



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:50 PM GMT

PDB ID : 4JNT  
Title : Crystal structure of the ectodomain of Bovine viral diarrhea virus 1 E2 envelope protein  
Authors : Li, Y.; Wang, J.; Modis, Y.  
Deposited on : 2013-03-15  
Resolution : 4.09 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

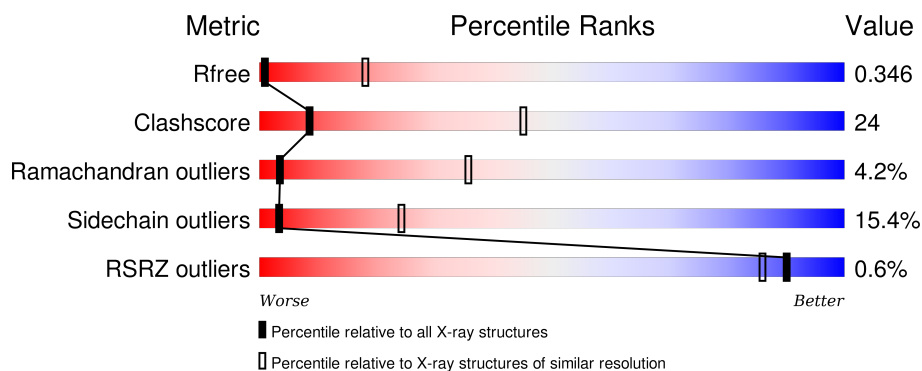
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.09 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	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

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	338	<div> <div></div> <div>48%</div> <div>38%</div> <div>9%</div> <div>...</div> </div>
1	B	338	<div> <div></div> <div>47%</div> <div>40%</div> <div>7%</div> <div>...</div> </div>

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	2405	-	-	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5380 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 Envelope glycoprotein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2578	1639	432	481	26			
1	B	324	Total	C	N	O	S	0	0	0
			2578	1639	432	481	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	788	ASP	ASN	VARIANT	UNP P19711
B	788	ASP	ASN	VARIANT	UNP P19711

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.63 Å 67.89 Å 139.41 Å 90.00° 121.89° 90.00°	Depositor
Resolution (Å)	48.57 – 4.09 48.53 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.9 (48.57-4.09) 89.9 (48.53-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 3.48 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.321 , 0.376 0.279 , 0.346	Depositor DCC
$R_{free}$ test set	486 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.1	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.15 , -57.0	EDS
Estimated twinning fraction	0.138 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	1 of 15505 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	5380	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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

### 5.1 Standard geometry

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	0.57	0/2639	0.84	2/3567 (0.1%)
1	B	0.59	0/2639	0.85	1/3567 (0.0%)
All	All	0.58	0/5278	0.84	3/7134 (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
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	965	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	879	TRP	N-CA-C	5.05	124.62	111.00
1	A	956	VAL	CB-CA-C	-5.03	101.85	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1011	MET	Peptide
1	A	986	ALA	Peptide
1	B	1010	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	B	968	MET	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	2578	0	2519	132	0
1	B	2578	0	2522	121	0
2	A	112	0	100	6	0
2	B	112	0	100	7	0
All	All	5380	0	5241	254	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 24.

