



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 07:39 AM BST

PDB ID : 1O8A
Title : Crystal Structure of Human Angiotensin Converting Enzyme (Native).
Authors : Natesh, R.; Schwager, S.L.U.; Sturrock, E.D.; Acharya, K.R.
Deposited on : 2002-11-26
Resolution : 2.00 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

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

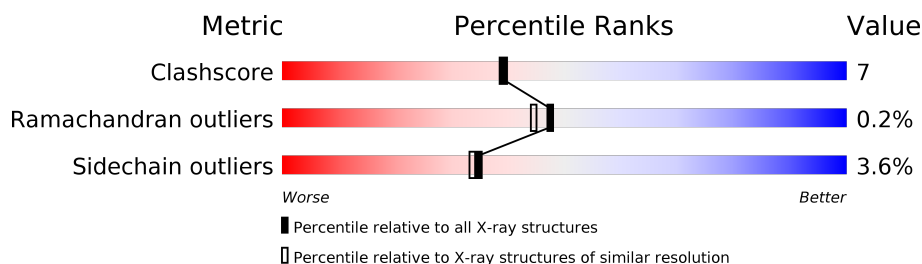
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	589	

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	695	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5264 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 ANGIOTENSIN CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	0	1
			4660	2991	798	847	24			

- 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		

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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

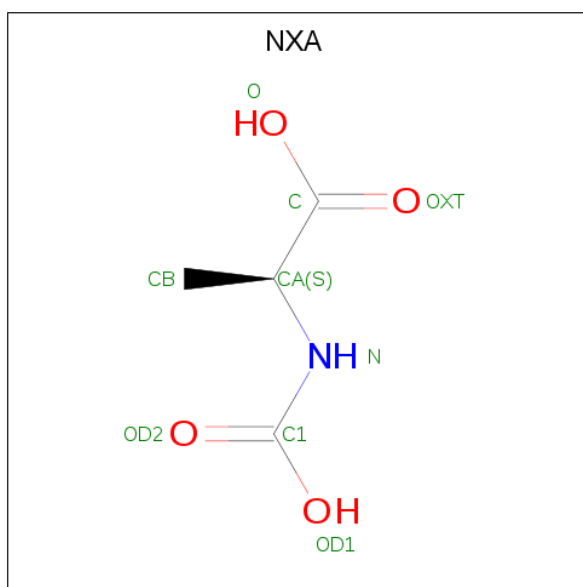


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is N-CARBOXYALANINE (three-letter code: NXA) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Cl	0	0
			2	2		

- Molecule 7 is water.

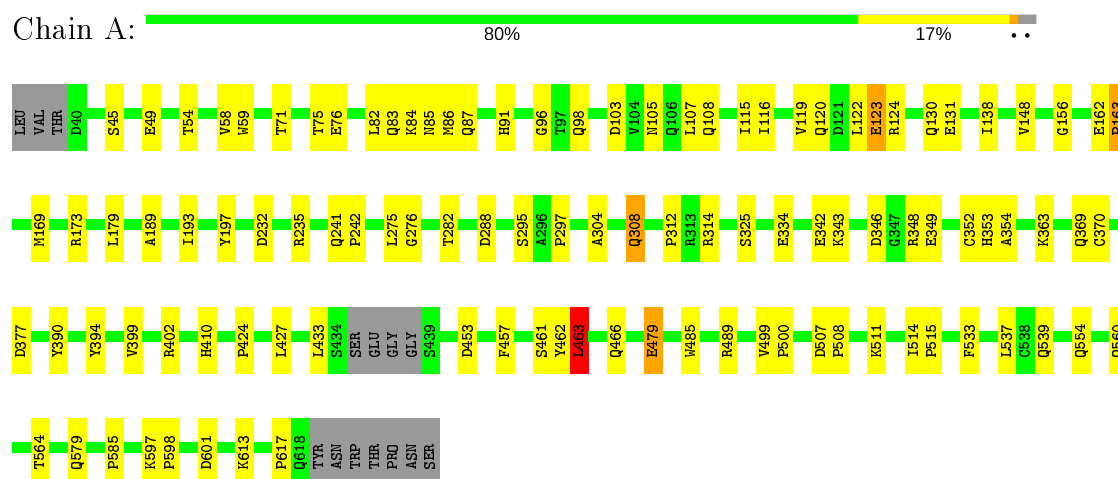
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	504	Total	O	0	0
			504	504		

