

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

#### Dec 16, 2023 - 08:28 am GMT

PDB ID	:	2XWT
Title	:	CRYSTAL STRUCTURE OF THE TSH RECEPTOR IN COMPLEX WITH
		A BLOCKING TYPE TSHR AUTOANTIBODY
Authors	:	Sanders, J.; Sanders, P.; Young, S.; Kabelis, K.; Baker, S.; Sullivan, A.; Evans,
		M.; Clark, J.; Wilmot, J.; Hu, X.; Roberts, E.; Powell, M.; Nunez Miguel, R.;
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Deposited on	:	2010-11-05
Resolution	:	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:

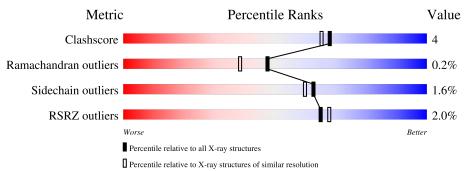
Xtriage (Phenix) EDS Percentile statistics Refmac	:::::::::::::::::::::::::::::::::::::::	1.8.4, CSD as $541$ be (2020)
Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	: :	Engh & Huber (2001)

# 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.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	$\begin{array}{l} {\rm Similar\ resolution} \\ (\# {\rm Entries,\ resolution\ range}({\rm \AA})) \end{array}$		
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	221	.% 93%	
2	В	214	% 92%	6% •
3	С	239	3% 89%	8% ••
4	D	2	100%	
5	Е	4	50% 50%	



#### 2XWT

# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5932 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 THYROID BLOCKING HUMAN AUTOANTIBODY K1-70 HEAVY CHAIN.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	215	Total 1617	C 1033	N 264	0 315	${S \atop 5}$	0	0	0

• Molecule 2 is a protein called THYROID BLOCKING HUMAN AUTOANTIBODY K1-70 LIGHT CHAIN.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	213	Total 1567	C 984	N 262	0 317	S 4	0	0	0

• Molecule 3 is a protein called THYROTROPIN RECEPTOR.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	С	234	Total 1844	C 1183	N 300	0 354	S 7	0	0	0

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



Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf	Trace
4	D	2	Total 28	C 16	N 2	0 10	0	0	0

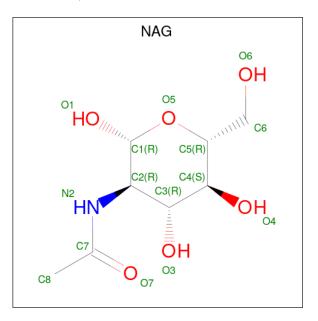
• Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.





Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
5	Е	4	Total 50	C 28	N 2	O 20	0	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	C	1	Total C N O 14 8 1 5	0	0
6	С	1	Total         C         N         O           14         8         1         5	0	0

• Molecule 7 is water.

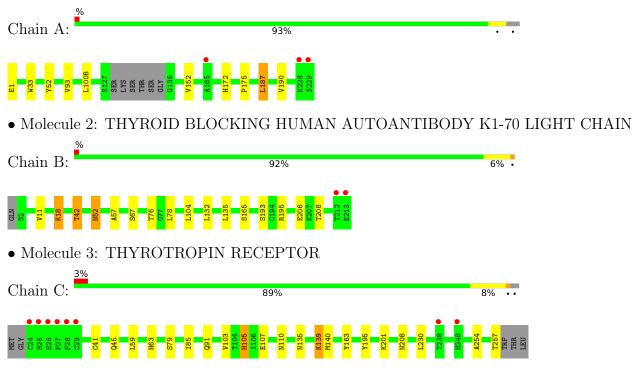
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	310	Total O 310 310	0	0
7	В	260	Total         O           260         260	0	0
7	С	228	Total         O           228         228	0	0



# 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: THYROID BLOCKING HUMAN AUTOANTIBODY K1-70 HEAVY CHAIN



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

Chain D:

100%

#### NAG1 NAG2

• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

50%

Chain E: 50%





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	83.02Å 89.30Å 101.27Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	66.98 - 1.90	Depositor
Resolution (A)	43.23 - 1.90	EDS
% Data completeness	94.2 (66.98-1.90)	Depositor
(in resolution range)	94.3 (43.23-1.90)	EDS
R <sub>merge</sub>	0.09	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.72 (at $1.89$ Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
D D.	0.177 , $0.227$	Depositor
$R, R_{free}$	0.185 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	22.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , $46.2$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.48, \langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5932	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.98% 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: NAG, BMA, MAN

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).

