



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 02:04 PM BST

PDB ID : 1N8Y  
Title : Crystal structure of the extracellular region of rat HER2  
Authors : Cho, H.-S.; Mason, K.; Ramyar, K.X.; Stanley, A.M.; Gabelli, S.B.; Denney Jr., D.W.; Leahy, D.J.  
Deposited on : 2002-11-21  
Resolution : 2.40 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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1  
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) : 2.13.1

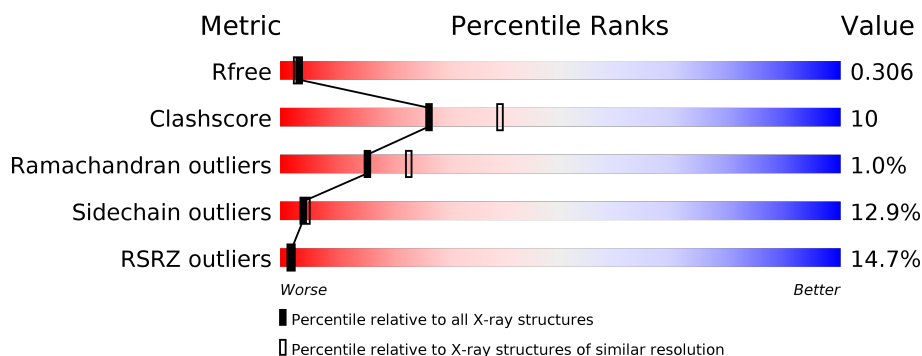
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	C	608	
2	A	2	
2	B	2	

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
2	NAG	B	2	-	-	-	X

## 2 Entry composition

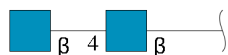
There are 4 unique types of molecules in this entry. The entry contains 4732 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 protooncoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	592	Total	C	N	O	S	0	0	0
			4578	2838	823	863	54			

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



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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

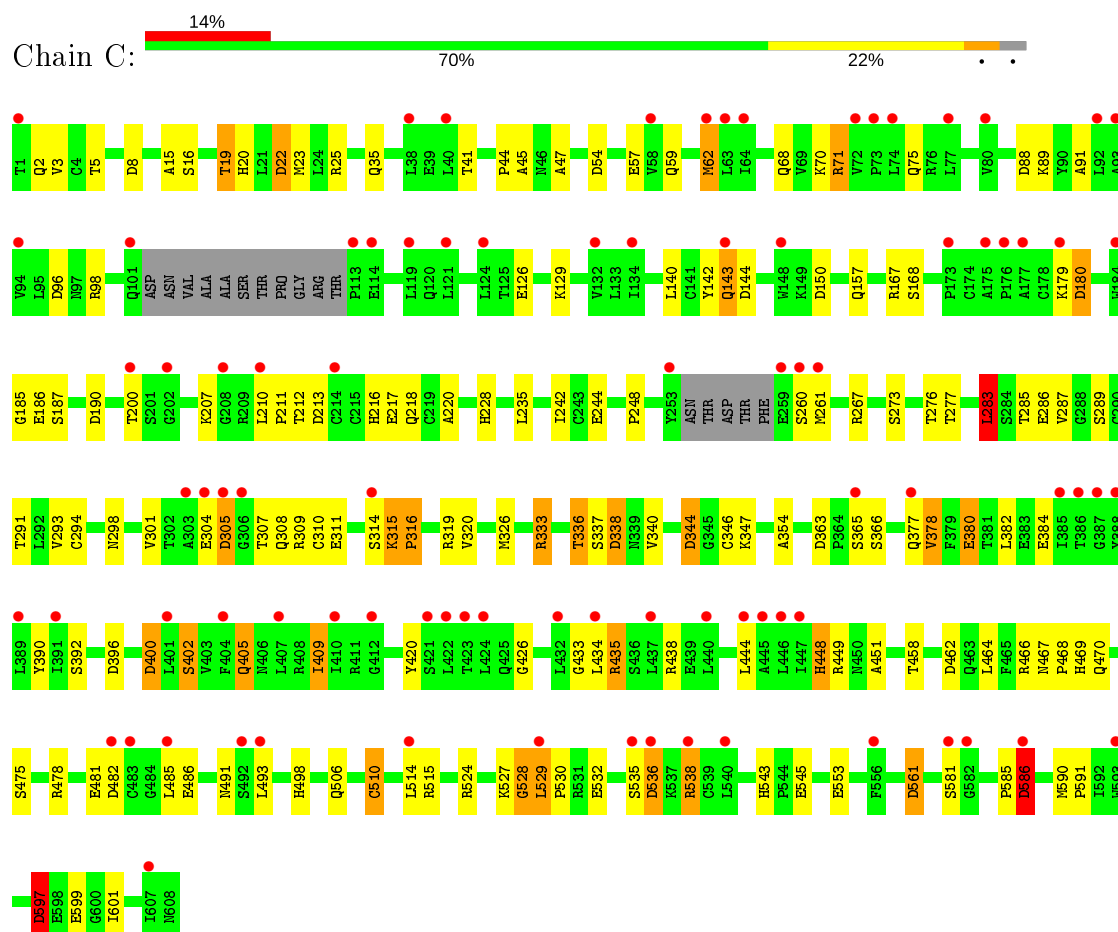
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	84	Total	O	0	0
			84	84		

