



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:48 PM GMT

PDB ID : 1XM1
Title : Nonbasic Thrombin Inhibitor Complex
Authors : Friedrich, R.; Bode, W.; Schwienhorst, A.
Deposited on : 2004-10-01
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

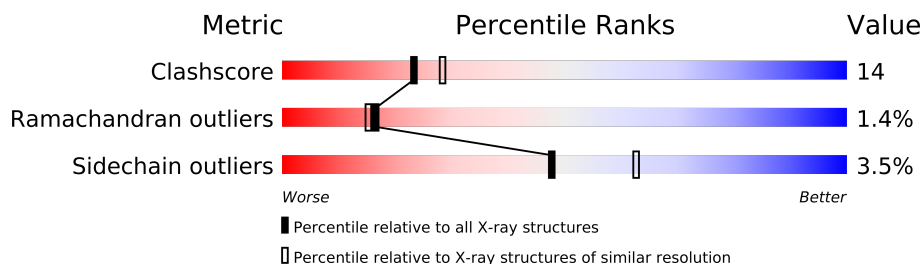
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	295	
2	H	10	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 2599 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

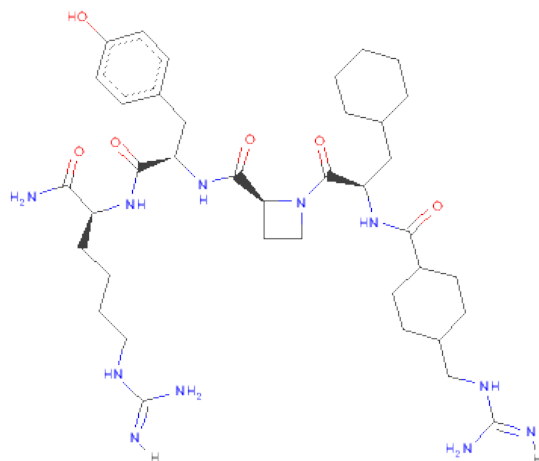
- Molecule 1 is a protein called thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	75	0	0
			2301	1467	404	415	15			

- Molecule 2 is a protein called Hirudin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	10	Total	C	N	O	S	0	0	0
			95	59	10	25	1			

- Molecule 3 is N-{[(2S)-1-(N-{[4-({[AMINO(IMINO)METHYL]AMINO}METHYL)CYCLOHEXYL]CARBONYL}-3-CYCLOHEXYL-L-ALANYL)AZETIDIN-2-YL]CARBONYL}-L-TYROSYL-N 6 -[AMINO(IMINO)METHYL]-L-LYSINAMIDE (three-letter code: GAH) (formula: C₃₈H₆₁N₁₁O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			55	38	11	6			

- Molecule 4 is water.

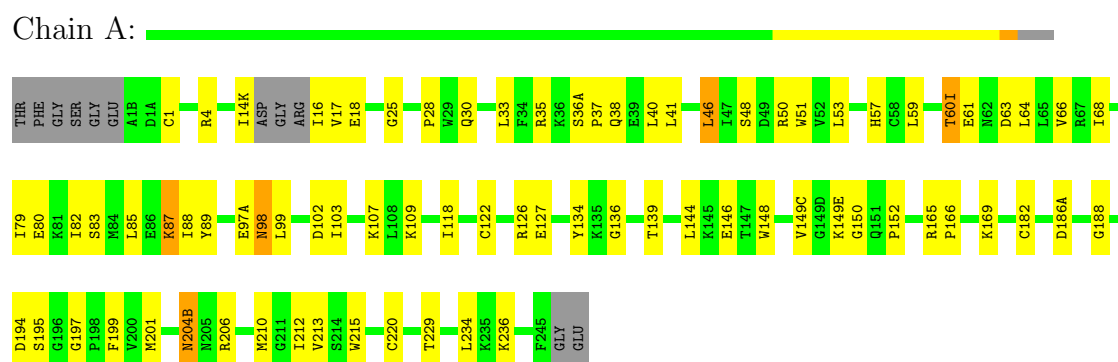
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	144	Total 144	O 144	0	0
4	H	4	Total 4	O 4	0	0

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 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.

Note EDS was not executed.

