



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:17 am GMT

PDB ID : 2VCB  
Title : FAMILY 89 GLYCOSIDE HYDROLASE FROM CLOSTRIDIUM PERFRINGENS IN COMPLEX WITH PUGNAC  
Authors : Ficko-Blean, E.; Stubbs, K.A.; Berg, O.; Vocadlo, D.J.; Boraston, A.B.  
Deposited on : 2007-09-19  
Resolution : 2.20 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

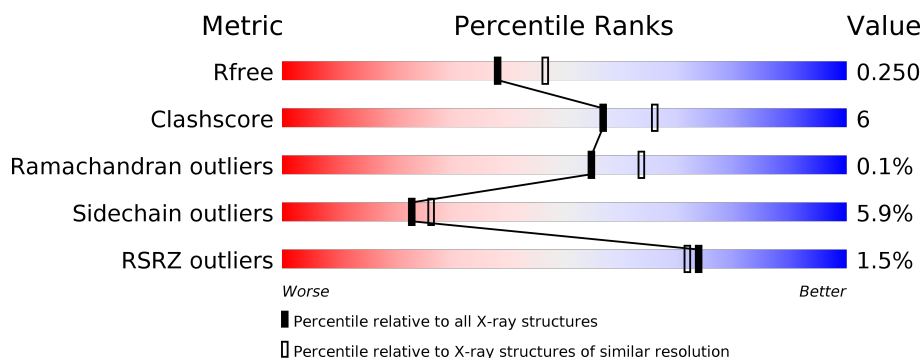
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	891	<div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

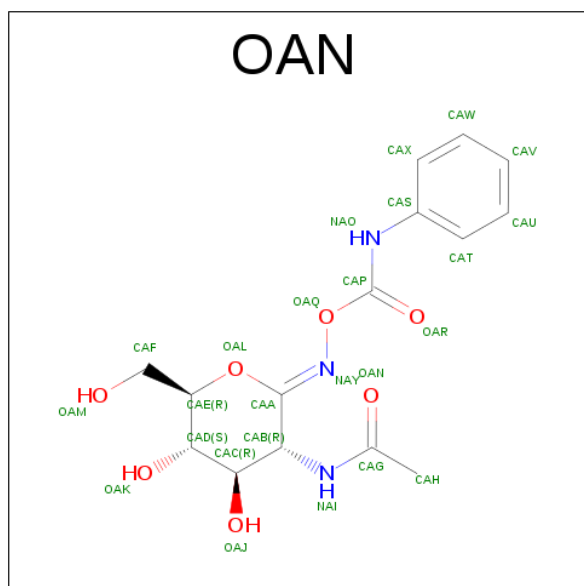
There are 4 unique types of molecules in this entry. The entry contains 7519 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALPHA-N-ACETYLGLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	883	7155	4535	1181	1410	29	103	1	1

- Molecule 2 is O-(2-ACETAMIDO-2-DEOXY D-GLUCOPYRANOSYLIDENE) AMINO-N-PHENYLCARBAMATE (three-letter code: OAN) (formula: C<sub>15</sub>H<sub>19</sub>N<sub>3</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	25	15	3	7	6	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

