



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:21 AM GMT

PDB ID : 2QF8  
Title : Crystal structure of the complex of Buffalo Secretory Glycoprotein with tetrasaccharide at 2.8Å resolution  
Authors : Singh,A.K.; Jain,R.; Sinha,M.; Kumar,A.; Singh,N.; Sharma,S.; Kaur,P.; Singh,T.P.  
Deposited on : 2007-06-27  
Resolution : 2.80 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

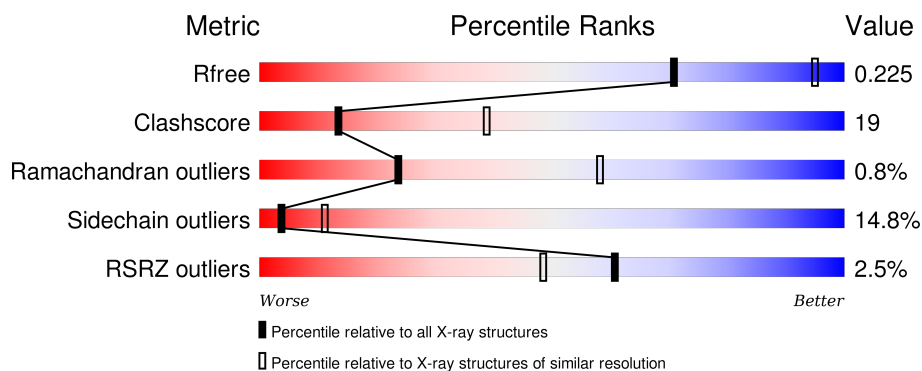
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

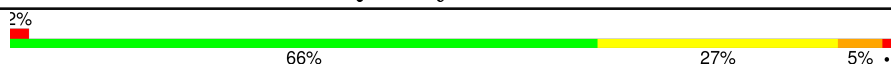
The reported resolution of this entry is 2.80 Å.

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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	A	361	

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
3	NAG	A	364	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	365	-	-	X	-
3	NAG	A	366	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3109 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 Chitinase-3-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2894	1851	507	527	9			

- Molecule 2 is SUGAR (2-MER) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			57	32	4	21		

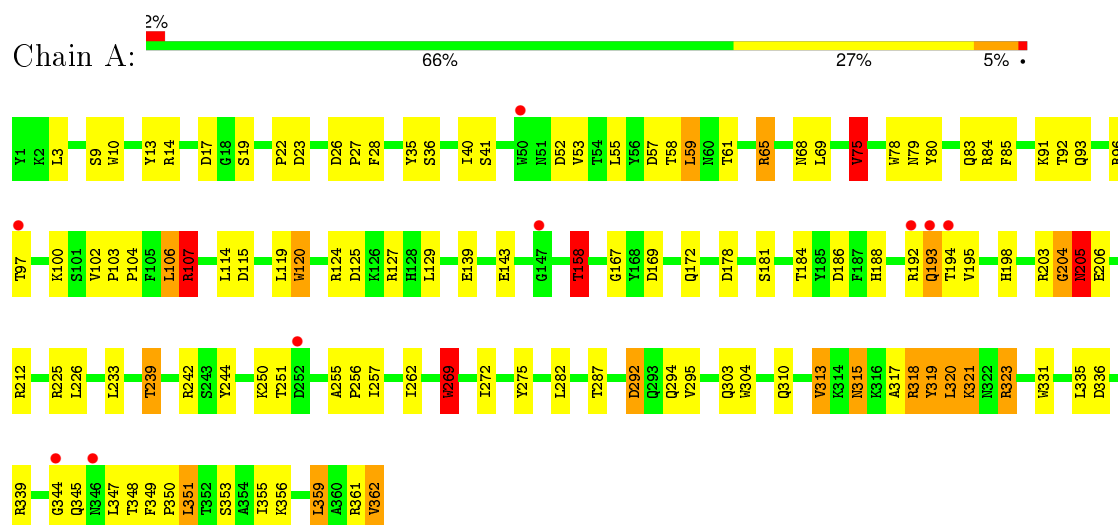
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	144	Total 144	O 144	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Chitinase-3-like protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.87Å 66.50Å 107.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.80 – 2.80 42.02 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.4 (56.80-2.80) 92.4 (42.02-2.80)	Depositor EDS
$R_{merge}$	0.00	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.187 , 0.227 0.195 , 0.225	Depositor DCC
$R_{free}$ test set	508 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.1	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 10690 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3109	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	A	1.16	3/2974 (0.1%)	1.17	21/4037 (0.5%)