- Molecule 1: thrombin



- Molecule 2: Hirudin



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	70.46Å 70.93Å 72.65Å 90.00° 100.38° 90.00°	Depositor
Resolution (Å)	14.93 – 2.30	Depositor
% Data completeness (in resolution range)	87.6 (14.93-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.201 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2599	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAH, TYS

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	0.55	0/2358	0.70	0/3184
2	H	0.53	0/79	0.58	0/103
All	All	0.55	0/2437	0.70	0/3287

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2301	0	2280	65	0
2	H	95	0	73	3	0
3	A	55	0	59	6	0
4	A	144	0	0	2	1
4	H	4	0	0	1	0
All	All	2599	0	2412	68	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (68) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:68:ILE:HD11	1:A:118:ILE:HG23	1.61	0.82
1:A:33:LEU:HD11	1:A:64:LEU:HD13	1.63	0.81
1:A:144:LEU:HD21	1:A:152:PRO:HB3	1.63	0.80
1:A:195:SER:HB3	3:A:1001:GAH:H332	1.67	0.76
1:A:61:GLU:OE1	1:A:87:LYS:HE3	1.93	0.68
1:A:66:VAL:CG2	1:A:83:SER:HB2	2.23	0.68
1:A:17:VAL:HG12	1:A:18:GLU:HG2	1.77	0.67
1:A:4:ARG:HG2	1:A:28:PRO:HG3	1.76	0.66
1:A:16:ILE:N	1:A:194:ASP:OD1	2.31	0.64
1:A:14(K):ILE:HG13	1:A:134:TYR:OH	1.98	0.64
1:A:82:ILE:HD12	1:A:82:ILE:N	2.14	0.62
1:A:146:GLU:HB2	1:A:220:CYS:HB2	1.86	0.58
1:A:4:ARG:HG2	1:A:28:PRO:CG	2.34	0.58
1:A:98:ASN:HD22	1:A:98:ASN:H	1.54	0.55
1:A:68:ILE:CD1	1:A:118:ILE:HG23	2.35	0.54
1:A:61:GLU:OE2	1:A:88:ILE:HG12	2.08	0.54
1:A:64:LEU:HD12	1:A:85:LEU:HD22	1.90	0.54
1:A:136:GLY:HA3	1:A:199:PHE:CZ	2.43	0.53
1:A:165:ARG:HB3	1:A:166:PRO:HD3	1.90	0.53
1:A:17:VAL:O	1:A:188:GLY:HA2	2.09	0.52
1:A:64:LEU:HD12	1:A:85:LEU:CD2	2.39	0.52
1:A:97(A):GLU:O	3:A:1001:GAH:H212	2.10	0.52
1:A:99:LEU:O	1:A:102:ASP:HB2	2.09	0.52
1:A:66:VAL:HG23	1:A:83:SER:HB2	1.91	0.51
1:A:30:GLN:NE2	1:A:139:THR:OG1	2.43	0.51
1:A:165:ARG:HG2	1:A:169:LYS:HE3	1.92	0.51
2:H:55:ASP:N	4:H:100:HOH:O	2.43	0.51
1:A:82:ILE:HD13	2:H:63:TYS:O1	2.11	0.50
1:A:85:LEU:N	1:A:85:LEU:HD12	2.27	0.49
1:A:98:ASN:HD22	1:A:98:ASN:N	2.10	0.48
1:A:50:ARG:NH1	1:A:109:LYS:O	2.47	0.48
1:A:46:LEU:HG	1:A:68:ILE:HD12	1.96	0.48
1:A:82:ILE:CD1	1:A:82:ILE:N	2.77	0.48
1:A:215:TRP:HB2	3:A:1001:GAH:H161	1.96	0.48
1:A:53:LEU:HD11	1:A:103:ILE:HD11	1.94	0.48
1:A:57:HIS:CE1	1:A:195:SER:HB2	2.49	0.47
1:A:25:GLY:O	1:A:28:PRO:HD3	2.13	0.47
1:A:126:ARG:HB2	1:A:126:ARG:NH2	2.29	0.47
1:A:212:ILE:HB	1:A:229:THR:HB	1.97	0.47
1:A:80:GLU:OE2	1:A:82:ILE:HD11	2.15	0.46
1:A:98:ASN:N	1:A:98:ASN:ND2	2.64	0.45
1:A:87:LYS:HB3	1:A:89:TYR:CE1	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:98:ASN:HA	3:A:1001:GAH:H201	1.99	0.45
1:A:197:GLY:O	1:A:213:VAL:HG23	2.16	0.45
1:A:36(A):SER:HA	1:A:37:PRO:C	2.37	0.45
1:A:201:MET:SD	1:A:210:MET:HG3	2.57	0.45
1:A:98:ASN:HA	3:A:1001:GAH:C20	2.47	0.44
1:A:46:LEU:HD22	1:A:48:SER:O	2.18	0.44
1:A:40:LEU:O	1:A:40:LEU:HD23	2.18	0.44
1:A:98:ASN:ND2	1:A:98:ASN:H	2.15	0.44
1:A:60(I):THR:HG23	1:A:63:ASP:OD2	2.18	0.43
1:A:236:LYS:HB2	4:A:1061:HOH:O	2.18	0.43
1:A:30:GLN:HB2	1:A:30:GLN:HE21	1.69	0.42
2:H:58:GLU:H	2:H:58:GLU:CD	2.21	0.42
1:A:204(B):ASN:C	1:A:204(B):ASN:HD22	2.23	0.42
1:A:204(B):ASN:ND2	1:A:206:ARG:H	2.17	0.42
1:A:46:LEU:HG	1:A:68:ILE:CD1	2.50	0.42
1:A:51:TRP:CH2	1:A:107:LYS:HB2	2.55	0.42
1:A:87:LYS:HD2	4:A:1139:HOH:O	2.19	0.42
1:A:46:LEU:CD2	1:A:48:SER:O	2.68	0.42
1:A:127:GLU:CD	1:A:127:GLU:H	2.23	0.42
1:A:41:LEU:CD1	1:A:64:LEU:HD22	2.50	0.41
3:A:1001:GAH:H231	3:A:1001:GAH:H15	1.96	0.41
1:A:61:GLU:HG2	1:A:61:GLU:H	1.61	0.41
1:A:1:CYS:C	1:A:122:CYS:SG	2.99	0.41
1:A:66:VAL:HG22	1:A:83:SER:HB2	2.00	0.41
1:A:35:ARG:O	1:A:38:GLN:HA	2.20	0.40
1:A:59:LEU:HD13	1:A:88:ILE:HD12	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:1082:HOH:O	4:A:1082:HOH:O[2_656]	1.82	0.38