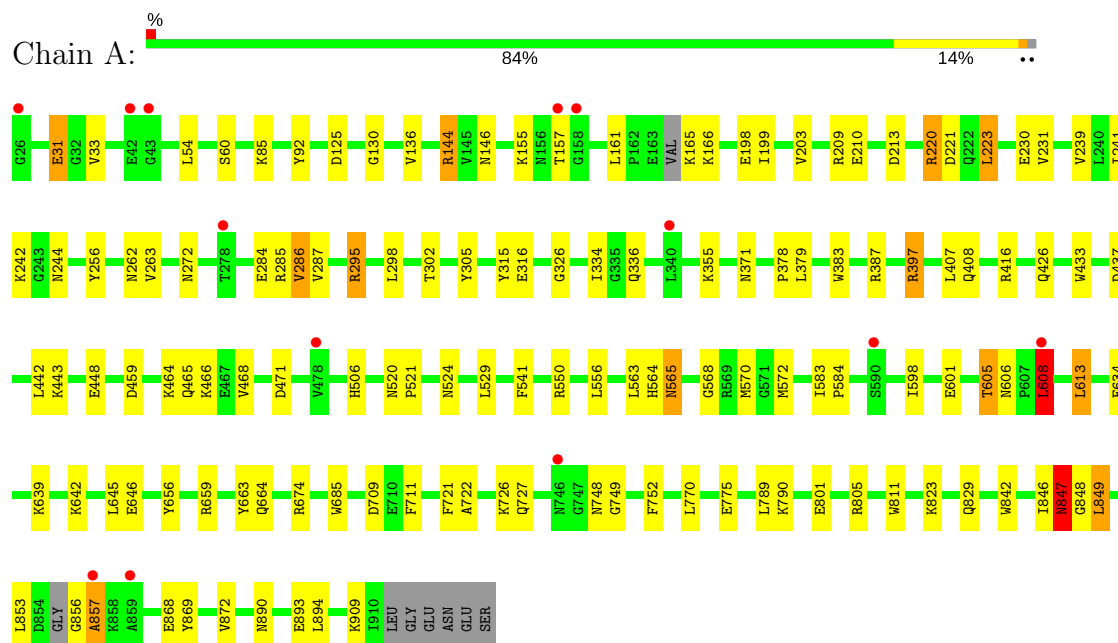
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	332	Total 338	O 338	0	6

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: ALPHA-N-ACETYLGLUCOSAMINIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.70Å 90.70Å 252.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20 29.69 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.3 (20.00-2.20) 90.2 (29.69-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.208 , 0.251 0.208 , 0.250	Depositor DCC
$R_{free}$ test set	2689 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OAN, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.54	0/7329	0.59	3/9917 (0.0%)

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	A	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	157	THR	OG1-CB-CG2	6.73	125.48	110.00
1	A	213	ASP	CB-CG-OD1	-6.19	112.73	118.30
1	A	608	LEU	CA-CB-CG	5.96	129.00	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	847	ASN	Peptide
1	A	857	ALA	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	A	7155	0	6747	78	0
2	A	25	0	18	2	0
3	A	1	0	0	0	0
4	A	338	0	0	9	0
All	All	7519	0	6765	78	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 6.