3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

• Molecule 1: ANGIOTENSIN CONVERTING ENZYME



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.62Å 85.06Å 133.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.14 – 2.00	Depositor
% Data completeness (in resolution range)	93.1 (47.14-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5264	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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: ZN, ACT, NXA, NAG, CL

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	0.32	0/4796	0.56	1/6524 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	463	LEU	CA-CB-CG	5.64	128.27	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4660	0	4482	69	0
2	A	84	0	78	0	0
3	A	4	0	3	0	0
4	A	1	0	0	0	0
5	A	9	0	5	0	0
6	A	2	0	0	0	0
7	A	504	0	0	10	0
All	All	5264	0	4568	69	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 7.

All (69) 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:82:LEU:HA	1:A:85:ASN:HD22	1.41	0.86
1:A:346:ASP:HB3	1:A:348:ARG:HB2	1.64	0.79
1:A:613:LYS:NZ	1:A:617:PRO:HG3	1.99	0.78
1:A:179:LEU:HD11	1:A:499:VAL:HG23	1.68	0.75
1:A:107:LEU:HD21	1:A:116:ILE:HD12	1.71	0.72
1:A:304:ALA:O	1:A:308:GLN:HG2	1.91	0.71
1:A:45:SER:O	1:A:49:GLU:HG3	1.96	0.66
1:A:560:GLN:HE21	1:A:564:THR:HG23	1.65	0.61
1:A:334:GLU:HG2	7:A:2327:HOH:O	2.02	0.59
1:A:96:GLY:HA3	1:A:122:LEU:HD22	1.87	0.56
1:A:462:TYR:O	1:A:466:GLN:HG2	2.05	0.56
1:A:560:GLN:HE21	1:A:564:THR:CG2	2.19	0.55
1:A:295:SER:O	1:A:297:PRO:HD3	2.07	0.54
1:A:343:LYS:HB2	1:A:370:CYS:HB3	1.90	0.53
1:A:511:LYS:O	1:A:515:PRO:HD2	2.10	0.52
1:A:116:ILE:O	1:A:120:GLN:HG3	2.09	0.51
1:A:533:PHE:O	1:A:537:LEU:HG	2.11	0.51
1:A:354:ALA:HB2	1:A:369:GLN:HG3	1.93	0.50
1:A:613:LYS:HZ3	1:A:617:PRO:HG3	1.76	0.50
1:A:312:PRO:HG2	1:A:342:GLU:HG2	1.93	0.49
1:A:84:LYS:HD3	1:A:87:GLN:OE1	2.12	0.49
1:A:98:GLN:HG2	7:A:2050:HOH:O	2.12	0.49
1:A:613:LYS:HZ1	1:A:617:PRO:HG3	1.75	0.49
1:A:424:PRO:HA	1:A:433:LEU:HD12	1.95	0.49
1:A:54:THR:O	1:A:58:VAL:HG12	2.13	0.49
1:A:463:LEU:C	1:A:463:LEU:HD23	2.33	0.49
1:A:96:GLY:HA3	1:A:122:LEU:CD2	2.43	0.48
1:A:58:VAL:HG13	1:A:59:TRP:CD1	2.49	0.48
1:A:173:ARG:NH1	1:A:288:ASP:OD1	2.46	0.48
1:A:353:HIS:HD2	7:A:2314:HOH:O	1.96	0.48
1:A:179:LEU:HD11	1:A:499:VAL:CG2	2.40	0.48
1:A:71:THR:O	1:A:348:ARG:HD2	2.13	0.48
1:A:107:LEU:CD2	1:A:116:ILE:HD12	2.44	0.47
1:A:427:LEU:HB2	1:A:433:LEU:HD12	1.97	0.47
1:A:325:SER:O	1:A:554:GLN:HA	2.14	0.47
1:A:169:MET:O	1:A:276:GLY:HA2	2.15	0.47
1:A:554:GLN:NE2	7:A:2447:HOH:O	2.46	0.46
1:A:91:HIS:HD2	7:A:2024:HOH:O	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:GLN:O	1:A:554:GLN:HG2	2.14	0.46
1:A:479:GLU:HG3	7:A:2394:HOH:O	2.15	0.46
1:A:485:TRP:CD2	1:A:508:PRO:HG3	2.51	0.46
1:A:58:VAL:HG13	1:A:59:TRP:HD1	1.79	0.46
1:A:514:ILE:HB	1:A:515:PRO:CD	2.47	0.45
1:A:597:LYS:HE3	1:A:601:ASP:OD2	2.16	0.45
1:A:130:GLN:HG2	7:A:2105:HOH:O	2.15	0.45
1:A:560:GLN:O	1:A:564:THR:HG23	2.16	0.45
1:A:457:PHE:CE2	1:A:461:SER:HB3	2.52	0.45
1:A:115:ILE:O	1:A:119:VAL:HG23	2.17	0.44
1:A:500:PRO:HG2	7:A:2413:HOH:O	2.18	0.44
1:A:83:GLN:HG3	7:A:2029:HOH:O	2.16	0.44
1:A:597:LYS:HB3	1:A:598:PRO:HD3	1.99	0.44
1:A:241:GLN:HB2	1:A:242:PRO:HD3	1.98	0.44
1:A:282:THR:HB	1:A:453:ASP:OD1	2.17	0.44
1:A:75:THR:HG22	1:A:76:GLU:OE1	2.18	0.44
1:A:123:GLU:HB3	1:A:124:ARG:H	1.68	0.43
1:A:554:GLN:CG	1:A:554:GLN:O	2.66	0.43
1:A:138:ILE:HG13	7:A:2104:HOH:O	2.17	0.43
1:A:275:LEU:HD22	1:A:275:LEU:N	2.33	0.43
1:A:162:GLU:OE1	1:A:352:CYS:HB3	2.19	0.43
1:A:148:VAL:HG12	1:A:349:GLU:CG	2.49	0.43
1:A:463:LEU:HD11	1:A:489:ARG:HA	2.01	0.42
1:A:399:VAL:HA	1:A:402:ARG:HG3	2.01	0.42
1:A:103:ASP:OD1	1:A:105:ASN:HB2	2.20	0.42
1:A:75:THR:CG2	1:A:76:GLU:OE1	2.69	0.41
1:A:308:GLN:HG2	1:A:308:GLN:H	1.68	0.41
1:A:189:ALA:O	1:A:193:ILE:HG12	2.20	0.41
1:A:162:GLU:HA	1:A:163:PRO:HA	1.79	0.41
1:A:232:ASP:OD1	1:A:235:ARG:NH2	2.54	0.41
1:A:507:ASP:N	1:A:508:PRO:CD	2.85	0.40