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
3	A	1	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	ASN	CB-CG	5.91	1.64	1.51
1	A	269	TRP	CB-CG	-5.54	1.40	1.50
1	A	319	TYR	CD2-CE2	-5.35	1.31	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ASN	CB-CA-C	12.40	135.20	110.40
1	A	292	ASP	CB-CG-OD1	8.49	125.94	118.30
1	A	269	TRP	CB-CA-C	-7.54	95.32	110.40
1	A	318	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	A	318	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	79	ASN	CA-CB-CG	6.91	128.60	113.40
1	A	336	ASP	CB-CG-OD2	6.88	124.49	118.30
1	A	107	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	107	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	79	ASN	N-CA-CB	-6.36	99.16	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ASP	CB-CG-OD2	6.35	124.01	118.30
1	A	65	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	52	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	84	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	120	TRP	CA-CB-CG	5.66	124.45	113.70
1	A	17	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	158	THR	N-CA-CB	-5.59	99.67	110.30
1	A	125	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	115	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	75	VAL	CB-CA-C	-5.19	101.53	111.40
1	A	167	GLY	N-CA-C	5.09	125.83	113.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	364	NAG	C1

There are no planarity outliers.

## 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	A	2894	0	2818	97	0
2	A	14	0	13	0	0
3	A	57	0	50	17	0
4	A	144	0	0	17	0
All	All	3109	0	2881	109	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 19.

