:LEU:HG	1.98	0.44
1:B:387:ARG:HA	1:B:396:VAL:HG22	1.99	0.44
1:G:230:PRO:HA	1:G:233:TRP:CE2	2.52	0.44
1:F:63:TRP:CD1	1:F:67:ARG:HG3	2.53	0.44
1:C:455:LEU:HB3	1:D:326:GLN:O	2.17	0.44
1:C:452:VAL:O	1:C:452:VAL:HG13	2.17	0.44
1:H:381:LEU:HD13	1:H:469:CYS:SG	2.58	0.44
1:H:457:ILE:HG22	1:H:458:LEU:N	2.32	0.44
1:C:367:THR:HG21	1:C:463:VAL:HG11	1.99	0.44
1:C:387:ARG:HA	1:C:396:VAL:HG22	2.00	0.44
1:G:233:TRP:HB2	1:G:299:PRO:HG2	1.99	0.44
1:G:381:LEU:HD13	1:G:469:CYS:SG	2.58	0.44
1:G:387:ARG:HA	1:G:396:VAL:HG22	2.00	0.43
1:A:3:THR:HG21	1:A:57:GLY:O	2.17	0.43
1:E:152:LEU:HD21	1:E:205:MET:HE1	2.00	0.43
1:G:48:PHE:CG	1:G:61:ILE:HD12	2.53	0.43
1:H:49:PRO:HA	1:H:76:LEU:HD13	1.99	0.43
1:C:152:LEU:HD21	1:C:205:MET:HE1	2.00	0.43
1:C:233:TRP:HB2	1:C:299:PRO:HG2	2.00	0.43
1:C:385:VAL:HG21	1:C:445:LEU:HD21	2.00	0.43
1:C:137:ASP:HA	1:C:147:ALA:HB2	2.01	0.43
1:C:381:LEU:HD13	1:C:469:CYS:SG	2.59	0.43
1:G:129:THR:HG22	1:G:250:THR:OG1	2.18	0.43
1:H:63:TRP:CD1	1:H:67:ARG:HG3	2.52	0.43
1:B:94:THR:HB	1:B:108:PRO:HB2	2.00	0.43
1:E:185:ASP:HB2	4:E:1195:HOH:O	2.18	0.43
1:A:233:TRP:HB2	1:A:299:PRO:HG2	2.01	0.43
1:A:261:GLY:HA2	1:A:331:MET:HE2	2.00	0.43
1:D:196:LEU:HD11	1:D:205:MET:HE1	2.01	0.43
1:E:381:LEU:HD13	1:E:469:CYS:SG	2.59	0.43