### 3 Residue-property plots

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: protooncoprotein



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

Chain A: 



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

Chain B:

100%

RMG1  
RMG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.87Å 116.40Å 55.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 29.53 – 2.39	Depositor EDS
% Data completeness (in resolution range)	94.4 (20.00-2.40) 92.7 (29.53-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.224 , 0.282 0.251 , 0.306	Depositor DCC
$R_{free}$ test set	1673 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.6	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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

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	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	C	0.70	1/4684 (0.0%)	0.92	21/6357 (0.3%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	57	GLU	CD-OE2	5.20	1.31	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	363	ASP	CB-CG-OD2	9.16	126.55	118.30
1	C	396	ASP	CB-CG-OD2	6.93	124.54	118.30
1	C	597	ASP	CB-CG-OD2	6.75	124.37	118.30
1	C	8	ASP	CB-CG-OD2	6.68	124.31	118.30
1	C	283	LEU	CA-CB-CG	6.53	130.31	115.30
1	C	144	ASP	CB-CG-OD2	6.41	124.06	118.30
1	C	462	ASP	CB-CG-OD2	6.40	124.06	118.30
1	C	400	ASP	CB-CG-OD1	6.28	123.95	118.30
1	C	190	ASP	CB-CG-OD2	6.06	123.75	118.30
1	C	54	ASP	CB-CG-OD2	5.97	123.68	118.30
1	C	536	ASP	CB-CG-OD2	5.94	123.64	118.30
1	C	150	ASP	CB-CG-OD2	5.85	123.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	344	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	88	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	586	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	305	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	338	ASP	CB-CG-OD2	5.27	123.04	118.30
1	C	96	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	213	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	180	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	482	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	528	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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	C	4578	0	4386	92	0
2	A	28	0	25	1	0
2	B	28	0	25	0	0
3	C	14	0	13	0	0
4	C	84	0	0	3	0
All	All	4732	0	4449	93	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (93) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:GLU:OE2	1:C:220:ALA:O	1.77	1.01
1:C:466:ARG:H	1:C:470:GLN:NE2	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:ARG:H	1:C:470:GLN:HE22	1.18	0.89
1:C:529:LEU:HB3	1:C:530:PRO:CD	2.04	0.88
1:C:143:GLN:NE2	1:C:167:ARG:HH21	1.72	0.87
1:C:143:GLN:HE21	1:C:167:ARG:HH21	1.28	0.81
1:C:529:LEU:CB	1:C:530:PRO:CD	2.58	0.80
1:C:283:LEU:HD13	1:C:308:GLN:HB3	1.63	0.80
1:C:529:LEU:CB	1:C:530:PRO:HD2	2.12	0.80
1:C:467:ASN:H	1:C:470:GLN:HE21	1.30	0.80
1:C:287:VAL:O	1:C:287:VAL:HG12	1.84	0.78
1:C:543:HIS:HD2	1:C:545:GLU:H	1.31	0.77
1:C:336:THR:HG22	1:C:338:ASP:H	1.50	0.77
1:C:15:ALA:O	1:C:449:ARG:NH2	2.20	0.75
1:C:377:GLN:O	1:C:380:GLU:CG	2.39	0.70
1:C:529:LEU:HB3	1:C:530:PRO:HD3	1.74	0.68
1:C:543:HIS:CD2	1:C:545:GLU:H	2.12	0.67
1:C:377:GLN:O	1:C:380:GLU:HG3	1.95	0.67
1:C:529:LEU:HB2	1:C:530:PRO:HD2	1.79	0.65
1:C:400:ASP:OD1	1:C:402:SER:HB2	1.97	0.65