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	571/589 (97%)	553 (97%)	17 (3%)	1 (0%)	47	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	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	494/515 (96%)	476 (96%)	18 (4%)	35	34

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	MET
1	A	108	GLN
1	A	123	GLU
1	A	131	GLU
1	A	163	PRO
1	A	197	TYR
1	A	308	GLN
1	A	314	ARG
1	A	363	LYS
1	A	377	ASP
1	A	390	TYR
1	A	394	TYR
1	A	410	HIS
1	A	463	LEU
1	A	479	GLU
1	A	539	GLN
1	A	579	GLN
1	A	585	PRO

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	83	GLN
1	A	85	ASN
1	A	91	HIS
1	A	231	GLN
1	A	248	HIS
1	A	539	GLN
1	A	554	GLN
1	A	560	GLN
1	A	579	GLN
1	A	610	HIS

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 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	694	1	14,14,15	2.10	6 (42%)	17,19,21	1.02	1 (5%)
5	NXA	A	702	-	2,8,8	0.96	0	3,10,10	5.83	3 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	695	1	14,14,15	2.10	6 (42%)	17,19,21	1.01	1 (5%)
2	NAG	A	692	1	14,14,15	2.19	7 (50%)	17,19,21	1.22	2 (11%)
2	NAG	A	696	1	14,14,15	2.03	6 (42%)	17,19,21	1.14	2 (11%)
2	NAG	A	691	1	14,14,15	2.06	6 (42%)	17,19,21	1.04	1 (5%)
2	NAG	A	693	1	14,14,15	2.03	5 (35%)	17,19,21	1.04	1 (5%)
3	ACT	A	700	4	1,3,3	3.42	1 (100%)	0,3,3	0.00	-