	is as page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:63:TRP:CD1	1:C:67:ARG:HG3	2.52	0.43	
1:B:49:PRO:HA	1:B:76:LEU:HD13	2.01	0.42	
1:D:416:THR:HG23	4:D:589:HOH:O	2.17	0.42	
1:E:159:TRP:N	1:E:160:PRO:CD	2.82	0.42	
1:E:367:THR:HG21	1:E:463:VAL:HG11	2.00	0.42	
1:G:94:THR:HB	1:G:108:PRO:HB2	2.00	0.42	
1:H:387:ARG:HA	1:H:396:VAL:HG22	2.01	0.42	
1:C:129:THR:HG22	1:C:250:THR:OG1	2.19	0.42	
1:F:159:TRP:N	1:F:160:PRO:CD	2.82	0.42	
1:A:196:LEU:HD11	1:A:205:MET:HE1	2.00	0.42	
1:C:455:LEU:HD22	1:D:328:GLY:O	2.19	0.42	
1:C:185:ASP:HB2	4:C:694:HOH:O	2.20	0.42	
1:C:4:GLU:HG3	1:C:7:LYS:HE2	2.02	0.42	
1:G:457:ILE:HD12	1:G:457:ILE:N	2.35	0.42	
1:E:196:LEU:HD11	1:E:205:MET:HE1	2.01	0.42	
1:A:49:PRO:HA	1:A:76:LEU:HD13	2.01	0.42	
1:B:457:ILE:CG2	1:B:458:LEU:HD13	2.49	0.42	
1:E:100:TYR:HB3	1:E:105:ILE:HD13	2.02	0.42	
1:G:152:LEU:HD21	1:G:205:MET:CE	2.50	0.42	
1:H:230:PRO:HA	1:H:233:TRP:CE2	2.55	0.42	
1:B:196:LEU:HD11	1:B:205:MET:HE1	2.02	0.42	
1:E:100:TYR:CB	1:E:105:ILE:HD13	2.50	0.42	
1:A:48:PHE:CB	1:A:61:ILE:HD12	2.50	0.42	
1:D:152:LEU:HD21	1:D:205:MET:HE1	2.02	0.42	
1:G:196:LEU:HD11	1:G:205:MET:HE1	2.01	0.42	
1:H:100:TYR:CB	1:H:105:ILE:HD13	2.49	0.42	
1:G:416:THR:HG23	4:G:587:HOH:O	2.20	0.41	
1:B:155:PRO:HB3	1:B:344:VAL:HG12	2.02	0.41	
1:B:416:THR:HG23	4:B:583:HOH:O	2.20	0.41	
1:B:152:LEU:HD12	1:B:206:ASN:O	2.21	0.41	
1:H:48:PHE:CG	1:H:61:ILE:HD12	2.56	0.41	
1:C:196:LEU:HD11	1:C:205:MET:HE1	2.01	0.41	
1:B:100:TYR:CB	1:B:105:ILE:HD13	2.51	0.41	
1:B:457:ILE:HG22	1:B:458:LEU:HD12	2.00	0.41	
1:B:129:THR:HG22	1:B:250:THR:OG1	2.21	0.41	
1:A:93:PHE:CE1	1:B:457:ILE:HG23	2.55	0.41	
1:C:159:TRP:N	1:C:160:PRO:CD	2.84	0.41	
1:B:152:LEU:HD21	1:B:205:MET:HE1	2.03	0.40	
1:E:349:ILE:HG21	1:E:470:ARG:NH2	2.35	0.40	
1:H:129:THR:HG22	1:H:250:THR:OG1	2.21	0.40	
1:H:166:GLY:O	1:H:186:ASN:ND2	2.53	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:A:159:TRP:N	1:A:160:PRO:CD	2.84	0.40	
1:A:185:ASP:HB2	4:A:691:HOH:O	2.21	0.40	
1:F:341:TRP:CE3	2:N:2:GLC:H61	2.56	0.40	
1:H:32:THR:CG2	1:H:34:ILE:HD13	2.34	0.40	
1:H:152:LEU:HD21	1:H:205:MET:HE1	2.04	0.40	
1:H:456:SER:C	1:H:457:ILE:HD12	2.42	0.40	
1:F:182:VAL:HG12	1:F:184:VAL:HG13	2.03	0.40	

There are no symmetry-related clashes.

### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	469/481~(98%)	457 (97%)	10 (2%)	2~(0%)	34	42
1	В	469/481~(98%)	458 (98%)	10 (2%)	1 (0%)	47	58
1	С	469/481 (98%)	458 (98%)	10 (2%)	1 (0%)	47	58
1	D	467/481~(97%)	457 (98%)	9 (2%)	1 (0%)	47	58
1	Е	470/481 (98%)	463 (98%)	6 (1%)	1 (0%)	47	58
1	F	470/481~(98%)	460 (98%)	9 (2%)	1 (0%)	47	58
1	G	470/481~(98%)	460 (98%)	9 (2%)	1 (0%)	47	58
1	Н	467/481 (97%)	457 (98%)	9 (2%)	1 (0%)	47	58
All	All	3751/3848 (98%)	3670 (98%)	72 (2%)	9 (0%)	47	58

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	378	GLU
1	F	378	GLU
1	А	378	GLU



Continued from previous page...

Mol	Chain	Res	Type
1	D	378	GLU
1	Е	378	GLU
1	G	378	GLU
1	А	4	GLU
1	В	378	GLU
1	Н	378	GLU

### 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	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	383/393~(98%)	383 (100%)	0	100	100
1	В	383/393~(98%)	383 (100%)	0	100	100
1	С	383/393~(98%)	383 (100%)	0	100	100
1	D	381/393~(97%)	381 (100%)	0	100	100
1	Ε	384/393~(98%)	384 (100%)	0	100	100
1	F	384/393~(98%)	384 (100%)	0	100	100
1	G	384/393~(98%)	384 (100%)	0	100	100
1	Н	381/393~(97%)	381 (100%)	0	100	100
All	All	3063/3144~(97%)	3063 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains identified.