Mol	Chain	Bo	nd lengths	Bond angles RMSZ $ \# Z  > 5$	
	Unam	RMSZ	RMSZ $\# Z  > 5$		# Z  > 5
1	А	0.59	1/1661~(0.1%)	0.61	0/2272
2	В	0.53	0/1606	0.63	0/2196
3	С	0.55	0/1885	0.66	0/2568
All	All	0.55	1/5152~(0.0%)	0.64	0/7036

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	А	1	GLU	CD-OE1	7.54	1.33	1.25

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	1617	0	1575	9	0
2	В	1567	0	1508	15	0
3	С	1844	0	1835	16	0
4	D	28	0	25	0	0
5	Е	50	0	43	1	0
6	С	28	0	26	0	0
7	А	310	0	0	1	0

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Mol		Non-H	1 0	H(added)	Clashes	Symm-Clashes
7	В	260	0	0	4	0
7	С	228	0	0	2	0
All	All	5932	0	5012	38	0

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

Atom 1	A +	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:110:ASN:HD22	3:C:135:ASN:HD22	1.25	0.81
3:C:139:LYS:HD3	3:C:163:TYR:O	1.83	0.79
2:B:18:LYS:HG2	2:B:76:THR:HG22	1.72	0.72
2:B:18:LYS:CG	2:B:76:THR:HG22	2.25	0.66
2:B:11:VAL:HG13	2:B:104:LEU:HD13	1.81	0.63
2:B:57:ALA:CB	7:B:355:HOH:O	2.48	0.62
3:C:254:ALA:O	3:C:257:THR:HG22	2.02	0.59
3:C:201:LYS:NZ	7:C:402:HOH:O	2.35	0.59
2:B:57:ALA:HB3	7:B:355:HOH:O	2.01	0.58
2:B:193:SER:HB3	2:B:208:THR:HG22	1.87	0.56
3:C:254:ALA:HB1	3:C:257:THR:CG2	2.36	0.56
2:B:78:LEU:HD11	2:B:104:LEU:HD21	1.90	0.54
2:B:42:THR:HG21	7:B:531:HOH:O	2.09	0.53
1:A:190:VAL:HG21	2:B:135:LEU:CD1	2.39	0.52
1:A:187:LEU:C	1:A:187:LEU:HD12	2.31	0.51
1:A:33:TRP:CE2	1:A:52:TYR:HB2	2.47	0.50
3:C:45:GLN:CG	3:C:63:HIS:CD2	2.95	0.50
3:C:195:TYR:CG	5:E:1:NAG:H82	2.48	0.49
3:C:79:SER:HA	3:C:103:VAL:HA	1.93	0.49
1:A:152:VAL:HG23	1:A:187:LEU:HD21	1.94	0.49
3:C:105:HIS:CE1	3:C:107:GLU:HG3	2.47	0.49
1:A:175:PRO:HG2	2:B:165:SER:OG	2.14	0.48
3:C:139:LYS:CD	3:C:163:TYR:O	2.61	0.47
1:A:172:HIS:HD2	7:B:501:HOH:O	1.97	0.46
2:B:195:ARG:NH1	2:B:206:GLU:OE1	2.49	0.46
3:C:45:GLN:HG3	3:C:63:HIS:CD2	2.51	0.46
3:C:45:GLN:HG2	3:C:63:HIS:CD2	2.52	0.44
2:B:193:SER:CB	2:B:208:THR:HG22	2.47	0.44
3:C:41:CYS:HB2	3:C:59:LEU:HD23	1.99	0.44
2:B:132:LEU:HD12	2:B:132:LEU:N	2.32	0.43
1:A:172:HIS:HE1	7:A:526:HOH:O	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:ASN:HD22	2:B:52:ASN:C	2.22	0.43
2:B:18:LYS:HG3	2:B:76:THR:HG22	1.98	0.42
1:A:93:VAL:HG11	1:A:100(B):LEU:HB3	2.00	0.42
3:C:91:GLN:NE2	7:C:416:HOH:O	2.52	0.41
1:A:152:VAL:CG2	1:A:187:LEU:HD21	2.50	0.41
3:C:254:ALA:HB1	3:C:257:THR:HG21	2.02	0.41
3:C:230:LEU:HD23	3:C:230:LEU:C	2.41	0.41

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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	211/221~(96%)	208 (99%)	3~(1%)	0	100	100
2	В	211/214~(99%)	206 (98%)	5(2%)	0	100	100
3	С	232/239~(97%)	223 (96%)	8 (3%)	1 (0%)	34	24
All	All	654/674~(97%)	637 (97%)	16 (2%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	С	85	ILE

