



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 06:28 PM BST

PDB ID : 1L3W
Title : C-cadherin Ectodomain
Authors : Boggon, T.J.; Murray, J.; Chappuis-Flament, S.; Wong, E.; Gumbiner, B.M.; Shapiro, L.
Deposited on : 2002-03-01
Resolution : 3.08 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

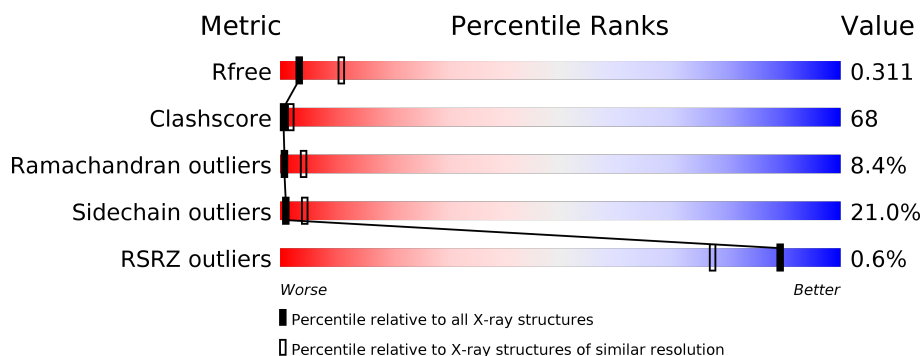
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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 ≥ 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	A	546	<div> <div></div> <div>32%</div> <div>45%</div> <div>17%</div> <div>5%</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	A	801	-	-	X	-
2	NAG	A	803	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	805	X	-	X	-
2	NAG	A	806	X	-	X	-
2	NAG	A	807	-	-	X	X
2	NAG	A	808	-	-	-	X
2	NAG	A	809	-	-	X	-
2	NAG	A	810	-	-	X	X
2	NAG	A	812	-	-	-	X
2	NAG	A	902	X	-	X	-
2	NAG	A	903	X	-	-	-
2	NAG	A	904	-	-	X	-
3	NDG	A	811	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4292 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.

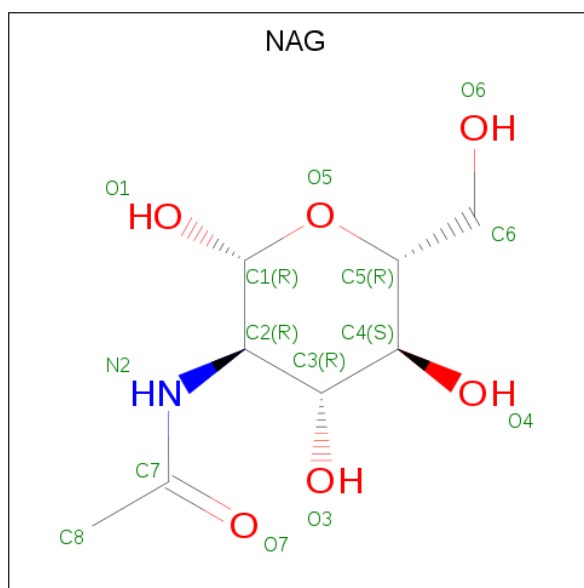
- Molecule 1 is a protein called EP-cadherin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	540	4032	2537	657	827	11	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

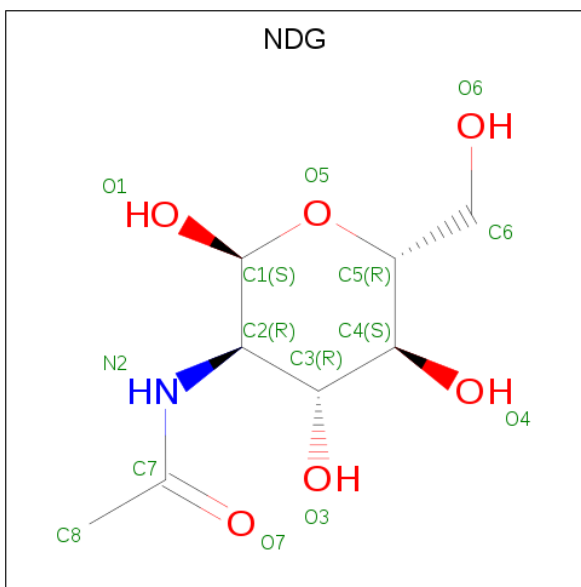
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P33148
A	-4	HIS	-	expression tag	UNP P33148
A	-3	HIS	-	expression tag	UNP P33148
A	-2	HIS	-	expression tag	UNP P33148
A	-1	HIS	-	expression tag	UNP P33148
A	0	HIS	-	expression tag	UNP P33148