### 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	Type	Chain	Bos	Link	Bo	ond leng	ths	Bond angles		les
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	GLC	Ι	1	2	12,12,12	0.99	0	$17,\!17,\!17$	0.76	0
2	GLC	Ι	2	2	11,11,12	0.46	0	$15,\!15,\!17$	0.97	0
2	GLC	J	1	2	12,12,12	1.01	0	$17,\!17,\!17$	0.85	0
2	GLC	J	2	2	11,11,12	0.76	0	$15,\!15,\!17$	1.15	1 (6%)
2	GLC	K	1	2	12,12,12	0.91	0	17,17,17	0.82	0
2	GLC	К	2	2	11,11,12	0.41	0	$15,\!15,\!17$	0.96	2 (13%)
2	GLC	L	1	2	12,12,12	1.02	0	$17,\!17,\!17$	0.68	0
2	GLC	L	2	2	11,11,12	0.73	0	$15,\!15,\!17$	1.02	1 (6%)
2	GLC	М	1	2	12,12,12	0.82	0	17,17,17	0.77	0
2	GLC	М	2	2	11,11,12	0.53	0	$15,\!15,\!17$	0.95	1 (6%)
2	GLC	Ν	1	2	12,12,12	0.90	0	17,17,17	0.68	0
2	GLC	N	2	2	11,11,12	0.46	0	$15,\!15,\!17$	0.86	0
2	GLC	0	1	2	12,12,12	0.96	0	$17,\!17,\!17$	0.73	0
2	GLC	0	2	2	11,11,12	0.80	0	$15,\!15,\!17$	0.98	1 (6%)
2	GLC	Р	1	2	12,12,12	1.02	0	17,17,17	0.82	0
2	GLC	Р	2	2	11,11,12	0.84	0	$15,\!15,\!17$	1.02	1 (6%)

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	GLC	Ι	1	2	-	0/2/22/22	0/1/1/1
2	GLC	Ι	2	2	-	0/2/19/22	0/1/1/1
2	GLC	J	1	2	-	0/2/22/22	0/1/1/1
2	GLC	J	2	2	-	0/2/19/22	0/1/1/1
2	GLC	Κ	1	2	-	0/2/22/22	0/1/1/1
2	GLC	Κ	2	2	-	0/2/19/22	0/1/1/1
2	GLC	L	1	2	-	1/2/22/22	0/1/1/1



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	L	2	2	-	0/2/19/22	0/1/1/1
2	GLC	М	1	2	-	1/2/22/22	0/1/1/1
2	GLC	М	2	2	-	0/2/19/22	0/1/1/1
2	GLC	N	1	2	-	0/2/22/22	0/1/1/1
2	GLC	N	2	2	-	0/2/19/22	0/1/1/1
2	GLC	0	1	2	-	0/2/22/22	0/1/1/1
2	GLC	0	2	2	-	0/2/19/22	0/1/1/1
2	GLC	Р	1	2	-	1/2/22/22	0/1/1/1
2	GLC	Р	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	L	2	GLC	C6-C5-C4	-2.64	106.81	113.00
2	J	2	GLC	C6-C5-C4	-2.61	106.90	113.00
2	Р	2	GLC	C6-C5-C4	-2.46	107.25	113.00
2	0	2	GLC	C6-C5-C4	-2.42	107.35	113.00
2	М	2	GLC	C6-C5-C4	-2.23	107.77	113.00
2	K	2	GLC	C1-O5-C5	2.15	115.11	112.19
2	K	2	GLC	C6-C5-C4	-2.09	108.11	113.00

All (7) bond angle outliers are listed below:

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	М	1	GLC	C4-C5-C6-O6
2	L	1	GLC	C4-C5-C6-O6
2	Р	1	GLC	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Ν	2	GLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



































## 5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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>	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	471/481~(97%)	0.24	11 (2%) 60 67	28, 52, 96, 152	0
1	В	471/481 (97%)	0.42	19 (4%) 38 45	29, 64, 111, 134	0
1	С	471/481~(97%)	0.19	16 (3%) 45 52	28, 52, 98, 161	0
1	D	469/481~(97%)	0.49	26 (5%) 25 31	30, 66, 117, 143	0
1	Е	472/481~(98%)	0.29	14 (2%) 50 57	28, 52, 97, 162	0
1	F	472/481~(98%)	0.25	18 (3%) 40 47	28, 53, 96, 166	0
1	G	472/481~(98%)	0.39	23 (4%) 29 36	30, 65, 114, 139	0
1	Н	469/481~(97%)	0.40	22 (4%) 31 38	30, 66, 113, 133	0
All	All	3767/3848~(97%)	0.34	149 (3%) 38 45	28, 58, 109, 166	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	454	GLY	9.0
1	Ε	453	SER	8.4
1	F	454	GLY	7.9
1	А	454	GLY	6.5
1	В	454	GLY	6.5
1	F	453	SER	6.2
1	F	455	LEU	6.0
1	D	455	LEU	5.4
1	А	457	ILE	5.3
1	Е	455	LEU	5.2
1	С	454	GLY	5.2
1	С	455	LEU	5.1
1	А	455	LEU	5.1
1	А	452	VAL	5.0
1	G	3	THR	4.9
1	В	453	SER	4.8