#### 5.3.2 Protein sidechains (i)

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

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



Mol	Chain	Analysed	lysed Rotameric Outliers		Percentiles		
1	А	180/189~(95%)	179~(99%)	1 (1%)	86 87		
2	В	172/178~(97%)	168~(98%)	4 (2%)	50 45		
3	С	214/220~(97%)	210~(98%)	4 (2%)	57 53		
All	All	566/587~(96%)	557~(98%)	9~(2%)	62 60		

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	187	LEU
2	В	18	LYS
2	В	42	THR
2	В	52	ASN
2	В	67	SER
3	С	105	HIS
3	С	139	LYS
3	С	140	MET
3	С	208	ASN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such side chains are listed below:

Mol	Chain	Res	Type
1	А	172	HIS
2	В	52	ASN
2	В	108	GLN
2	В	128	ASN
2	В	189	HIS
3	С	45	GLN
3	С	63	HIS
3	С	91	GLN
3	С	105	HIS
3	С	110	ASN
3	С	186	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)

6 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	Mol Type Chain R		Chain Res Link		Bo	Bond lengths			Bond angles		
MOI	IOI Type Cham	Counts			RMSZ	# Z >2	Counts	RMSZ	# Z >2		
4	NAG	D	1	4,3	14,14,15	0.40	0	17,19,21	0.90	1 (5%)	
4	NAG	D	2	4	14,14,15	0.51	0	17,19,21	1.05	1 (5%)	
5	NAG	Е	1	5,3	14,14,15	0.56	0	17,19,21	0.95	0	
5	NAG	Е	2	5	14,14,15	0.56	0	17,19,21	0.65	0	
5	BMA	Е	3	5	11,11,12	0.53	0	$15,\!15,\!17$	0.97	0	
5	MAN	Е	4	5	11,11,12	0.62	0	15,15,17	1.16	2 (13%)	

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
4	NAG	D	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
5	NAG	Е	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	Е	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Е	3	5	-	0/2/19/22	0/1/1/1
5	MAN	Е	4	5	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	Ε	4	MAN	C1-C2-C3	2.73	113.02	109.67
4	D	1	NAG	O5-C5-C6	2.43	111.02	107.20
5	Е	4	MAN	C1-O5-C5	2.27	115.27	112.19
4	D	2	NAG	C8-C7-N2	2.07	119.61	116.10

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
5	Ε	4	MAN	O5-C5-C6-O6

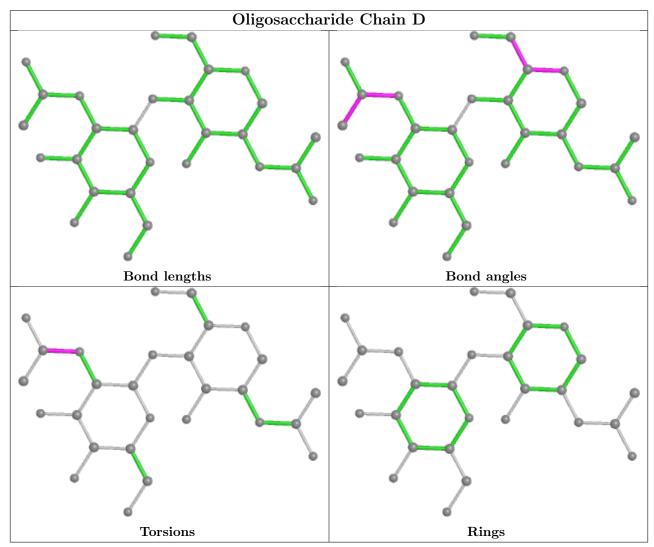
All (3) torsion outliers are listed below:

There are no ring outliers.

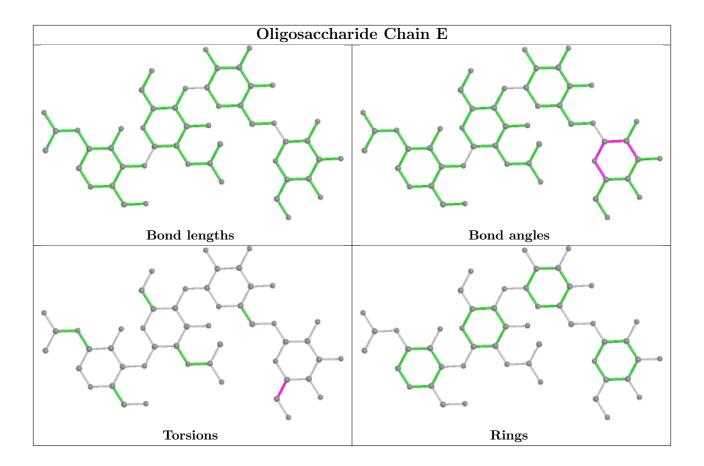
1 monomer is involved in 1 short contact:

Mo	Chain	Res	Type	Clashes	Symm-Clashes
5	Е	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)

2 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).