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	280/295 (95%)	259 (92%)	17 (6%)	4 (1%)	16	15
2	H	7/10 (70%)	7 (100%)	0	0	100	100
All	All	287/305 (94%)	266 (93%)	17 (6%)	4 (1%)	16	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149(C)	VAL
1	A	150	GLY
1	A	148	TRP
1	A	149(E)	LYS

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	249/256 (97%)	240 (96%)	9 (4%)	47	61
2	H	9/9 (100%)	9 (100%)	0	100	100
All	All	258/265 (97%)	249 (96%)	9 (4%)	48	63

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	60(I)	THR
1	A	79	ILE
1	A	87	LYS
1	A	98	ASN
1	A	182	CYS
1	A	186(A)	ASP
1	A	204(B)	ASN
1	A	234	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	62	ASN
1	A	78	ASN
1	A	98	ASN
1	A	131	GLN
1	A	204(B)	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue 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	TYS	H	63	2	16,16,17	4.80	4 (25%)	20,22,24	0.82	1 (5%)

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	TYS	H	63	2	-	0/9/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	63	TYS	O-C	17.77	1.23	1.11
2	H	63	TYS	OH-S	-5.21	1.54	1.63
2	H	63	TYS	OH-CZ	-2.81	1.39	1.42
2	H	63	TYS	CA-C	2.11	1.52	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	63	TYS	OH-S-O1	2.80	115.72	107.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates i

There are no carbohydrates in this entry.

5.6 Ligand geometry i

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	$\# Z > 2$
3	GAH	A	1001	-	58,58,58	3.34	31 (53%)	78,78,78	3.43	34 (43%)