All (109) 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:A:323:ARG:HG2	1:A:323:ARG:HH11	0.92	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ASP:HB2	4:A:498:HOH:O	1.59	1.02
1:A:317:ALA:HA	1:A:320:LEU:CD1	1.91	1.00
3:A:365:NAG:H62	3:A:366:NAG:C8	1.91	0.99
1:A:323:ARG:CG	1:A:323:ARG:HH11	1.83	0.89
3:A:365:NAG:H62	3:A:366:NAG:H81	1.53	0.89
1:A:323:ARG:NH1	1:A:323:ARG:HG2	1.67	0.87
1:A:317:ALA:HA	1:A:320:LEU:HD13	1.58	0.85
1:A:269:TRP:CZ2	3:A:364:NAG:H3	2.11	0.84
1:A:310:GLN:HE22	1:A:345:GLN:HE22	1.23	0.83
1:A:269:TRP:CE3	1:A:272:ILE:CG1	2.61	0.82
1:A:269:TRP:CE3	1:A:272:ILE:HG13	2.14	0.81
3:A:365:NAG:H62	3:A:366:NAG:H82	1.62	0.80
1:A:212:ARG:HD2	1:A:212:ARG:O	1.83	0.77
1:A:10:TRP:CH2	3:A:364:NAG:H61	2.22	0.75
1:A:269:TRP:CH2	4:A:485:HOH:O	2.41	0.73
1:A:331:TRP:CZ3	4:A:433:HOH:O	2.42	0.72
1:A:269:TRP:CZ3	1:A:272:ILE:HG13	2.25	0.72
1:A:313:VAL:HG13	1:A:355:ILE:HG13	1.71	0.72
1:A:269:TRP:CZ3	4:A:485:HOH:O	2.45	0.70
1:A:262:ILE:H	1:A:303:GLN:HE22	1.42	0.68
1:A:313:VAL:CG1	1:A:355:ILE:HG13	2.22	0.68
1:A:78:TRP:CZ2	4:A:486:HOH:O	2.47	0.68
1:A:22:PRO:HB2	1:A:58:THR:HG22	1.75	0.67
1:A:78:TRP:CH2	4:A:486:HOH:O	2.47	0.67
1:A:204:GLY:HA2	1:A:292:ASP:HB3	1.76	0.66
1:A:310:GLN:HE22	1:A:345:GLN:NE2	1.92	0.65
1:A:103:PRO:HB2	1:A:104:PRO:HD3	1.78	0.65
1:A:35:TYR:OH	1:A:55:LEU:HD12	1.97	0.64
1:A:127:ARG:NH1	4:A:390:HOH:O	2.30	0.63
1:A:10:TRP:CZ2	3:A:364:NAG:H4	2.34	0.62
1:A:317:ALA:HA	1:A:320:LEU:HD11	1.78	0.62
1:A:57:ASP:O	1:A:61:THR:HG23	1.99	0.61
1:A:269:TRP:CE3	1:A:272:ILE:HG12	2.35	0.61
1:A:120:TRP:CZ3	1:A:158:THR:HB	2.35	0.61
3:A:367:NAG:C8	3:A:367:NAG:O3	2.49	0.60
1:A:320:LEU:HD22	1:A:321:LYS:N	2.16	0.59
1:A:204:GLY:CA	1:A:292:ASP:HB3	2.32	0.59
1:A:212:ARG:CD	1:A:212:ARG:O	2.51	0.59
1:A:269:TRP:CZ3	1:A:272:ILE:CG1	2.86	0.58
3:A:364:NAG:H62	3:A:365:NAG:N2	2.18	0.58
1:A:269:TRP:HE3	1:A:272:ILE:CG1	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:VAL:HG13	1:A:355:ILE:CG1	2.34	0.57
1:A:319:TYR:CZ	1:A:323:ARG:HD2	2.39	0.56
1:A:198:HIS:CE1	4:A:452:HOH:O	2.57	0.56
3:A:366:NAG:O3	3:A:367:NAG:O5	2.23	0.56
1:A:93:GLN:HE21	1:A:96:ARG:HH22	1.52	0.56
1:A:75:VAL:HG22	1:A:114:LEU:HD11	1.88	0.56
1:A:262:ILE:H	1:A:303:GLN:NE2	2.03	0.56
1:A:317:ALA:CA	1:A:320:LEU:HD13	2.33	0.55
3:A:367:NAG:H83	3:A:367:NAG:O3	2.07	0.55
1:A:349:PHE:N	1:A:350:PRO:HD3	2.21	0.54
1:A:239:THR:HG22	1:A:335:LEU:HB2	1.88	0.54
1:A:198:HIS:HE1	4:A:452:HOH:O	1.90	0.54
1:A:192:ARG:O	1:A:194:THR:N	2.41	0.53
1:A:269:TRP:HE3	1:A:272:ILE:HG12	1.74	0.52
1:A:28:PHE:O	1:A:356:LYS:NZ	2.42	0.52
1:A:244:TYR:HB3	1:A:257:ILE:HD12	1.91	0.52
3:A:364:NAG:H62	3:A:365:NAG:HN2	1.73	0.52
1:A:119:LEU:HD22	1:A:120:TRP:CZ3	2.44	0.51
3:A:365:NAG:O4	3:A:366:NAG:C7	2.59	0.51
1:A:40:ILE:HD12	1:A:80:TYR:OH	2.10	0.51
1:A:348:THR:HG22	4:A:465:HOH:O	2.11	0.51
1:A:212:ARG:NH1	4:A:368:HOH:O	2.44	0.50
1:A:353:SER:OG	4:A:488:HOH:O	2.20	0.50
1:A:78:TRP:C	1:A:80:TYR:H	2.15	0.50
3:A:365:NAG:C6	3:A:366:NAG:H82	2.36	0.50
1:A:124:ARG:HG3	1:A:124:ARG:HH11	1.77	0.50
1:A:294:GLN:NE2	1:A:315:ASN:OD1	2.45	0.49
1:A:78:TRP:CZ2	4:A:438:HOH:O	2.55	0.49
1:A:22:PRO:HB2	1:A:58:THR:CG2	2.42	0.49
1:A:188:HIS:HE1	1:A:194:THR:O	1.96	0.49
1:A:206:GLU:HG3	1:A:292:ASP:OD2	2.14	0.48
1:A:212:ARG:CG	1:A:212:ARG:O	2.61	0.48
1:A:100:LYS:HD3	1:A:139:GLU:OE2	2.14	0.47
1:A:242:ARG:NH1	4:A:507:HOH:O	2.45	0.47
1:A:186:ASP:OD1	1:A:242:ARG:NH1	2.43	0.47
1:A:13:TYR:O	1:A:14:ARG:C	2.51	0.47
3:A:366:NAG:HO3	3:A:367:NAG:C1	2.28	0.47
1:A:107:ARG:HD3	1:A:143:GLU:OE2	2.15	0.47
1:A:205:ASN:HD22	1:A:205:ASN:C	2.18	0.47
1:A:344:GLY:O	1:A:345:GLN:C	2.53	0.46
1:A:275:TYR:CD2	1:A:351:LEU:HD22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:VAL:HG13	1:A:304:TRP:CZ2	2.51	0.46
1:A:310:GLN:NE2	1:A:345:GLN:HE22	2.02	0.45
1:A:124:ARG:NH1	1:A:124:ARG:HG3	2.30	0.45
1:A:78:TRP:CH2	4:A:438:HOH:O	2.69	0.45
1:A:269:TRP:CZ2	3:A:364:NAG:C3	2.94	0.45
1:A:320:LEU:HD21	1:A:359:LEU:HD11	1.98	0.44
1:A:169:ASP:OD2	1:A:172:GLN:HG3	2.18	0.44
1:A:339:ARG:HH11	1:A:339:ARG:HG2	1.82	0.44
1:A:127:ARG:NH1	4:A:481:HOH:O	2.50	0.44
1:A:269:TRP:CD1	3:A:365:NAG:O6	2.67	0.44
1:A:204:GLY:C	1:A:206:GLU:H	2.20	0.44
1:A:204:GLY:O	1:A:206:GLU:N	2.51	0.44
1:A:96:ARG:NH1	4:A:500:HOH:O	2.51	0.44
1:A:320:LEU:HD22	1:A:320:LEU:C	2.38	0.43
1:A:35:TYR:HD1	1:A:59:LEU:HD22	1.84	0.43
1:A:119:LEU:HD22	1:A:120:TRP:HZ3	1.84	0.43
3:A:366:NAG:O3	3:A:367:NAG:C1	2.66	0.42
1:A:362:VAL:H	1:A:362:VAL:HG23	1.34	0.42
1:A:255:ALA:HA	1:A:256:PRO:HD3	1.85	0.42
1:A:158:THR:H	1:A:158:THR:HG22	1.22	0.42
1:A:26:ASP:HA	1:A:27:PRO:HD3	1.82	0.41
1:A:198:HIS:CD2	1:A:198:HIS:H	2.39	0.41
1:A:318:ARG:O	1:A:319:TYR:C	2.59	0.41
1:A:78:TRP:CD1	1:A:119:LEU:HD13	2.56	0.41
1:A:351:LEU:HA	1:A:351:LEU:HD12	1.74	0.41
1:A:102:VAL:CG1	1:A:106:LEU:HD22	2.51	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	A	359/361 (99%)	334 (93%)	22 (6%)	3 (1%)	24 58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	193	GLN
1	A	204	GLY