All (78) 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:847:ASN:N	1:A:848:GLY:HA3	1.83	0.93
1:A:198:GLU:OE1	4:A:3065[A]:HOH:O	1.94	0.85
1:A:605:THR:HG21	4:A:2223:HOH:O	1.81	0.79
1:A:664:GLN:OE1	2:A:1911:OAN:OAR	1.99	0.79
1:A:674:ARG:HD2	1:A:868:GLU:OE1	1.84	0.76
1:A:521:PRO:O	1:A:550:ARG:NH2	2.13	0.75
1:A:408:GLN:H	1:A:465:GLN:HE22	1.33	0.75
1:A:336:GLN:HE22	1:A:465:GLN:HE21	1.38	0.71
1:A:659:ARG:HD2	1:A:663:TYR:CE2	2.27	0.69
1:A:572:MET:H	1:A:727:GLN:HE21	1.40	0.69
1:A:85:LYS:H	1:A:146:ASN:HD21	1.43	0.64
1:A:664:GLN:OE1	2:A:1911:OAN:CAP	2.46	0.64
1:A:263:VAL:HG13	1:A:272:ASN:O	1.98	0.64
1:A:565:ASN:HD21	1:A:568:GLY:H	1.46	0.63
1:A:572:MET:H	1:A:727:GLN:NE2	1.96	0.62
1:A:316:GLU:OE2	1:A:397:ARG:NH2	2.33	0.61
1:A:85:LYS:H	1:A:146:ASN:ND2	1.98	0.61
1:A:231:VAL:HG22	1:A:286:VAL:HG23	1.83	0.60
1:A:295:ARG:HD2	1:A:326:GLY:O	2.03	0.59
1:A:598:ILE:HG23	1:A:613:LEU:HD22	1.85	0.58
1:A:262:ASN:HD21	1:A:634:GLU:HG2	1.70	0.56
1:A:426:GLN:HB3	1:A:443:LYS:HD2	1.88	0.55
1:A:60:SER:O	1:A:144:ARG:HG2	2.07	0.55
1:A:605:THR:HG23	1:A:606:ASN:OD1	2.06	0.55
1:A:598:ILE:CG2	1:A:613:LEU:HD22	2.37	0.55
1:A:749:GLY:H	1:A:752:PHE:H	1.54	0.55
1:A:722:ALA:O	1:A:726:LYS:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:GLN:H	1:A:465:GLN:NE2	2.04	0.54
1:A:31:GLU:C	1:A:31:GLU:OE1	2.46	0.54
1:A:383:TRP:CE2	1:A:387:ARG:HG3	2.43	0.53
1:A:770:LEU:HD22	1:A:829:GLN:O	2.09	0.53
1:A:459:ASP:OD1	1:A:506:HIS:HE1	1.93	0.52
1:A:92:TYR:HB3	1:A:136:VAL:HA	1.91	0.52
1:A:563:LEU:O	1:A:564:HIS:HB3	2.11	0.51
1:A:231:VAL:HG12	1:A:241:ILE:HG12	1.92	0.51
1:A:464:LYS:O	1:A:468:VAL:HG23	2.09	0.51
1:A:849:LEU:CD1	1:A:849:LEU:N	2.73	0.51
1:A:408:GLN:N	1:A:465:GLN:HE22	2.07	0.51
1:A:31:GLU:OE1	1:A:31:GLU:O	2.29	0.50
1:A:847:ASN:N	1:A:848:GLY:CA	2.64	0.50
1:A:846:ILE:C	1:A:848:GLY:HA3	2.32	0.50
1:A:60:SER:O	1:A:144:ARG:CG	2.61	0.48
1:A:130:GLY:HA3	1:A:161:LEU:HD13	1.96	0.48
1:A:407:LEU:HD22	4:A:2119:HOH:O	2.15	0.47
1:A:210:GLU:HG3	4:A:2068:HOH:O	2.14	0.46
1:A:890:ASN:HB3	1:A:893:GLU:HB2	1.98	0.46
1:A:565:ASN:ND2	1:A:568:GLY:H	2.12	0.46
1:A:790:LYS:HD2	1:A:790:LYS:HA	1.73	0.46
1:A:315:TYR:CE2	1:A:334:ILE:HD11	2.51	0.45
1:A:230:GLU:HB2	1:A:242:LYS:HB2	1.98	0.45
1:A:608:LEU:HG	1:A:656:TYR:HE2	1.82	0.45
1:A:371:ASN:ND2	4:A:2137:HOH:O	2.48	0.45
1:A:416:ARG:CZ	1:A:437:ASP:HB3	2.46	0.45
1:A:659:ARG:HD2	1:A:663:TYR:CD2	2.51	0.45
1:A:664:GLN:HG3	4:A:2274:HOH:O	2.17	0.45
1:A:565:ASN:HD21	1:A:568:GLY:N	2.14	0.44
1:A:220:ARG:HD3	1:A:221:ASP:O	2.18	0.43
1:A:775:GLU:CD	1:A:775:GLU:H	2.22	0.43
1:A:230:GLU:HG2	1:A:287:VAL:HG22	2.00	0.43
1:A:565:ASN:HD22	1:A:565:ASN:C	2.22	0.43
1:A:239:VAL:HG21	1:A:256:TYR:CZ	2.54	0.42
1:A:355:LYS:HE3	1:A:378:PRO:HB2	2.00	0.42
1:A:371:ASN:HB3	1:A:433:TRP:CD2	2.55	0.42
1:A:466:LYS:HE2	1:A:466:LYS:HB3	1.83	0.42
1:A:199:ILE:O	1:A:203:VAL:HG23	2.20	0.42
1:A:378:PRO:HG2	4:A:2132:HOH:O	2.20	0.42
1:A:355:LYS:HB3	1:A:355:LYS:HE3	1.84	0.42
1:A:520:ASN:HB3	4:A:2207:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:GLY:O	1:A:857:ALA:HB2	2.20	0.41
1:A:639:LYS:HG3	1:A:711:PHE:CE1	2.55	0.41
1:A:868:GLU:O	1:A:872:VAL:HG23	2.21	0.41
1:A:570:MET:HB2	1:A:829:GLN:HG3	2.03	0.41
1:A:220:ARG:O	1:A:244:ASN:HA	2.20	0.41
1:A:801:GLU:O	1:A:805:ARG:HG3	2.20	0.41
1:A:223:LEU:HD23	4:A:2074:HOH:O	2.22	0.40
1:A:305:TYR:HB2	1:A:601:GLU:O	2.21	0.40
1:A:583:ILE:HB	1:A:584:PRO:HD3	2.03	0.40
1:A:842:TRP:O	1:A:846:ILE:HD12	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	A	878/891 (98%)	846 (96%)	31 (4%)	1 (0%)	55 63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	LEU