All (254) 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:B:890:LYS:HE3	2:B:2406:NAG:O3	1.51	1.10
1:B:1009:GLN:O	1:B:1011:MET:SD	2.19	0.99
1:B:796:CYS:HB2	1:B:816:PRO:O	1.66	0.96
1:A:939:VAL:HG11	1:A:969:PRO:HD3	1.49	0.94
1:A:741:GLU:OE2	1:A:746:MET:SD	2.30	0.90
1:B:890:LYS:NZ	2:B:2406:NAG:H4	1.90	0.86
1:B:947:LEU:HD12	1:B:948:LYS:N	1.95	0.81
1:A:878:ASN:O	1:A:880:THR:N	2.12	0.81
1:A:947:LEU:HD12	1:A:948:LYS:N	1.95	0.81
1:A:727:PRO:O	1:A:742:ASP:O	1.99	0.80
1:A:963:THR:O	1:A:997:ASN:ND2	2.16	0.79
1:A:750:ARG:HG3	1:A:750:ARG:O	1.82	0.79
1:A:952:GLY:O	1:A:971:ARG:NH2	2.16	0.78
1:B:878:ASN:O	1:B:880:THR:N	2.17	0.78
1:B:761:LEU:HB2	1:B:770:VAL:HG12	1.66	0.77
1:B:797:PRO:CG	1:B:845:VAL:HG21	2.16	0.75
1:B:836:ASN:O	1:B:839:THR:O	2.05	0.74
1:B:890:LYS:HZ1	2:B:2406:NAG:H4	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:890:LYS:CE	2:B:2406:NAG:O3	2.34	0.74
1:A:797:PRO:HG2	1:A:845:VAL:HG21	1.71	0.73
1:A:951:ILE:HG13	1:A:956:VAL:HG21	1.71	0.73
1:B:890:LYS:HZ2	2:B:2406:NAG:C4	2.02	0.72
1:A:836:ASN:O	1:A:839:THR:O	2.08	0.71
1:A:741:GLU:OE1	1:A:741:GLU:N	2.23	0.71
1:A:968:MET:HG3	1:A:1000:PHE:CE1	2.26	0.71
1:B:1006:TYR:CE1	1:B:1022:LEU:HD23	2.26	0.70
1:B:708:GLU:HG3	1:B:772:PHE:CD2	2.27	0.69
1:A:960:ALA:HB2	1:A:995:LEU:HD23	1.73	0.69
1:B:837:MET:SD	1:B:837:MET:N	2.63	0.69
1:B:942:VAL:HB	1:B:943:PRO:CD	2.24	0.68
1:B:890:LYS:NZ	2:B:2406:NAG:C4	2.56	0.68
1:A:694:LEU:O	1:A:745:LEU:HG	1.93	0.68
1:B:967:PRO:O	1:B:968:MET:HB2	1.94	0.68
1:B:877:GLY:O	1:B:878:ASN:C	2.31	0.67
1:A:1006:TYR:CE1	1:A:1022:LEU:HD23	2.30	0.67
1:A:923:GLU:HG2	2:A:2405:NAG:C7	2.25	0.67
1:A:796:CYS:HB2	1:A:816:PRO:O	1.96	0.66
1:A:939:VAL:CG1	1:A:969:PRO:HD3	2.22	0.65
1:B:711:GLY:HA3	1:B:716:GLU:OE2	1.97	0.65
1:B:968:MET:HG3	1:B:1000:PHE:CD1	2.31	0.65
1:B:736:VAL:HG23	1:B:749:GLN:HA	1.79	0.65
1:B:797:PRO:HG2	1:B:845:VAL:HG21	1.79	0.64
1:B:832:CYS:HB2	1:B:845:VAL:HG22	1.78	0.63
1:A:994:THR:HG23	1:A:995:LEU:N	2.14	0.63
1:A:850:ARG:NE	1:A:852:LYS:O	2.32	0.63
1:B:951:ILE:HD11	1:B:956:VAL:HG21	1.81	0.62
1:B:833:THR:HA	1:B:844:VAL:HA	1.81	0.62
1:B:703:ALA:O	1:B:758:LEU:HD12	2.00	0.61
1:B:756:ARG:HB2	1:B:776:PHE:HE2	1.65	0.61
1:B:999:TYR:CE2	1:B:1010:TYR:CE2	2.88	0.61
1:A:833:THR:HA	1:A:844:VAL:HA	1.82	0.61
1:B:942:VAL:HB	1:B:943:PRO:HD2	1.83	0.61
1:A:966:GLY:O	1:A:998:LYS:HA	2.00	0.61
1:A:960:ALA:HB2	1:A:995:LEU:CD2	2.31	0.60
1:B:938:GLY:O	1:B:961:MET:HB3	2.02	0.60
1:B:787:MET:HB3	1:B:791:PHE:CB	2.32	0.59
1:B:935:ASN:OD1	1:B:940:ALA:HB2	2.02	0.59
1:A:740:CYS:C	1:A:741:GLU:OE1	2.40	0.59
1:B:696:CYS:SG	1:B:725:TYR:HE1	2.24	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:PRO:HA	1:A:725:TYR:CD2	2.38	0.59
1:A:951:ILE:HG13	1:A:956:VAL:CG2	2.32	0.58
1:A:923:GLU:HG2	2:A:2405:NAG:O7	2.03	0.58
1:A:939:VAL:HG22	1:A:958:VAL:CG2	2.32	0.58