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	Ca	0	0
			12	12		

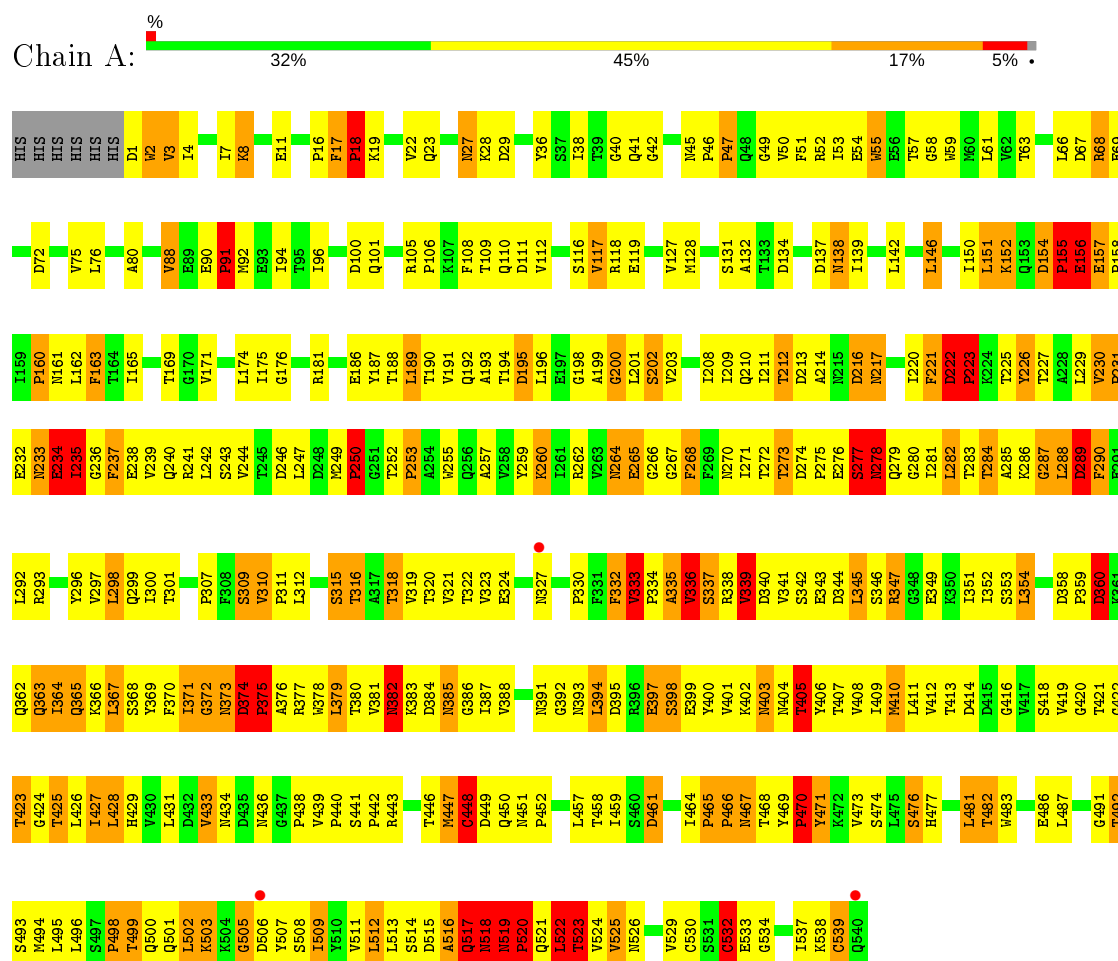
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		

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: EP-cadherin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.17Å 75.14Å 129.81Å 90.00° 105.50° 90.00°	Depositor
Resolution (Å)	20.00 – 3.08 19.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	69.8 (20.00-3.08) 85.4 (19.88-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.71 (at 2.98Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.243 , 0.276 0.280 , 0.311	Depositor DCC
R_{free} test set	1052 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 75.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4292	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CA, NAG, NDG