### 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	A	761/767 (99%)	716 (94%)	45 (6%)	23	26

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

Mol	Chain	Res	Type
1	A	31	GLU
1	A	33	VAL
1	A	54	LEU
1	A	125	ASP
1	A	144	ARG
1	A	155	LYS
1	A	165	LYS
1	A	166	LYS
1	A	209	ARG
1	A	220	ARG
1	A	223	LEU
1	A	284	GLU
1	A	285	ARG
1	A	286	VAL
1	A	295	ARG
1	A	302	THR
1	A	379	LEU
1	A	397	ARG
1	A	442	LEU
1	A	448	GLU
1	A	471	ASP
1	A	524	ASN
1	A	529	LEU
1	A	541	PHE
1	A	556	LEU
1	A	565	ASN
1	A	605	THR
1	A	608	LEU
1	A	613	LEU
1	A	642	LYS
1	A	645	LEU
1	A	646	GLU
1	A	685	TRP
1	A	709	ASP
1	A	721	PHE
1	A	748	ASN
1	A	789	LEU
1	A	811	TRP

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Mol	Chain	Res	Type
1	A	823	LYS
1	A	847	ASN
1	A	849	LEU
1	A	853	LEU
1	A	869	TYR
1	A	894	LEU
1	A	909	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	146	ASN
1	A	151	ASN
1	A	192	ASN
1	A	201	ASN
1	A	222	GLN
1	A	262	ASN
1	A	325	ASN
1	A	370	GLN
1	A	371	ASN
1	A	455	GLN
1	A	465	GLN
1	A	506	HIS
1	A	518	GLN
1	A	523	ASN
1	A	534	GLN
1	A	565	ASN
1	A	727	GLN
1	A	746	ASN
1	A	847	ASN
1	A	888	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	OAN	A	1911	-	23,26,26	4.66	2 (8%)	23,35,35	2.78	4 (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
2	OAN	A	1911	-	-	2/12/35/35	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1911	OAN	CAS-NAO	-21.76	0.99	1.41
2	A	1911	OAN	OAQ-NAY	-3.39	1.36	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1911	OAN	CAT-CAS-NAO	-2.56	111.83	120.41
2	A	1911	OAN	CAX-CAS-NAO	2.49	128.74	120.41
2	A	1911	OAN	CAA-CAB-NAI	3.60	115.07	109.26
2	A	1911	OAN	CAS-NAO-CAP	11.47	145.47	126.41

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1911	OAN	NAY-OAQ-CAP-NAO
2	A	1911	OAN	NAY-OAQ-CAP-OAR

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1911	OAN	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	882/891 (98%)	-0.21	13 (1%) 74 72	20, 39, 54, 66	30 (3%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	GLY	3.8
1	A	158	GLY	3.7
1	A	857	ALA	3.6
1	A	478	VAL	3.0
1	A	608	LEU	2.5
1	A	340	LEU	2.2
1	A	43	GLY	2.2
1	A	859	ALA	2.2
1	A	42[A]	GLU	2.2
1	A	590	SER	2.1
1	A	746	ASN	2.1
1	A	278	THR	2.1
1	A	157	THR	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](#)

There are no carbohydrates in this entry.

## 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	OAN	A	1911	25/25	0.95	0.08	-1.25	32,36,65,66	6
3	CA	A	1912	1/1	0.99	0.06	-1.81	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.