1:A:750:ARG:O	1:A:751:CYS:HB2	2.04	0.58
1:B:907:SER:HA	1:B:913:TYR:CD2	2.38	0.58
1:B:910:LEU:HD13	1:B:915:ILE:HG21	1.86	0.58
1:A:706:LYS:O	1:A:757:TYR:HE1	1.85	0.58
1:B:824:ILE:HG13	1:B:856:HIS:HA	1.85	0.57
1:A:823:PRO:O	1:A:826:TRP:HB2	2.04	0.57
1:A:783:ASP:O	1:A:784:VAL:HG13	2.04	0.57
1:B:835:PHE:HD1	1:B:842:THR:HG22	1.70	0.57
1:A:856:HIS:O	1:A:857:ARG:HG2	2.04	0.57
1:B:794:GLY:HA3	1:B:818:PHE:CZ	2.40	0.57
1:A:951:ILE:CG1	1:A:956:VAL:HG21	2.34	0.57
1:A:879:TRP:O	1:A:879:TRP:HE3	1.87	0.57
1:A:877:GLY:O	1:A:878:ASN:C	2.42	0.56
1:A:824:ILE:HG12	1:A:856:HIS:HA	1.87	0.56
1:B:787:MET:HB3	1:B:791:PHE:CG	2.41	0.56
1:B:826:TRP:O	1:B:853:PRO:HA	2.06	0.56
1:A:897:CYS:SG	1:A:914:PRO:HB3	2.46	0.56
1:A:821:VAL:HG11	1:A:879:TRP:CZ2	2.41	0.55
1:B:850:ARG:NE	1:B:852:LYS:O	2.39	0.55
1:B:735:MET:CE	1:B:751:CYS:SG	2.94	0.55
1:A:755:THR:HB	1:A:778:GLY:HA3	1.87	0.55
1:A:777:ASP:O	1:A:779:ARG:NH2	2.40	0.55
1:A:999:TYR:CD2	1:A:1010:TYR:CE2	2.95	0.54
1:A:756:ARG:CG	1:A:776:PHE:HE2	2.20	0.54
1:A:935:ASN:HA	1:A:940:ALA:HA	1.89	0.54
1:A:740:CYS:HA	1:A:744:LYS:O	2.08	0.54
1:B:877:GLY:O	1:B:878:ASN:O	2.26	0.54
1:A:971:ARG:HG3	1:A:972:PRO:HD2	1.89	0.54
1:A:1003:ARG:HG3	1:A:1010:TYR:CE1	2.44	0.53
1:A:877:GLY:O	1:A:878:ASN:O	2.26	0.53
1:B:790:ASN:O	1:B:792:GLU:OE1	2.27	0.53
1:A:997:ASN:C	1:A:998:LYS:HD3	2.29	0.53
1:A:793:PHE:CZ	1:A:795:LEU:HD12	2.45	0.52
1:A:808:PHE:CE1	1:A:826:TRP:HD1	2.27	0.52
1:B:735:MET:HE1	1:B:751:CYS:SG	2.48	0.52
1:B:720:THR:HG21	1:B:731:LEU:HD22	1.92	0.52
1:A:797:PRO:CG	1:A:845:VAL:HG21	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:939:VAL:HG11	1:B:968:MET:O	2.09	0.51
1:A:709:ARG:O	1:A:716:GLU:HB3	2.10	0.51
1:A:750:ARG:O	1:A:750:ARG:CG	2.56	0.51
1:B:971:ARG:HG3	1:B:972:PRO:HD2	1.92	0.51
1:A:985:THR:HG22	1:A:988:THR:OG1	2.10	0.51
1:B:878:ASN:ND2	2:B:2403:NAG:H83	2.26	0.51
1:B:783:ASP:OD1	1:B:846:ARG:HG3	2.11	0.51
1:B:753:ARG:HA	1:B:779:ARG:O	2.11	0.51
1:B:966:GLY:O	1:B:998:LYS:HA	2.10	0.51
1:A:923:GLU:HG2	2:A:2405:NAG:N2	2.26	0.51
1:B:706:LYS:HA	1:B:756:ARG:HD3	1.92	0.51
1:B:949:CYS:HB2	1:B:971:ARG:O	2.11	0.50
1:A:750:ARG:O	1:A:751:CYS:CB	2.58	0.50
1:A:753:ARG:HB3	1:A:780:LYS:HD3	1.93	0.50
1:A:735:MET:O	1:A:736:VAL:HG23	2.11	0.50
1:B:767:PRO:O	1:B:770:VAL:HG13	2.12	0.50
1:B:861:ILE:O	1:B:877:GLY:HA2	2.12	0.49
1:A:976:ILE:HG23	1:A:991:TYR:CE1	2.47	0.49
1:B:987:CYS:HB3	1:B:1022:LEU:CD1	2.42	0.49
1:A:826:TRP:O	1:A:853:PRO:HA	2.12	0.49
1:B:999:TYR:CE2	1:B:1010:TYR:CZ	3.00	0.49
1:A:725:TYR:HA	1:A:729:MET:CE	2.42	0.49
1:A:732:GLU:OE2	1:A:750:ARG:NH2	2.45	0.49
1:B:912:HIS:CD2	1:B:915:ILE:HD12	2.48	0.49
1:A:803:ILE:HD12	1:A:833:THR:HG21	1.94	0.49
1:A:856:HIS:C	1:A:857:ARG:CG	2.81	0.49
1:B:940:ALA:O	1:B:958:VAL:HG23	2.13	0.49
1:A:780:LYS:HG2	1:A:781:GLN:HG3	1.94	0.49
1:A:788:ASP:OD1	1:A:789:ASP:N	2.46	0.48