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	GAH	A	1001	-	-	0/56/84/84	1/3/4/4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	GAH	C27-C28	-8.01	1.46	1.55
3	A	1001	GAH	C35-C36	6.31	1.50	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	GAH	C2-C3	6.27	1.70	1.53
3	A	1001	GAH	C2-C1	6.01	1.68	1.52
3	A	1001	GAH	C7-C6	5.77	1.62	1.51
3	A	1001	GAH	C17-N25	5.43	1.45	1.34
3	A	1001	GAH	C23-C18	5.18	1.66	1.52
3	A	1001	GAH	C1-C6	5.03	1.65	1.52
3	A	1001	GAH	C19-C18	4.58	1.64	1.52
3	A	1001	GAH	C29-N31	4.56	1.44	1.34
3	A	1001	GAH	C33-C34	4.49	1.62	1.51
3	A	1001	GAH	C35-C34	4.39	1.48	1.38
3	A	1001	GAH	C15-N14	4.31	1.55	1.45
3	A	1001	GAH	C16-C18	4.13	1.60	1.53
3	A	1001	GAH	C9-N8	4.12	1.42	1.33
3	A	1001	GAH	C45-N47	4.07	1.41	1.33
3	A	1001	GAH	C3-C12	3.98	1.58	1.51
3	A	1001	GAH	C32-N31	3.93	1.54	1.45
3	A	1001	GAH	C15-C17	3.78	1.61	1.53
3	A	1001	GAH	C28-C29	3.62	1.60	1.52
3	A	1001	GAH	C33-C32	3.56	1.62	1.54
3	A	1001	GAH	C12-N14	3.52	1.42	1.34
3	A	1001	GAH	C36-C37	3.46	1.46	1.38
3	A	1001	GAH	C38-C39	3.35	1.45	1.38
3	A	1001	GAH	C27-C26	3.30	1.57	1.54
3	A	1001	GAH	O46-C45	-3.22	1.17	1.23
3	A	1001	GAH	C7-N8	3.21	1.55	1.46
3	A	1001	GAH	C39-C34	2.91	1.45	1.38
3	A	1001	GAH	C16-C15	2.46	1.61	1.53
3	A	1001	GAH	C38-C37	2.23	1.43	1.38
3	A	1001	GAH	C21-C22	2.01	1.59	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	GAH	C44-N43-C41	11.98	148.13	121.63
3	A	1001	GAH	C15-N14-C12	10.89	145.71	121.63
3	A	1001	GAH	C32-C41-N43	8.50	136.54	116.81
3	A	1001	GAH	C27-C26-N25	-7.66	83.15	88.37
3	A	1001	GAH	O42-C41-N43	-7.49	108.51	122.93
3	A	1001	GAH	C15-C17-N25	6.84	131.01	118.70
3	A	1001	GAH	C41-C32-N31	6.56	129.73	111.28
3	A	1001	GAH	C28-C29-N31	6.07	130.09	116.70
3	A	1001	GAH	C29-C28-N25	-5.84	104.81	114.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	GAH	C2-C3-C12	4.65	121.40	110.63
3	A	1001	GAH	C1-C6-C7	4.44	122.75	111.65
3	A	1001	GAH	C26-C27-C28	4.30	93.90	87.79
3	A	1001	GAH	O24-C17-N25	-3.77	115.38	121.38
3	A	1001	GAH	C28-N25-C17	3.68	143.77	128.76
3	A	1001	GAH	C16-C15-N14	3.59	119.46	110.52
3	A	1001	GAH	C4-C5-C6	3.53	118.83	112.47
3	A	1001	GAH	C5-C4-C3	3.45	116.63	110.81
3	A	1001	GAH	C33-C32-N31	-3.38	103.71	110.80
3	A	1001	GAH	C17-C15-N14	3.36	116.63	108.76
3	A	1001	GAH	O46-C45-N47	-3.32	117.42	123.03
3	A	1001	GAH	O30-C29-N31	-3.27	116.62	122.93
3	A	1001	GAH	C3-C12-N14	-3.26	111.02	116.19
3	A	1001	GAH	C1-C2-C3	3.25	116.29	110.81
3	A	1001	GAH	O30-C29-C28	-3.19	113.29	120.38
3	A	1001	GAH	O24-C17-C15	-3.10	113.55	119.60
3	A	1001	GAH	N52-C53-N55	2.99	126.08	120.35
3	A	1001	GAH	C26-N25-C17	-2.83	119.72	132.39
3	A	1001	GAH	O42-C41-C32	-2.44	114.94	120.31
3	A	1001	GAH	C32-N31-C29	2.41	126.95	121.63
3	A	1001	GAH	C48-C44-N43	-2.34	106.38	110.83
3	A	1001	GAH	O13-C12-N14	2.25	127.26	122.93
3	A	1001	GAH	C27-C28-N25	-2.13	86.46	88.08
3	A	1001	GAH	C2-C3-C4	-2.04	104.93	109.70
3	A	1001	GAH	C44-C45-N47	2.03	120.72	116.78

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	GAH	C1-C2-C3-C4-C5-C6

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.