### 5.3.2 Protein sidechains ⓘ

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	A	304/304 (100%)	259 (85%)	45 (15%)	4 11

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	9	SER
1	A	19	SER
1	A	23	ASP
1	A	36	SER
1	A	41	SER
1	A	53	VAL
1	A	59	LEU
1	A	65	ARG
1	A	69	LEU
1	A	75	VAL
1	A	83	GLN
1	A	85	PHE
1	A	91	LYS
1	A	92	THR
1	A	97	THR
1	A	106	LEU
1	A	107	ARG

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Mol	Chain	Res	Type
1	A	129	LEU
1	A	158	THR
1	A	181	SER
1	A	184	THR
1	A	193	GLN
1	A	203	ARG
1	A	205	ASN
1	A	225	ARG
1	A	226	LEU
1	A	233	LEU
1	A	239	THR
1	A	250	LYS
1	A	251	THR
1	A	269	TRP
1	A	282	LEU
1	A	287	THR
1	A	295	VAL
1	A	313	VAL
1	A	315	ASN
1	A	320	LEU
1	A	321	LYS
1	A	323	ARG
1	A	347	LEU
1	A	351	LEU
1	A	359	LEU
1	A	361	ARG
1	A	362	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	79	ASN
1	A	93	GLN
1	A	188	HIS
1	A	193	GLN
1	A	198	HIS
1	A	205	ASN
1	A	294	GLN
1	A	303	GLN
1	A	345	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