1:B:951:ILE:CD1	1:B:956:VAL:HG21	2.43	0.48
1:B:696:CYS:SG	1:B:725:TYR:CE1	3.06	0.48
1:A:745:LEU:O	1:A:745:LEU:HD12	2.13	0.48
1:A:1004:ASP:HB3	1:A:1011:MET:SD	2.54	0.48
1:B:703:ALA:HB1	1:B:720:THR:OG1	2.12	0.48
1:B:1006:TYR:CZ	1:B:1022:LEU:HD23	2.48	0.48
1:A:704:ILE:HG22	1:A:705:ALA:N	2.28	0.48
2:A:2401:NAG:O3	2:A:2402:NAG:O5	2.24	0.48
1:B:752:THR:HG23	1:B:779:ARG:NH2	2.29	0.48
1:B:843:THR:HG22	1:B:844:VAL:N	2.29	0.48
1:B:755:THR:OG1	1:B:777:ASP:HA	2.14	0.48
1:B:756:ARG:HB2	1:B:776:PHE:CE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:999:TYR:HB3	1:B:1012:LEU:HD21	1.96	0.47
1:A:725:TYR:HA	1:A:729:MET:HE3	1.95	0.47
1:B:899:TRP:CD2	1:B:900:CYS:SG	3.08	0.47
1:B:797:PRO:CD	1:B:845:VAL:HG21	2.44	0.47
1:A:783:ASP:HB2	1:A:846:ARG:HA	1.96	0.47
1:A:889:TYR:CE1	1:A:894:ILE:HD11	2.49	0.47
1:B:782:GLU:OE2	1:B:844:VAL:HG13	2.15	0.47
1:A:698:PRO:HA	1:A:725:TYR:CG	2.50	0.47
1:A:753:ARG:HA	1:A:779:ARG:O	2.15	0.47
1:A:803:ILE:HG21	1:A:805:ARG:NH2	2.30	0.47
1:B:823:PRO:O	1:B:826:TRP:HB2	2.15	0.47
1:A:754:GLU:O	1:A:776:PHE:CZ	2.67	0.47
1:B:995:LEU:O	1:B:996:LYS:C	2.53	0.47
1:B:947:LEU:O	1:B:958:VAL:HG12	2.15	0.46
1:B:844:VAL:HG22	1:B:846:ARG:N	2.31	0.46
1:B:939:VAL:CG1	1:B:968:MET:O	2.64	0.46
1:A:708:GLU:O	1:A:709:ARG:C	2.52	0.46
1:A:755:THR:HB	1:A:778:GLY:N	2.31	0.46
1:A:824:ILE:CG1	1:A:856:HIS:HA	2.45	0.46
1:B:782:GLU:CD	1:B:844:VAL:HG13	2.36	0.46
1:A:995:LEU:O	1:A:996:LYS:C	2.54	0.46
1:A:895:GLU:OE2	1:A:905:LYS:NZ	2.37	0.46
1:A:939:VAL:HG13	1:A:939:VAL:O	2.15	0.46
1:B:834:SER:N	1:B:843:THR:O	2.49	0.46
1:A:706:LYS:O	1:A:757:TYR:CE1	2.67	0.46
1:B:969:PRO:O	1:B:970:CYS:CB	2.64	0.46
1:A:963:THR:HG22	1:A:963:THR:O	2.16	0.46
1:B:703:ALA:HB2	1:B:722:TRP:HA	1.97	0.45
1:A:870:LEU:O	1:A:886:GLN:HG2	2.16	0.45
1:A:755:THR:HB	1:A:778:GLY:CA	2.46	0.45
1:A:888:LEU:CD2	1:A:928:LEU:HD22	2.47	0.45
1:B:775:LEU:HD23	1:B:775:LEU:N	2.29	0.45
1:B:821:VAL:O	1:B:880:THR:HG21	2.17	0.45
1:B:751:CYS:SG	1:B:752:THR:N	2.89	0.45
1:A:895:GLU:HB2	1:A:921:GLU:HG3	1.98	0.45
1:A:946:THR:CG2	1:A:959:ILE:HD13	2.47	0.45
1:B:783:ASP:O	1:B:784:VAL:HB	2.16	0.45
1:A:968:MET:HG3	1:A:1000:PHE:CZ	2.52	0.45
1:A:761:LEU:HB2	1:A:770:VAL:HG12	1.98	0.45
1:A:923:GLU:CG	2:A:2405:NAG:N2	2.80	0.45
1:A:889:TYR:CE2	1:A:891:GLY:HA2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1004:ASP:OD2	1:B:1020:PHE:HB2	2.16	0.45
1:A:696:CYS:SG	1:A:725:TYR:HE1	2.40	0.45
1:A:783:ASP:OD2	1:A:846:ARG:HD3	2.16	0.45
1:A:941:ILE:HG21	1:A:956:VAL:HG11	1.99	0.45
1:A:1006:TYR:CZ	1:A:1022:LEU:HD23	2.51	0.44
1:B:733:ASP:OD2	1:B:756:ARG:NH1	2.50	0.44
1:B:916:GLY:O	1:B:930:ASP:O	2.35	0.44
1:B:965:LEU:C	1:B:965:LEU:HD12	2.37	0.44
1:A:929:VAL:HG22	1:A:930:ASP:HB2	1.98	0.44
1:B:761:LEU:HD11	1:B:765:ALA:HB3	1.98	0.44
1:A:939:VAL:HG22	1:A:958:VAL:HG21	2.00	0.44