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	0.70	8/4115 (0.2%)	1.37	76/5651 (1.3%)

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	A	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ALA	CA-CB	-8.34	1.34	1.52
1	A	539	CYS	CB-SG	8.16	1.96	1.82
1	A	223	PRO	CG-CD	7.01	1.73	1.50
1	A	523	THR	N-CA	-6.24	1.33	1.46
1	A	522	LEU	N-CA	-5.97	1.34	1.46

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	520	PRO	CA-C-N	-13.28	87.99	117.20
1	A	235	ILE	N-CA-C	12.73	145.36	111.00
1	A	290	PHE	N-CA-C	12.73	145.36	111.00
1	A	374	ASP	N-CA-C	11.61	142.34	111.00
1	A	17	PHE	C-N-CD	-11.54	95.22	120.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	PHE	Sidechain
1	A	18	PRO	Mainchain
1	A	222	ASP	Mainchain
1	A	520	PRO	Mainchain

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	4032	0	3772	539	0
2	A	182	0	169	89	0
3	A	28	0	24	9	0
4	A	12	0	0	0	0
5	A	38	0	0	3	0
All	All	4292	0	3965	554	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 68.

The worst 5 of 554 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:482:THR:HG23	1:A:499:THR:CG2	1.75	1.17
1:A:234:GLU:H	1:A:235:ILE:HG23	1.08	1.15
1:A:423:THR:HB	2:A:810:NAG:C7	1.76	1.15
1:A:8:LYS:H	1:A:8:LYS:HD2	1.04	1.14
1:A:474:SER:HB2	1:A:512:LEU:HG	1.25	1.12

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	538/546 (98%)	401 (74%)	92 (17%)	45 (8%)	1 4

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	A	155	PRO
1	A	235	ILE
1	A	347	ARG
1	A	363	GLN

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	438/486 (90%)	346 (79%)	92 (21%)	1 4

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	LEU
1	A	353	SER
1	A	512	LEU
1	A	309	SER
1	A	318	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	233	ASN
1	A	385	ASN
1	A	138	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	391	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 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	NAG	A	903	1	14,14,15	0.53	0	17,19,21	0.76	0
2	NAG	A	807	1	14,14,15	0.63	0	17,19,21	1.15	2 (11%)
2	NAG	A	902	1	14,14,15	1.08	1 (7%)	17,19,21	1.07	1 (5%)
3	NDG	A	804	1	14,14,15	0.64	0	17,19,21	0.77	0
2	NAG	A	802	1	14,14,15	0.73	0	17,19,21	0.82	0
2	NAG	A	808	1	14,14,15	0.66	0	17,19,21	0.68	0
2	NAG	A	904	1	14,14,15	0.72	1 (7%)	17,19,21	0.68	0
2	NAG	A	806	1	14,14,15	0.56	0	17,19,21	1.34	2 (11%)
2	NAG	A	812	1	14,14,15	0.80	1 (7%)	17,19,21	0.73	1 (5%)
2	NAG	A	801	1	14,14,15	0.68	0	17,19,21	0.95	1 (5%)
2	NAG	A	805	1	14,14,15	0.71	0	17,19,21	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	810	1	14,14,15	0.66	0	17,19,21	1.34	4 (23%)
3	NDG	A	811	1	14,14,15	0.85	0	17,19,21	1.86	1 (5%)
2	NAG	A	809	1	14,14,15	0.74	0	17,19,21	0.93	0
2	NAG	A	803	1	14,14,15	0.97	1 (7%)	17,19,21	1.13	2 (11%)