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Mol	Chain	Res	Type	RSRZ
1	А	453	SER	4.6
1	F	452	VAL	4.6
1	Е	458	LEU	4.6
1	F	456	SER	4.6
1	G	454	GLY	4.3
1	D	281	LEU	4.1
1	D	285	LEU	4.1
1	D	456	SER	4.0
1	Н	455	LEU	3.8
1	D	280	PHE	3.7
1	Е	224	ALA	3.7
1	Н	454	GLY	3.7
1	D	236	ILE	3.6
1	G	455	LEU	3.6
1	D	454	GLY	3.6
1	G	322	MET	3.6
1	D	453	SER	3.5
1	F	3	THR	3.5
1	А	458	LEU	3.5
1	Е	452	VAL	3.5
1	Н	458	LEU	3.5
1	D	111	VAL	3.5
1	С	221	GLY	3.5
1	Н	281	LEU	3.4
1	С	452	VAL	3.4
1	В	458	LEU	3.4
1	С	3	THR	3.3
1	Н	93	PHE	3.3
1	С	453	SER	3.2
1	D	390	PHE	3.2
1	C	148	LEU	3.2
1	F	458	LEU	3.2
1	С	457	ILE	3.2
1	C	456	SER	3.2
1	F	133	ILE	3.1
1	G	458	LEU	3.1
1	Е	456	SER	3.1
1	Н	310	GLU	3.1
1	D	28	PHE	3.0
1	В	20	GLY	3.0
1	Н	28	PHE	3.0
1	G	281	LEU	3.0



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Mol	Chain	Res	Type	RSRZ
1	Н	285	LEU	3.0
1	Н	457	ILE	3.0
1	Н	294	VAL	2.9
1	В	93	PHE	2.9
1	G	326	GLN	2.9
1	Н	133	ILE	2.9
1	G	133	ILE	2.8
1	D	276	LEU	2.8
1	D	294	VAL	2.8
1	G	285	LEU	2.8
1	D	300	LEU	2.7
1	F	236	ILE	2.7
1	F	243	TYR	2.7
1	H	88	ASP	2.7
1	G	236	ILE	2.7
1	F	135	ALA	2.7
1	D	458	LEU	2.7
1	Н	84	LYS	2.6
1	F	457	ILE	2.6
1	В	455	LEU	2.6
1	D	8	LEU	2.6
1	А	3	THR	2.6
1	Е	118	TYR	2.6
1	А	135	ALA	2.6
1	G	304	ALA	2.6
1	Е	457	ILE	2.6
1	С	458	LEU	2.5
1	D	34	ILE	2.5
1	Е	133	ILE	2.5
1	D	86	PHE	2.5
1	C	326	GLN	2.5
1	G	196	LEU	2.5
1	D	93	PHE	2.5
1	H	451	PRO	2.5
1	G	453	SER	2.4
1	H	36	VAL	2.4
1	В	326	GLN	2.4
1	В	104	LEU	2.4
1	D	451	PRO	2.4
1	С	133	ILE	2.4
1	А	196	LEU	2.4
1	В	123	LEU	2.4



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Mol	Chain	Res   Type		RSRZ
1	Н	196	LEU	2.4
1	В	224	ALA	2.4
1	D	457	ILE	2.4
1	D	24	VAL	2.4
1	Н	86	PHE	2.4
1	Е	459	ARG	2.4
1	G	313	ALA	2.4
1	G	300	LEU	2.3
1	С	451	PRO	2.3
1	F	459	ARG	2.2
1	Н	107	TYR	2.2
1	Е	474	LEU	2.2
1	В	88	ASP	2.2
1	В	243	TYR	2.2
1	F	390	PHE	2.2
1	G	28	PHE	2.2
1	D	326	GLN	2.2
1	D	166	GLY	2.2
1	G	4	GLU	2.2
1	G	450	ARG	2.2
1	D	322	MET	2.2
1	Е	236	ILE	2.2
1	Е	221	GLY	2.2
1	В	36	VAL	2.1
1	С	224	ALA	2.1
1	В	457	ILE	2.1
1	G	474	LEU	2.1
1	F	219	ASN	2.1
1	А	4	GLU	2.1
1	G	93	PHE	2.1
1	G	330	ILE	2.1
1	Н	236	ILE	2.1
1	G	166	GLY	2.1
1	Н	35	LYS	2.1
1	В	130	TRP	2.1
1	A	463	VAL	2.1
1	В	86	PHE	2.1
1	В	451	PRO	2.1
1	D	140	LEU	2.1
1	C	459	ARG	2.1
1	С	226	THR	2.1
1	В	92	PRO	2.1