1:A:840:LEU:N	1:A:840:LEU:HD22	2.33	0.44
1:B:750:ARG:O	1:B:751:CYS:CB	2.66	0.44
1:A:704:ILE:CG2	1:A:705:ALA:N	2.81	0.44
1:B:832:CYS:N	1:B:844:VAL:HG23	2.33	0.43
1:A:947:LEU:C	1:A:947:LEU:HD12	2.37	0.43
1:B:844:VAL:HG22	1:B:846:ARG:H	1.83	0.43
1:B:758:LEU:O	1:B:772:PHE:HA	2.19	0.43
1:A:810:THR:HG21	1:A:826:TRP:CD1	2.54	0.43
1:A:929:VAL:HG13	1:A:930:ASP:N	2.33	0.43
1:B:845:VAL:HG23	1:B:846:ARG:N	2.34	0.43
1:A:757:TYR:CE2	1:A:774:LYS:HE2	2.53	0.43
1:A:794:GLY:HA3	1:A:818:PHE:CE1	2.53	0.43
1:B:844:VAL:HG22	1:B:845:VAL:N	2.34	0.43
1:B:794:GLY:HA3	1:B:818:PHE:CE2	2.53	0.43
1:B:972:PRO:HG2	1:B:975:ILE:HD11	2.01	0.43
1:A:709:ARG:NH1	1:A:710:ILE:O	2.52	0.42
1:B:698:PRO:HA	1:B:725:TYR:CG	2.54	0.42
1:B:857:ARG:O	1:B:859:GLY:N	2.52	0.42
1:A:741:GLU:OE2	1:A:746:MET:CG	2.68	0.42
1:A:923:GLU:CG	2:A:2405:NAG:HN2	2.33	0.42
1:B:695:ASP:HB3	1:B:743:GLY:O	2.19	0.42
1:A:940:ALA:O	1:A:958:VAL:HG23	2.20	0.42
1:B:946:THR:HG23	1:B:959:ILE:HD13	2.02	0.42
1:B:943:PRO:O	1:B:957:GLN:OE1	2.38	0.42
1:B:824:ILE:CG1	1:B:856:HIS:HA	2.49	0.42
1:A:935:ASN:C	1:A:935:ASN:OD1	2.58	0.41
1:A:823:PRO:HB2	1:A:826:TRP:HB2	2.02	0.41
1:A:749:GLN:OE1	1:A:776:PHE:HD1	2.03	0.41
1:B:909:GLY:O	1:B:951:ILE:HG21	2.21	0.41
1:A:803:ILE:HD12	1:A:833:THR:CG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:810:THR:HG21	1:B:826:TRP:CD1	2.55	0.41
1:A:736:VAL:CG1	1:A:737:ILE:N	2.83	0.41
1:B:835:PHE:HZ	1:B:840:LEU:HD12	1.86	0.41
1:A:894:ILE:CG2	1:A:895:GLU:N	2.83	0.41
1:B:868:GLU:OE1	1:B:926:TYR:CE1	2.74	0.41
1:B:843:THR:HG22	1:B:844:VAL:H	1.85	0.41
1:A:856:HIS:C	1:A:857:ARG:HG2	2.40	0.41
1:B:713:LEU:HD23	1:B:713:LEU:O	2.21	0.41
1:A:1017:GLN:NE2	1:A:1019:TRP:CZ2	2.88	0.41
1:B:784:VAL:HA	1:B:847:THR:O	2.20	0.41
1:B:899:TRP:CZ2	1:B:932:THR:OG1	2.72	0.41
1:B:920:LEU:CD1	1:B:927:ARG:HD2	2.51	0.41
1:A:767:PRO:O	1:A:770:VAL:HG13	2.20	0.41
1:A:907:SER:HA	1:A:913:TYR:HB2	2.03	0.41
1:B:787:MET:HB3	1:B:791:PHE:HB2	2.03	0.41
1:B:835:PHE:CD1	1:B:842:THR:HG22	2.53	0.41
1:B:840:LEU:HD22	1:B:840:LEU:N	2.36	0.41
1:A:733:ASP:OD1	1:A:736:VAL:N	2.53	0.41
1:A:877:GLY:C	1:A:878:ASN:O	2.58	0.41
1:A:755:THR:N	1:A:778:GLY:HA3	2.36	0.41
1:B:761:LEU:CD1	1:B:765:ALA:HB3	2.51	0.40
1:A:888:LEU:HD21	1:A:928:LEU:HD22	2.04	0.40
1:A:1015:GLU:HB3	1:A:1016:TYR:CE1	2.56	0.40
1:A:968:MET:CB	1:A:1000:PHE:CE1	3.03	0.40
1:A:781:GLN:OE1	1:A:781:GLN:N	2.54	0.40
1:A:966:GLY:O	1:A:999:TYR:CD1	2.75	0.40
1:B:969:PRO:O	1:B:970:CYS:HB3	2.22	0.40
1:B:757:TYR:HD1	1:B:774:LYS:HA	1.86	0.40
1:B:829:THR:HA	1:B:848:TYR:O	2.21	0.40
1:A:830:VAL:HG13	1:A:848:TYR:HB2	2.03	0.40
1:A:766:LEU:HD11	1:A:768:THR:OG1	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	320/338 (95%)	274 (86%)	32 (10%)	14 (4%)	3	35
1	B	320/338 (95%)	274 (86%)	33 (10%)	13 (4%)	3	36
All	All	640/676 (95%)	548 (86%)	65 (10%)	27 (4%)	3	36