1:C:35:GLN:HG2	1:C:59:GLN:NE2	2.11	0.65
1:C:597:ASP:HB2	1:C:601:ILE:H	1.63	0.64
1:C:466:ARG:N	1:C:470:GLN:HE22	1.95	0.63
1:C:529:LEU:HB3	1:C:530:PRO:HD2	1.76	0.63
1:C:71:ARG:HB2	1:C:71:ARG:NH1	2.16	0.60
1:C:377:GLN:O	1:C:380:GLU:HG2	2.00	0.60
1:C:143:GLN:NE2	1:C:167:ARG:NH2	2.48	0.60
1:C:451:ALA:O	1:C:478:ARG:HG3	2.02	0.59
1:C:390:TYR:CE2	1:C:392:SER:HB2	2.38	0.59
1:C:216:HIS:HD2	1:C:218:GLN:H	1.51	0.59
1:C:333:ARG:HG2	1:C:333:ARG:HH11	1.69	0.58
1:C:515:ARG:HD3	1:C:532:GLU:OE2	2.04	0.57
1:C:289:SER:HB2	4:C:820:HOH:O	2.03	0.57
1:C:298:ASN:HD22	1:C:310:CYS:HB3	1.70	0.57
1:C:315:LYS:HB2	1:C:316:PRO:HD2	1.87	0.56
1:C:585:PRO:O	1:C:586:ASP:C	2.42	0.56
1:C:481:GLU:O	1:C:485:LEU:HD12	2.05	0.55
1:C:242:ILE:HG22	1:C:244:GLU:HG3	1.87	0.55
1:C:344:ASP:HA	1:C:378:VAL:HG22	1.87	0.55
1:C:287:VAL:O	1:C:287:VAL:CG1	2.54	0.54
1:C:433:GLY:HA2	1:C:506:GLN:OE1	2.09	0.53
1:C:285:THR:HG22	1:C:286:GLU:N	2.23	0.52
1:C:2:GLN:HG3	1:C:3:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:561:ASP:N	1:C:561:ASP:OD1	2.43	0.52
1:C:20:HIS:HE1	1:C:41:THR:O	1.93	0.52
1:C:467:ASN:H	1:C:470:GLN:NE2	2.04	0.52
1:C:491:ASN:ND2	1:C:493:LEU:H	2.08	0.52
1:C:16:SER:OG	1:C:19:THR:HB	2.11	0.51
1:C:524:ARG:HG2	1:C:528:GLY:HA3	1.93	0.51
1:C:535:SER:O	1:C:538:ARG:HB2	2.10	0.51
1:C:405:GLN:HG2	1:C:435:ARG:CZ	2.41	0.50
1:C:142:TYR:CD1	1:C:185:GLY:HA2	2.47	0.49
1:C:510:CYS:SG	1:C:514:LEU:HD23	2.53	0.48
1:C:20:HIS:CE1	1:C:41:THR:O	2.67	0.47
1:C:216:HIS:CD2	1:C:218:GLN:H	2.31	0.47
1:C:333:ARG:HG2	1:C:333:ARG:NH1	2.28	0.47
1:C:143:GLN:HE21	1:C:167:ARG:NH2	2.03	0.47
1:C:143:GLN:NE2	1:C:167:ARG:HE	2.13	0.47
1:C:336:THR:CG2	1:C:337:SER:N	2.77	0.47
1:C:478:ARG:HH22	1:C:486:GLU:CD	2.18	0.46
1:C:597:ASP:HB3	1:C:599:GLU:H	1.80	0.46
1:C:285:THR:HG22	1:C:287:VAL:H	1.82	0.45
1:C:384:GLU:HB2	1:C:409:ILE:HD12	1.99	0.45
1:C:210:LEU:HB3	1:C:211:PRO:HD2	1.98	0.45
1:C:44:PRO:HD2	1:C:47:ALA:HB2	1.99	0.45
1:C:283:LEU:CD1	1:C:308:GLN:HB3	2.43	0.45
1:C:242:ILE:HG22	1:C:244:GLU:CG	2.47	0.44
1:C:597:ASP:HB2	1:C:601:ILE:N	2.30	0.44
1:C:23:MET:HG3	1:C:420:TYR:OH	2.18	0.44
1:C:467:ASN:HB2	1:C:468:PRO:CD	2.49	0.43
1:C:448:HIS:HA	1:C:475:SER:O	2.19	0.43
1:C:71:ARG:HB2	1:C:71:ARG:HH11	1.84	0.43
1:C:478:ARG:NH2	1:C:486:GLU:OE1	2.49	0.43
1:C:22:ASP:OD1	1:C:25:ARG:NH1	2.52	0.42
1:C:384:GLU:CG	1:C:409:ILE:HD12	2.49	0.42
1:C:248:PRO:HD2	1:C:267:ARG:HB2	2.01	0.42
1:C:444:LEU:HD23	1:C:470:GLN:HA	1.99	0.42
1:C:5:THR:HG22	4:C:840:HOH:O	2.18	0.42
1:C:91:ALA:HB2	1:C:129:LYS:O	2.20	0.42
1:C:142:TYR:OH	1:C:186:GLU:HB3	2.20	0.42
1:C:143:GLN:HG3	1:C:143:GLN:H	1.26	0.42
1:C:62:MET:HB2	1:C:62:MET:HE3	1.81	0.41
1:C:590:MET:HA	1:C:591:PRO:HD3	1.90	0.41
1:C:467:ASN:HD22	1:C:469:HIS:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:CYS:HB3	1:C:298:ASN:HB2	2.03	0.41
1:C:23:MET:HG2	1:C:444:LEU:CD1	2.51	0.41
2:A:1:NAG:O6	2:A:2:NAG:H82	2.20	0.41
1:C:35:GLN:HG2	1:C:59:GLN:HE22	1.82	0.41
1:C:354:ALA:HA	1:C:390:TYR:O	2.21	0.40
1:C:458:THR:O	1:C:498:HIS:HA	2.21	0.40
1:C:433:GLY:O	1:C:435:ARG:N	2.54	0.40
1:C:346:CYS:HB2	4:C:808:HOH:O	2.21	0.40
1:C:426:GLY:HA2	1:C:449:ARG:O	2.21	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	Percentiles	
1	C	586/608 (96%)	548 (94%)	32 (6%)	6 (1%)	15	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	45	ALA
1	C	529	LEU
1	C	597	ASP
1	C	434	LEU
1	C	586	ASP
1	C	316	PRO