Mol Type	Chain	Res	Link	Bond lengths			Bond angles			
IVIOI	Moi Type Chain F	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2	
6	NAG	С	304	3	14,14,15	0.60	0	17,19,21	1.69	4 (23%)
6	NAG	С	303	3	14,14,15	0.41	0	17,19,21	0.97	1 (5%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	С	304	3	-	0/6/23/26	0/1/1/1
6	NAG	С	303	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
6	С	304	NAG	C4-C3-C2	3.78	116.56	111.02
6	С	304	NAG	C3-C4-C5	3.35	116.21	110.24
6	С	303	NAG	O5-C5-C6	2.87	111.70	107.20
6	С	304	NAG	O5-C1-C2	-2.43	107.46	111.29
6	С	304	NAG	C1-O5-C5	2.10	115.04	112.19

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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	215/221~(97%)	-0.16	3 (1%) 75 77	11, 18, 33, 43	0
2	В	213/214~(99%)	-0.04	2 (0%) 84 85	12, 20, 33, 44	0
3	С	234/239~(97%)	0.03	8 (3%) 45 48	11, 21, 42, 48	0
All	All	662/674~(98%)	-0.05	13 (1%) 65 68	11, 20, 35, 48	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	С	25	SER	6.4
2	В	212	THR	5.3
3	С	24	CYS	4.9
3	С	28	PRO	4.8
3	С	29	CYS	4.5
1	А	229	SER	4.1
3	С	26	SER	3.9
3	С	239	THR	3.6
3	С	248	HIS	3.1
2	В	213	GLU	2.8
3	С	27	PRO	2.7
1	А	228	LYS	2.6
1	А	165	ALA	2.5

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

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

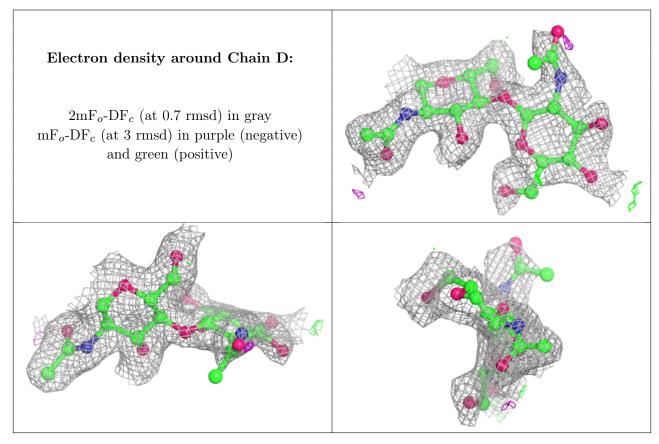


### 6.3 Carbohydrates (i)

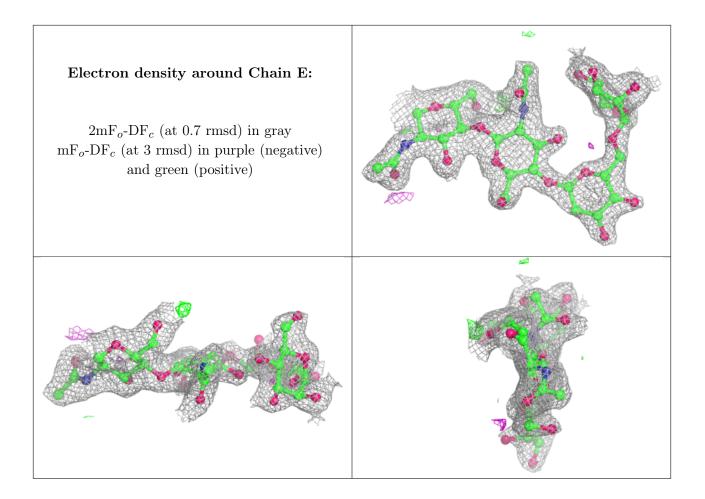
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	NAG	D	2	14/15	0.77	0.36	$49,\!52,\!53,\!53$	0
5	MAN	Е	4	11/12	0.79	0.21	$50,\!53,\!54,\!55$	0
5	BMA	Е	3	11/12	0.80	0.29	$54,\!55,\!55,\!56$	0
5	NAG	Е	2	14/15	0.81	0.19	45,48,50,51	0
4	NAG	D	1	14/15	0.86	0.13	26,32,38,44	0
5	NAG	Е	1	14/15	0.94	0.09	26,30,34,39	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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
6	NAG	С	304	14/15	0.80	0.17	38,44,46,46	0
6	NAG	С	303	14/15	0.91	0.19	36,39,40,40	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