Mol	Chain	Res	Type	RSRZ
1	F	4	GLU	2.0
1	Н	87	GLN	2.0
1	F	389	LEU	2.0
1	В	28	PHE	2.0
1	G	84	LYS	2.0
1	F	451	PRO	2.0
1	Н	330	ILE	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	$B-factors(A^2)$	Q<0.9
2	GLC	L	1	12/12	0.93	0.17	$47,\!53,\!56,\!57$	0
2	GLC	J	1	12/12	0.94	0.15	45,49,51,52	0
2	GLC	Р	1	12/12	0.94	0.15	45,50,51,52	0
2	GLC	K	2	11/12	0.95	0.14	$29,\!32,\!34,\!35$	0
2	GLC	J	2	11/12	0.95	0.12	39,41,44,44	0
2	GLC	L	2	11/12	0.95	0.14	40,43,45,46	0
2	GLC	М	1	12/12	0.95	0.14	33,38,40,41	0
2	GLC	N	1	12/12	0.95	0.15	36,41,42,42	0
2	GLC	0	2	11/12	0.95	0.14	39,40,42,43	0
2	GLC	K	1	12/12	0.95	0.13	35,39,41,41	0
2	GLC	N	2	11/12	0.96	0.12	30,33,36,37	0
2	GLC	0	1	12/12	0.96	0.15	44,48,50,50	0
2	GLC	М	2	11/12	0.96	0.15	28,31,34,35	0
2	GLC	Ι	2	11/12	0.96	0.15	27,30,32,33	0
2	GLC	Р	2	11/12	0.96	0.15	39,41,43,43	0
2	GLC	Ι	1	12/12	0.97	0.12	33,37,39,40	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
3	CA	F	483	1/1	0.64	0.10	71,71,71,71	0
3	CA	А	485	1/1	0.77	0.08	$61,\!61,\!61,\!61$	0
3	CA	А	483	1/1	0.81	0.06	70,70,70,70	0
3	CA	D	483	1/1	0.83	0.09	$95,\!95,\!95,\!95$	0
3	CA	G	485	1/1	0.83	0.07	59, 59, 59, 59, 59	0
3	CA	А	484	1/1	0.85	0.19	57,57,57,57	0
3	CA	С	485	1/1	0.86	0.06	61,61,61,61	0



Mol	Type	Chain	$\operatorname{Res}$	Atoms	RSCC	RSR	$B$ -factors $(A^2)$	$Q{<}0.9$
3	CA	В	483	1/1	0.87	0.05	$93,\!93,\!93,\!93$	0
3	CA	F	485	1/1	0.88	0.07	60,60,60,60	0
3	CA	F	484	1/1	0.88	0.24	57,57,57,57	0
3	CA	Е	484	1/1	0.89	0.20	58, 58, 58, 58	0
3	CA	D	485	1/1	0.90	0.14	58, 58, 58, 58	0
3	CA	С	483	1/1	0.90	0.06	64,64,64,64	0
3	CA	Е	485	1/1	0.91	0.06	61,61,61,61	0
3	CA	G	483	1/1	0.92	0.09	85,85,85,85	0
3	CA	С	484	1/1	0.92	0.15	$57,\!57,\!57,\!57$	0
3	CA	В	484	1/1	0.93	0.05	$54,\!54,\!54,\!54$	0
3	CA	Е	483	1/1	0.94	0.05	67,67,67,67	0
3	CA	G	484	1/1	0.95	0.06	$54,\!54,\!54,\!54$	0
3	CA	Н	485	1/1	0.95	0.05	$59,\!59,\!59,\!59$	0
3	CA	Н	484	1/1	0.96	0.03	54,54,54,54	0
3	CA	Н	483	1/1	0.97	0.08	89,89,89,89	0
3	CA	В	485	1/1	0.97	0.07	59, 59, 59, 59, 59	0
3	CA	D	484	1/1	0.97	0.04	$55,\!55,\!55,\!55$	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