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	751	CYS
1	A	797	PRO
1	A	858	GLN
1	A	879	TRP
1	A	996	LYS
1	B	765	ALA
1	B	797	PRO
1	B	858	GLN
1	B	879	TRP
1	B	968	MET
1	B	970	CYS
1	B	973	TYR
1	A	765	ALA
1	A	885	ASP
1	A	928	LEU
1	B	751	CYS
1	B	784	VAL
1	B	996	LYS
1	A	878	ASN
1	B	967	PRO
1	A	709	ARG
1	A	810	THR
1	B	878	ASN
1	B	943	PRO
1	A	1008	GLN
1	A	824	ILE
1	A	855	PRO

### 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	285/298 (96%)	243 (85%)	42 (15%)	4	26
1	B	285/298 (96%)	239 (84%)	46 (16%)	3	22
All	All	570/596 (96%)	482 (85%)	88 (15%)	3	24

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	709	ARG
1	A	713	LEU
1	A	740	CYS
1	A	742	ASP
1	A	744	LYS
1	A	750	ARG
1	A	756	ARG
1	A	766	LEU
1	A	767	PRO
1	A	771	VAL
1	A	773	LYS
1	A	776	PHE
1	A	779	ARG
1	A	788	ASP
1	A	790	ASN
1	A	805	ARG
1	A	812	LEU
1	A	827	THR
1	A	830	VAL
1	A	831	SER
1	A	834	SER
1	A	842	THR
1	A	845	VAL
1	A	848	TYR
1	A	879	TRP
1	A	885	ASP
1	A	888	LEU
1	A	928	LEU
1	A	935	ASN
1	A	936	ARG
1	A	941	ILE