### 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	Percentiles
1	C	513/526 (98%)	447 (87%)	66 (13%)	<b>4</b> <b>5</b>

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	19	THR
1	C	22	ASP
1	C	62	MET
1	C	68	GLN
1	C	70	LYS
1	C	71	ARG
1	C	75	GLN
1	C	89	LYS
1	C	98	ARG
1	C	140	LEU
1	C	143	GLN
1	C	157	GLN
1	C	168	SER
1	C	179	LYS
1	C	180	ASP
1	C	187	SER
1	C	200	THR
1	C	207	LYS
1	C	212	THR
1	C	217	GLU
1	C	228	HIS
1	C	235	LEU
1	C	260	SER
1	C	261	MET
1	C	273	SER
1	C	276	THR
1	C	277	THR
1	C	283	LEU
1	C	291	THR
1	C	293	VAL
1	C	301	VAL
1	C	304	GLU
1	C	305	ASP
1	C	307	THR

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Mol	Chain	Res	Type
1	C	309	ARG
1	C	311	GLU
1	C	314	SER
1	C	315	LYS
1	C	319	ARG
1	C	320	VAL
1	C	326	MET
1	C	333	ARG
1	C	336	THR
1	C	340	VAL
1	C	347	LYS
1	C	365	SER
1	C	366	SER
1	C	378	VAL
1	C	380	GLU
1	C	382	LEU
1	C	402	SER
1	C	405	GLN
1	C	409	ILE
1	C	435	ARG
1	C	438	ARG
1	C	448	HIS
1	C	464	LEU
1	C	510	CYS
1	C	527	LYS
1	C	536	ASP
1	C	538	ARG
1	C	553	GLU
1	C	561	ASP
1	C	581	SER
1	C	586	ASP
1	C	597	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	20	HIS
1	C	59	GLN
1	C	68	GLN
1	C	75	GLN
1	C	143	GLN
1	C	216	HIS

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Mol	Chain	Res	Type
1	C	218	GLN
1	C	236	HIS
1	C	298	ASN
1	C	308	GLN
1	C	406	ASN
1	C	416	HIS
1	C	467	ASN
1	C	470	GLN
1	C	491	ASN
1	C	509	ASN
1	C	543	HIS
1	C	547	GLN