4 carbohydrates 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$
3	NAG	A	364	3	15,15,15	1.12	2 (13%)	17,21,21	1.97	4 (23%)
3	NAG	A	365	3	14,14,15	1.35	2 (14%)	15,19,21	2.18	4 (26%)
3	NAG	A	366	3	14,14,15	1.75	3 (21%)	15,19,21	1.79	5 (33%)
3	NAG	A	367	3	14,14,15	0.69	0	15,19,21	1.08	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
3	NAG	A	364	3	1/1/6/7	0/6/26/26	0/1/1/1
3	NAG	A	365	3	-	0/6/23/26	0/1/1/1
3	NAG	A	366	3	-	0/6/23/26	0/1/1/1
3	NAG	A	367	3	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	366	NAG	O5-C1	-4.73	1.35	1.43
3	A	364	NAG	C1-C2	-3.14	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	364	NAG	O5-C1	-2.29	1.38	1.43
3	A	366	NAG	O5-C5	2.39	1.48	1.43
3	A	365	NAG	C4-C5	2.54	1.58	1.53
3	A	365	NAG	O4-C4	3.31	1.50	1.43
3	A	366	NAG	C1-C2	3.46	1.57	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	364	NAG	C1-O5-C5	-5.22	103.82	113.47
3	A	365	NAG	C2-N2-C7	-4.11	117.77	123.04
3	A	366	NAG	C6-C5-C4	-3.83	103.56	113.02
3	A	364	NAG	C4-C3-C2	-3.72	105.28	110.43
3	A	366	NAG	C1-O5-C5	-2.40	109.20	112.25
3	A	367	NAG	C2-N2-C7	-2.06	120.39	123.04
3	A	364	NAG	C6-C5-C4	-2.02	108.04	113.02
3	A	367	NAG	O3-C3-C2	2.14	113.34	109.11
3	A	365	NAG	C4-C3-C2	2.36	114.90	111.23
3	A	366	NAG	O3-C3-C2	2.54	114.14	109.11
3	A	366	NAG	O4-C4-C5	2.57	116.05	109.24
3	A	366	NAG	O5-C5-C6	2.77	113.34	107.35
3	A	364	NAG	O1-C1-O5	2.79	117.87	110.25
3	A	365	NAG	O4-C4-C5	4.43	120.98	109.24
3	A	365	NAG	C1-O5-C5	4.48	117.93	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	364	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	364	NAG	6	0
3	A	365	NAG	8	0
3	A	366	NAG	8	0
3	A	367	NAG	5	0



## 5.6 Ligand geometry ⓘ

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$
2	NAG	A	363	1	14,14,15	0.95	0	15,19,21	2.23	5 (33%)

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	363	1	-	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	Z	Observed(°)	Ideal(°)
2	A	363	NAG	O7-C7-C8	-4.76	113.34	122.06
2	A	363	NAG	O4-C4-C5	-3.80	99.16	109.24
2	A	363	NAG	C6-C5-C4	-2.50	106.84	113.02
2	A	363	NAG	C8-C7-N2	3.15	122.14	116.11
2	A	363	NAG	C3-C4-C5	3.24	115.85	110.20

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 ⓘ

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 [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<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	A	361/361 (100%)	-0.07	9 (2%) 61 48	11, 27, 54, 80	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	TRP	3.2
1	A	194	THR	2.8
1	A	193	GLN	2.6
1	A	344	GLY	2.5
1	A	346	ASN	2.5
1	A	252	ASP	2.4
1	A	97	THR	2.4
1	A	147	GLY	2.2
1	A	192	ARG	2.2

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	364	15/15	0.83	0.38	5.71	23,25,58,63	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	366	14/15	0.67	0.37	-	23,25,26,26	14
3	NAG	A	367	14/15	0.36	0.90	-	24,25,27,28	14
3	NAG	A	365	14/15	0.71	0.39	-	21,24,25,25	14

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	363	14/15	0.87	0.25	1.67	21,24,28,34	14

## 6.5 Other polymers [i](#)

There are no such residues in this entry.