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Mol	Chain	Res	Type
1	A	942	VAL
1	A	947	LEU
1	A	951	ILE
1	A	953	LYS
1	A	962	ASP
1	A	964	LYS
1	A	970	CYS
1	A	973	TYR
1	A	989	PHE
1	A	994	THR
1	A	995	LEU
1	B	694	LEU
1	B	696	CYS
1	B	712	GLN
1	B	713	LEU
1	B	721	THR
1	B	726	SER
1	B	746	MET
1	B	768	THR
1	B	771	VAL
1	B	776	PHE
1	B	777	ASP
1	B	787	MET
1	B	792	GLU
1	B	801	LYS
1	B	811	THR
1	B	812	LEU
1	B	827	THR
1	B	831	SER
1	B	834	SER
1	B	837	MET
1	B	842	THR
1	B	843	THR
1	B	862	THR
1	B	870	LEU
1	B	878	ASN
1	B	905	LYS
1	B	912	HIS
1	B	924	THR
1	B	929	VAL
1	B	936	ARG
1	B	937	GLU

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Mol	Chain	Res	Type
1	B	941	ILE
1	B	947	LEU
1	B	951	ILE
1	B	953	LYS
1	B	962	ASP
1	B	964	LYS
1	B	965	LEU
1	B	968	MET
1	B	971	ARG
1	B	988	THR
1	B	989	PHE
1	B	1012	LEU
1	B	1015	GLU
1	B	1022	LEU
1	B	1023	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	712	GLN
1	A	749	GLN
1	B	865	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](#)

16 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	$\# Z  > 2$
2	NAG	A	2401	1,2	14,14,15	0.67	0	15,19,21	2.54	5 (33%)
2	NAG	A	2402	2	14,14,15	0.71	0	15,19,21	1.74	4 (26%)
2	NAG	A	2403	1,2	14,14,15	0.55	0	15,19,21	1.72	4 (26%)
2	NAG	A	2404	2	14,14,15	0.80	1 (7%)	15,19,21	1.15	0
2	NAG	A	2405	1,2	14,14,15	0.47	0	15,19,21	1.52	3 (20%)
2	NAG	A	2406	2	14,14,15	0.58	0	15,19,21	1.55	1 (6%)
2	NAG	A	2407	1,2	14,14,15	0.53	0	15,19,21	1.92	5 (33%)
2	NAG	A	2408	2	14,14,15	0.82	1 (7%)	15,19,21	1.70	1 (6%)
2	NAG	B	2401	1,2	14,14,15	0.50	0	15,19,21	3.28	6 (40%)
2	NAG	B	2402	2	14,14,15	0.62	0	15,19,21	0.86	0
2	NAG	B	2403	1,2	14,14,15	0.91	0	15,19,21	2.84	8 (53%)
2	NAG	B	2404	2	14,14,15	0.75	0	15,19,21	2.23	3 (20%)
2	NAG	B	2405	1,2	14,14,15	0.47	0	15,19,21	1.52	3 (20%)
2	NAG	B	2406	2	14,14,15	0.56	0	15,19,21	1.54	1 (6%)
2	NAG	B	2407	1,2	14,14,15	0.43	0	15,19,21	2.04	5 (33%)
2	NAG	B	2408	2	14,14,15	0.60	0	15,19,21	1.61	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2402	2	-	0/6/23/26	0/1/1/1
2	NAG	A	2403	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2404	2	-	0/6/23/26	0/1/1/1
2	NAG	A	2405	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2406	2	-	0/6/23/26	0/1/1/1
2	NAG	A	2407	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2408	2	-	0/6/23/26	0/1/1/1
2	NAG	B	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2402	2	-	0/6/23/26	0/1/1/1
2	NAG	B	2403	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2404	2	-	0/6/23/26	0/1/1/1
2	NAG	B	2405	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	2406	2	-	0/6/23/26	0/1/1/1
2	NAG	B	2407	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2408	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2408	NAG	C1-C2	2.32	1.55	1.52
2	A	2404	NAG	C1-C2	2.49	1.55	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2401	NAG	C4-C3-C2	-6.26	101.50	111.23
2	A	2407	NAG	C4-C3-C2	-4.13	104.81	111.23
2	B	2403	NAG	O7-C7-C8	-3.85	115.00	122.06
2	B	2401	NAG	O7-C7-C8	-3.08	116.41	122.06
2	B	2407	NAG	O7-C7-C8	-3.01	116.53	122.06
2	B	2403	NAG	C3-C4-C5	-2.93	105.09	110.20
2	A	2401	NAG	C4-C3-C2	-2.79	106.89	111.23
2	A	2403	NAG	O7-C7-C8	-2.54	117.40	122.06
2	B	2407	NAG	C4-C3-C2	-2.44	107.44	111.23
2	B	2403	NAG	C4-C3-C2	-2.37	107.55	111.23
2	A	2402	NAG	O7-C7-C8	-2.35	117.75	122.06
2	A	2403	NAG	C3-C4-C5	-2.26	106.25	110.20
2	B	2404	NAG	C3-C2-N2	-2.25	105.17	110.56
2	A	2405	NAG	C3-C4-C5	-2.18	106.40	110.20
2	B	2405	NAG	C3-C4-C5	-2.15	106.44	110.20
2	A	2407	NAG	C3-C4-C5	-2.05	106.62	110.20
2	A	2407	NAG	O4-C4-C3	2.19	115.27	110.34
2	A	2405	NAG	C2-N2-C7	2.20	125.87	123.04
2	B	2405	NAG	C2-N2-C7	2.22	125.89	123.04
2	A	2402	NAG	C1-O5-C5	2.29	115.16	112.25
2	B	2401	NAG	O4-C4-C5	2.36	115.50	109.24
2	A	2407	NAG	C3-C2-N2	2.37	116.23	110.56
2	A	2401	NAG	C8-C7-N2	2.51	120.90	116.11
2	B	2403	NAG	C3-C2-N2	2.57	116.72	110.56
2	B	2407	NAG	C2-N2-C7	2.68	126.48	123.04
2	B	2404	NAG	C2-N2-C7	2.69	126.50	123.04
2	B	2401	NAG	C8-C7-N2	2.77	121.41	116.11
2	A	2407	NAG	C8-C7-N2	2.81	121.49	116.11
2	A	2405	NAG	C1-O5-C5	2.87	115.89	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2405	NAG	C1-O5-C5	2.88	115.90	112.25
2	A	2402	NAG	C2-N2-C7	2.89	126.75	123.04
2	A	2403	NAG	C8-C7-N2	3.07	121.97	116.11
2	B	2401	NAG	O3-C3-C2	3.14	115.33	109.11
2	B	2403	NAG	C8-C7-N2	3.16	122.16	116.11
2	A	2401	NAG	C3-C4-C5	3.32	115.99	110.20
2	A	2401	NAG	O3-C3-C4	3.34	117.86	110.34
2	A	2403	NAG	C1-O5-C5	3.39	116.55	112.25
2	B	2403	NAG	O5-C5-C6	3.56	115.05	107.35
2	B	2407	NAG	C1-O5-C5	3.86	117.15	112.25
2	B	2407	NAG	C8-C7-N2	4.01	123.77	116.11
2	A	2402	NAG	C4-C3-C2	4.19	117.75	111.23
2	B	2403	NAG	O4-C4-C3	4.41	120.27	110.34
2	B	2406	NAG	C1-O5-C5	5.00	118.59	112.25
2	A	2406	NAG	C1-O5-C5	5.04	118.64	112.25
2	A	2408	NAG	C1-O5-C5	5.26	118.93	112.25
2	B	2408	NAG	C1-O5-C5	5.50	119.23	112.25
2	B	2403	NAG	C1-O5-C5	5.90	119.74	112.25
2	A	2401	NAG	C1-O5-C5	6.91	121.02	112.25
2	B	2404	NAG	C1-O5-C5	7.18	121.36	112.25
2	B	2401	NAG	C1-O5-C5	9.10	123.80	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2401	NAG	1	0
2	A	2402	NAG	1	0
2	A	2405	NAG	5	0
2	B	2403	NAG	1	0
2	B	2406	NAG	6	0