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	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	807	1	-	5/6/23/26	0/1/1/1
2	NAG	A	902	1	1/1/5/7	1/6/23/26	0/1/1/1
3	NDG	A	804	1	-	0/6/23/26	0/1/1/1
2	NAG	A	802	1	-	2/6/23/26	0/1/1/1
2	NAG	A	808	1	-	3/6/23/26	0/1/1/1
2	NAG	A	904	1	-	3/6/23/26	0/1/1/1
2	NAG	A	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	812	1	-	4/6/23/26	0/1/1/1
2	NAG	A	801	1	-	3/6/23/26	0/1/1/1
2	NAG	A	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	810	1	-	3/6/23/26	0/1/1/1
3	NDG	A	811	1	-	2/6/23/26	0/1/1/1
2	NAG	A	809	1	-	2/6/23/26	0/1/1/1
2	NAG	A	803	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	NAG	C1-C2	3.10	1.57	1.52
2	A	803	NAG	O5-C5	2.53	1.48	1.43
2	A	904	NAG	C1-C2	-2.19	1.49	1.52
2	A	812	NAG	C1-C2	-2.11	1.49	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	811	NDG	C2-N2-C7	-6.99	112.95	122.90
2	A	806	NAG	C2-N2-C7	-3.41	118.04	122.90
2	A	805	NAG	C2-N2-C7	-2.98	118.66	122.90
2	A	807	NAG	C2-N2-C7	-2.88	118.80	122.90
2	A	803	NAG	C2-N2-C7	-2.82	118.88	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	902	NAG	C1
2	A	806	NAG	C1
2	A	903	NAG	C1
2	A	805	NAG	C1

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	807	NAG	C3-C2-N2-C7
2	A	902	NAG	C3-C2-N2-C7
2	A	904	NAG	C3-C2-N2-C7
2	A	807	NAG	C4-C5-C6-O6
2	A	802	NAG	C4-C5-C6-O6

There are no ring outliers.

13 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	807	NAG	17	0
2	A	902	NAG	8	0
3	A	804	NDG	2	0
2	A	808	NAG	2	0
2	A	904	NAG	8	0
2	A	806	NAG	9	0
2	A	812	NAG	3	0
2	A	801	NAG	21	0
2	A	805	NAG	7	0
2	A	810	NAG	12	0
3	A	811	NDG	7	0
2	A	809	NAG	8	0
2	A	803	NAG	4	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, 95th 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 ²)	Q<0.9
1	A	540/546 (98%)	-0.43	3 (0%) 89 77	6, 68, 100, 100	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	540	GLN	2.6
1	A	506	ASP	2.4
1	A	327	ASN	2.1

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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
2	NAG	A	810	14/15	0.56	0.63	78,78,78,78	14
2	NAG	A	904	14/15	0.64	0.28	27,27,27,27	14
2	NAG	A	903	14/15	0.66	0.25	56,56,56,56	14
2	NAG	A	801	14/15	0.69	0.36	39,39,39,39	14

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	A	812	14/15	0.72	0.43	67,67,67,67	14
3	NDG	A	811	14/15	0.73	0.36	100,100,100,100	14
2	NAG	A	802	14/15	0.74	0.37	99,99,99,99	14
2	NAG	A	803	14/15	0.74	0.44	63,63,63,63	14
2	NAG	A	808	14/15	0.76	0.46	83,83,83,83	14
2	NAG	A	805	14/15	0.76	0.31	89,89,89,89	0
3	NDG	A	804	14/15	0.79	0.28	51,51,51,51	14
2	NAG	A	807	14/15	0.80	0.43	62,62,62,62	14
2	NAG	A	806	14/15	0.80	0.30	64,64,64,64	14
2	NAG	A	902	14/15	0.81	0.29	37,37,37,37	14
4	CA	A	607	1/1	0.84	0.12	90,90,90,90	0
4	CA	A	610	1/1	0.84	0.06	70,70,70,70	0
2	NAG	A	809	14/15	0.88	0.25	100,100,100,100	0
4	CA	A	609	1/1	0.92	0.05	69,69,69,69	0
4	CA	A	611	1/1	0.93	0.08	85,85,85,85	0
4	CA	A	602	1/1	0.93	0.13	15,15,15,15	0
4	CA	A	605	1/1	0.97	0.11	10,10,10,10	0
4	CA	A	606	1/1	0.97	0.08	37,37,37,37	0
4	CA	A	608	1/1	0.98	0.05	34,34,34,34	0
4	CA	A	604	1/1	0.98	0.14	12,12,12,12	0
4	CA	A	603	1/1	0.98	0.12	10,10,10,10	0
4	CA	A	601	1/1	0.99	0.11	5,5,5,5	0
4	CA	A	600	1/1	0.99	0.05	22,22,22,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.