### 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](#)

4 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAG	A	1	1,2	14,14,15	0.80	1 (7%)	17,19,21	1.24	3 (17%)
2	NAG	A	2	2	14,14,15	0.71	0	17,19,21	1.27	2 (11%)
2	NAG	B	1	1,2	14,14,15	0.58	0	17,19,21	1.70	2 (11%)
2	NAG	B	2	2	14,14,15	0.56	0	17,19,21	1.11	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
2	NAG	A	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	A	2	2	-	4/6/23/26	0/1/1/1
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAG	O5-C1	-2.22	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	5.48	119.62	112.19
2	B	1	NAG	O5-C1-C2	2.76	115.65	111.29
2	A	1	NAG	C4-C3-C2	2.49	114.67	111.02
2	A	2	NAG	C1-O5-C5	2.38	115.41	112.19
2	B	2	NAG	C8-C7-N2	2.27	119.94	116.10
2	A	1	NAG	O4-C4-C3	-2.21	105.23	110.35
2	A	1	NAG	C1-C2-N2	-2.12	106.86	110.49
2	A	2	NAG	O4-C4-C5	2.00	114.27	109.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

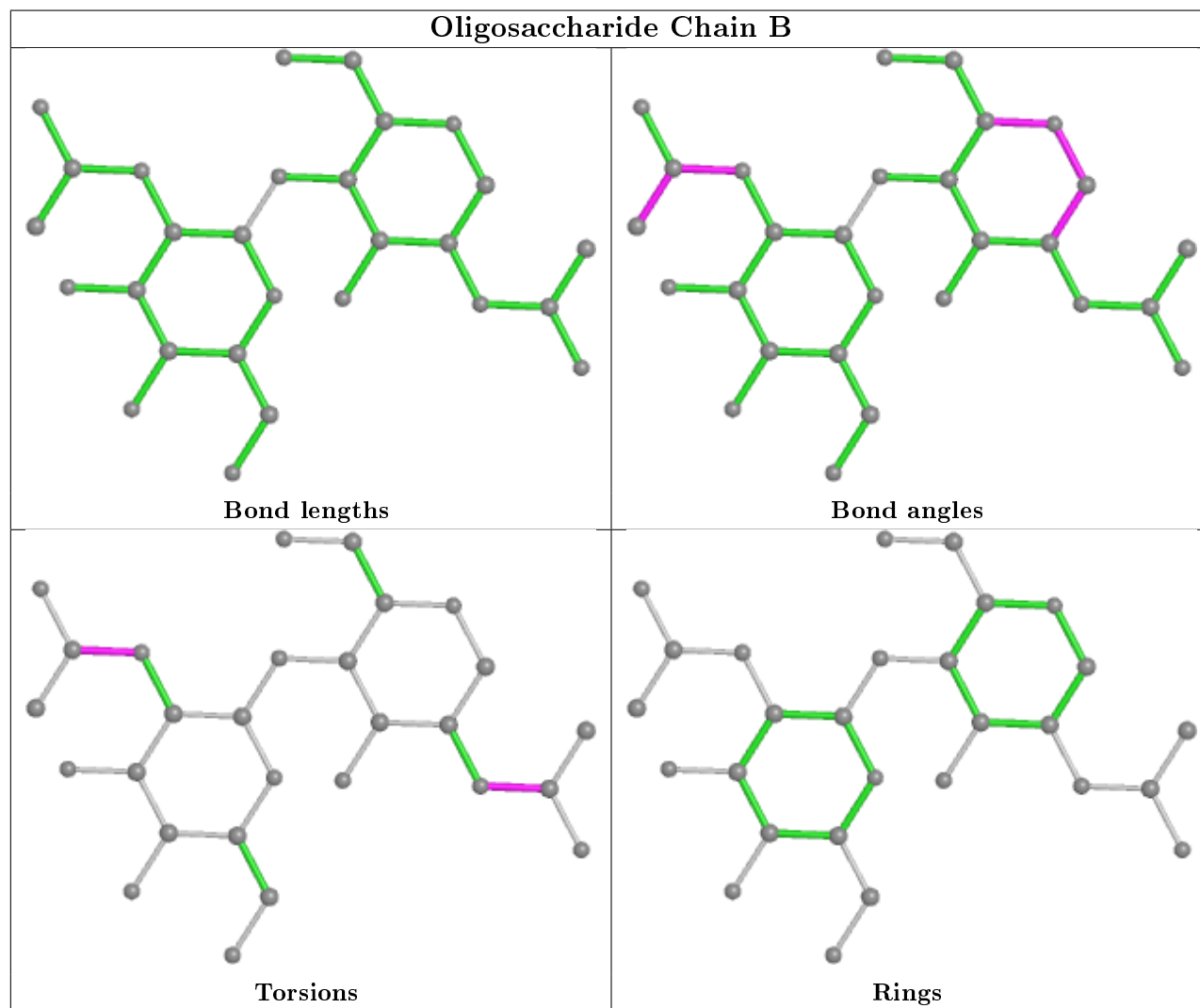
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	A	2	NAG	C8-C7-N2-C2
2	A	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	A	2	NAG	O7-C7-N2-C2
2	A	2	NAG	C4-C5-C6-O6
2	A	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O7-C7-N2-C2
2	A	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	NAG	1	0
2	A	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](#)