## 5.6 Ligand geometry

There are no ligands in this entry.

## 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	324/338 (95%)	-0.49	4 (1%) 81 73	63, 112, 172, 210	0
1	B	324/338 (95%)	-0.61	0 100 100	62, 108, 149, 177	0
All	All	648/676 (95%)	-0.55	4 (0%) 90 86	62, 109, 162, 210	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	838	ASP	2.8
1	A	1013	LYS	2.4
1	A	1023	GLU	2.2
1	A	1014	GLY	2.0

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

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	NAG	B	2405	14/15	0.88	0.42	0.75	92,105,118,130	0
2	NAG	A	2403	14/15	0.80	0.20	0.10	128,169,206,223	0
2	NAG	B	2403	14/15	0.86	0.19	-1.02	101,159,192,206	0
2	NAG	A	2401	14/15	0.95	0.12	-1.64	59,73,92,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	2404	14/15	0.81	0.18	-	99,162,186,198	0
2	NAG	B	2401	14/15	0.86	0.14	-	97,177,229,235	0
2	NAG	B	2407	14/15	0.87	0.22	-	119,171,232,241	0
2	NAG	B	2406	14/15	0.62	0.53	-	136,143,145,146	0
2	NAG	A	2406	14/15	0.53	0.47	-	136,143,145,146	0
2	NAG	B	2402	14/15	0.86	0.21	-	140,225,283,337	0
2	NAG	A	2402	14/15	0.91	0.13	-	71,117,157,163	0
2	NAG	A	2408	14/15	0.72	0.41	-	137,202,231,236	0
2	NAG	A	2405	14/15	0.84	0.34	-	92,105,118,130	0
2	NAG	A	2407	14/15	0.86	0.32	-	129,201,215,223	0
2	NAG	B	2408	14/15	0.68	0.43	-	136,200,227,240	0
2	NAG	B	2404	14/15	0.78	0.43	-	112,181,230,239	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.