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	694	1	-	2/6/23/26	0/1/1/1
5	NXA	A	702	-	-	0/2/8/8	-
2	NAG	A	695	1	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	A	692	1	-	2/6/23/26	0/1/1/1
2	NAG	A	696	1	-	0/6/23/26	0/1/1/1
2	NAG	A	691	1	-	0/6/23/26	0/1/1/1
2	NAG	A	693	1	-	0/6/23/26	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	692	NAG	C1-C2	4.32	1.58	1.52
2	A	694	NAG	C1-C2	4.13	1.58	1.52
2	A	696	NAG	C1-C2	4.09	1.58	1.52
2	A	695	NAG	C1-C2	4.07	1.58	1.52
2	A	691	NAG	C1-C2	4.00	1.58	1.52
2	A	693	NAG	C1-C2	3.73	1.57	1.52
3	A	700	ACT	CH3-C	3.42	1.53	1.48
2	A	694	NAG	O7-C7	-3.33	1.15	1.23
2	A	692	NAG	O7-C7	-3.30	1.15	1.23
2	A	695	NAG	O7-C7	-3.28	1.15	1.23
2	A	695	NAG	O5-C5	3.28	1.50	1.43
2	A	693	NAG	O7-C7	-3.28	1.15	1.23
2	A	696	NAG	O7-C7	-3.26	1.15	1.23
2	A	691	NAG	O7-C7	-3.24	1.15	1.23
2	A	693	NAG	O5-C5	3.22	1.50	1.43
2	A	693	NAG	C4-C5	3.22	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	695	NAG	C4-C5	3.19	1.59	1.53
2	A	691	NAG	O5-C5	3.18	1.49	1.43
2	A	694	NAG	O5-C5	3.12	1.49	1.43
2	A	692	NAG	C4-C5	3.12	1.59	1.53
2	A	694	NAG	C4-C5	3.10	1.59	1.53
2	A	691	NAG	C4-C5	3.05	1.59	1.53
2	A	696	NAG	C4-C5	2.98	1.59	1.53
2	A	692	NAG	O5-C5	2.93	1.49	1.43
2	A	696	NAG	O5-C5	2.62	1.48	1.43
2	A	696	NAG	C8-C7	-2.39	1.45	1.50
2	A	691	NAG	C8-C7	-2.34	1.45	1.50
2	A	693	NAG	C8-C7	-2.28	1.45	1.50
2	A	694	NAG	C8-C7	-2.26	1.45	1.50
2	A	692	NAG	C3-C2	2.25	1.57	1.52
2	A	694	NAG	C3-C2	2.22	1.57	1.52
2	A	695	NAG	C8-C7	-2.21	1.45	1.50
2	A	692	NAG	C8-C7	-2.21	1.46	1.50
2	A	695	NAG	C3-C2	2.15	1.57	1.52
2	A	691	NAG	C3-C2	2.09	1.56	1.52
2	A	696	NAG	C3-C2	2.08	1.56	1.52
2	A	692	NAG	C2-N2	2.07	1.49	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	702	NXA	C-CA-N	7.44	122.32	111.81
5	A	702	NXA	CB-CA-N	-5.99	97.59	108.95
5	A	702	NXA	CB-CA-C	-3.27	105.92	110.93
2	A	692	NAG	C2-N2-C7	3.01	127.19	122.90
2	A	691	NAG	C4-C3-C2	-2.73	107.01	111.02
2	A	696	NAG	O5-C1-C2	-2.67	107.07	111.29
2	A	695	NAG	C4-C3-C2	-2.48	107.39	111.02
2	A	694	NAG	C4-C3-C2	-2.48	107.39	111.02
2	A	693	NAG	C4-C3-C2	-2.46	107.42	111.02
2	A	692	NAG	C4-C3-C2	-2.19	107.80	111.02
2	A	696	NAG	C4-C3-C2	-2.19	107.81	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	695	NAG	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	694	NAG	O5-C5-C6-O6
2	A	694	NAG	C4-C5-C6-O6
2	A	692	NAG	C3-C2-N2-C7
2	A	692	NAG	C1-C2-N2-C7
2	A	695	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.