1 ligand is 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		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	766	1	14,14,15	0.75	0	17,19,21	1.83	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	766	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	766	NAG	C1-O5-C5	5.85	120.12	112.19
3	C	766	NAG	O4-C4-C5	2.58	115.69	109.30
3	C	766	NAG	C3-C4-C5	-2.45	105.86	110.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	766	NAG	C8-C7-N2-C2
3	C	766	NAG	O7-C7-N2-C2
3	C	766	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	592/608 (97%)	0.72	87 (14%) 2 2	11, 26, 36, 47	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	121	LEU	5.9
1	C	1	THR	5.4
1	C	389	LEU	5.4
1	C	304	GLU	5.3
1	C	422	LEU	5.3
1	C	593	TRP	5.0
1	C	119	LEU	5.0
1	C	253	TYR	4.9
1	C	124	LEU	4.6
1	C	74	LEU	4.3
1	C	529	LEU	4.3
1	C	72	VAL	4.3
1	C	64	ILE	4.3
1	C	581	SER	4.2
1	C	62	MET	3.9
1	C	77	LEU	3.9
1	C	424	LEU	3.9
1	C	493	LEU	3.8
1	C	38	LEU	3.8
1	C	385	ILE	3.8
1	C	421	SER	3.8
1	C	440	LEU	3.7
1	C	94	VAL	3.6
1	C	184	TRP	3.5
1	C	377	GLN	3.5
1	C	101	GLN	3.4
1	C	410	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	173	PRO	3.3
1	C	92	LEU	3.2
1	C	607	ILE	3.2
1	C	391	ILE	3.1
1	C	586	ASP	3.1
1	C	432	LEU	3.1
1	C	434	LEU	3.1
1	C	259	GLU	3.0
1	C	93	ALA	3.0
1	C	175	ALA	3.0
1	C	423	THR	3.0
1	C	437	LEU	3.0
1	C	535	SER	3.0
1	C	538	ARG	2.9
1	C	540	LEU	2.9
1	C	132	VAL	2.8
1	C	303	ALA	2.8
1	C	387	GLY	2.8
1	C	73	PRO	2.8
1	C	40	LEU	2.8
1	C	482	ASP	2.7
1	C	388	TYR	2.7
1	C	261	MET	2.7
1	C	305	ASP	2.7
1	C	582	GLY	2.6
1	C	445	ALA	2.6
1	C	113	PRO	2.6
1	C	485	LEU	2.5
1	C	404	PHE	2.5
1	C	114	GLU	2.5
1	C	386	THR	2.5
1	C	446	LEU	2.5
1	C	492	SER	2.5
1	C	177	ALA	2.5
1	C	58	VAL	2.4
1	C	179	LYS	2.4
1	C	63	LEU	2.4
1	C	134	ILE	2.4
1	C	148	TRP	2.4
1	C	314	SER	2.4
1	C	365	SER	2.3
1	C	407	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	514	LEU	2.3
1	C	176	PRO	2.3
1	C	306	GLY	2.3
1	C	556	PHE	2.3
1	C	80	VAL	2.3
1	C	143	GLN	2.2
1	C	483	CYS	2.2
1	C	401	LEU	2.2
1	C	447	ILE	2.2
1	C	214	CYS	2.2
1	C	208	GLY	2.1
1	C	200	THR	2.1
1	C	210	LEU	2.1
1	C	260	SER	2.0
1	C	202	GLY	2.0
1	C	412	GLY	2.0
1	C	444	LEU	2.0
1	C	536	ASP	2.0

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

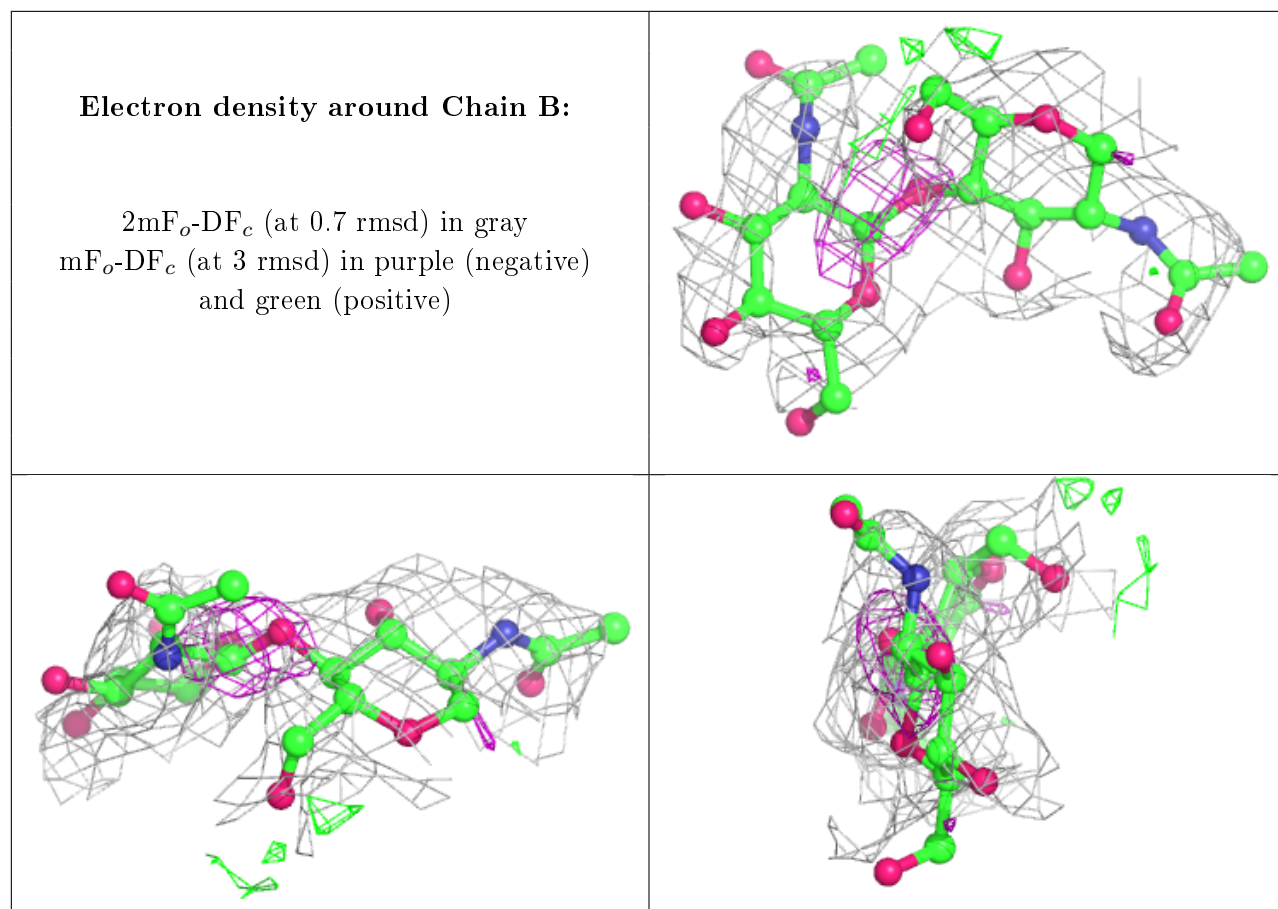
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	B	2	14/15	0.67	0.62	62,63,64,65	0
2	NAG	B	1	14/15	0.69	0.35	53,55,58,60	0
2	NAG	A	2	14/15	0.75	0.28	51,53,54,55	0
2	NAG	A	1	14/15	0.88	0.15	37,40,45,47	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	NAG	C	766	14/15	0.82	0.12	65,74,77,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.