



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2021 – 05:36 PM EDT

PDB ID : 3HVG
Title : Structure of bace (beta secretase) in Complex with EV0
Authors : Godemann, R.; Madden, J.; Kramer, J.; Smith, M.A.; Barker, J.; Ebner, A.
Deposited on : 2009-06-16
Resolution : 2.26 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) : 1.13
EDS : 2.23.2
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) : 2.23.2

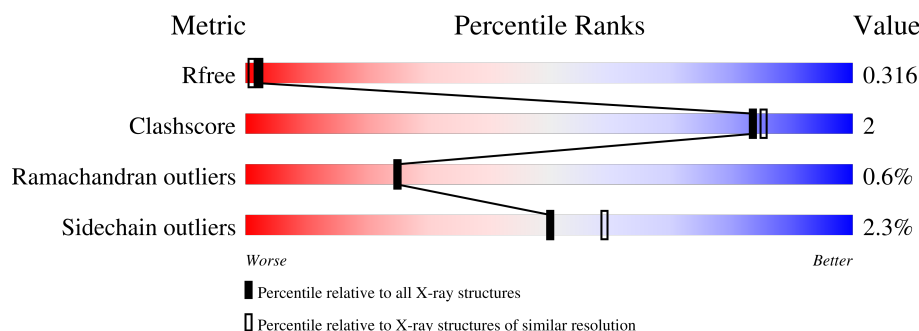
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

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 of 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	411	
1	B	411	
1	C	411	

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	EV0	B	441	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EV0	B	442	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9063 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.

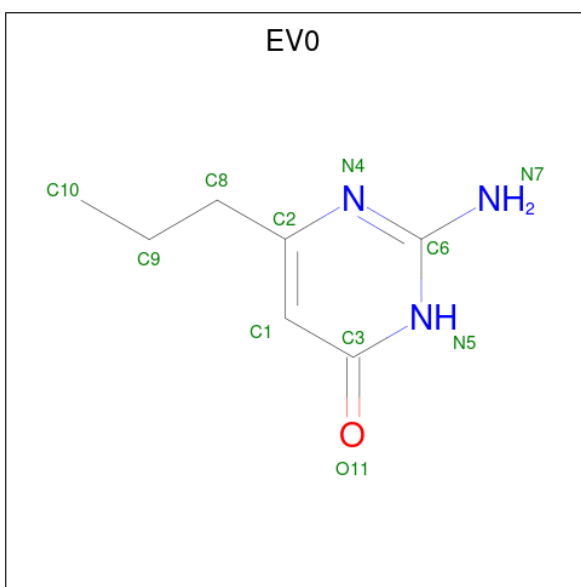
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2977	1904	495	564	14			
1	B	370	Total	C	N	O	S	0	1	0
			2921	1871	486	550	14			
1	C	373	Total	C	N	O	S	0	1	0
			2946	1887	492	553	14			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	LEU	-	expression tag	UNP P56817
A	-17	PRO	-	expression tag	UNP P56817
A	-16	ARG	-	expression tag	UNP P56817
A	-5	LYS	ARG	engineered mutation	UNP P56817
A	-4	THR	ARG	engineered mutation	UNP P56817
B	-18	LEU	-	expression tag	UNP P56817
B	-17	PRO	-	expression tag	UNP P56817
B	-16	ARG	-	expression tag	UNP P56817
B	-5	LYS	ARG	engineered mutation	UNP P56817
B	-4	THR	ARG	engineered mutation	UNP P56817
C	-18	LEU	-	expression tag	UNP P56817
C	-17	PRO	-	expression tag	UNP P56817
C	-16	ARG	-	expression tag	UNP P56817
C	-5	LYS	ARG	engineered mutation	UNP P56817
C	-4	THR	ARG	engineered mutation	UNP P56817

- Molecule 2 is 2-amino-6-propylpyrimidin-4(3H)-one (three-letter code: EV0) (formula: $C_7H_{11}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	7	3	1		
2	B	1	Total	C	N	O	0	0
			11	7	3	1		
2	B	1	Total	C	N	O	0	0
			11	7	3	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		

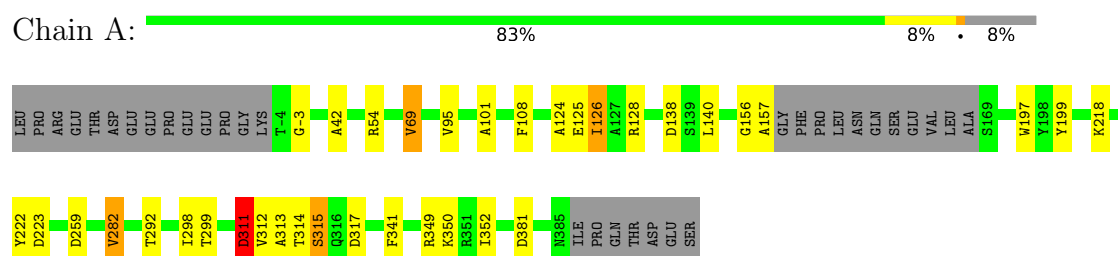
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total 46	O 46	0	0
4	B	67	Total 67	O 67	0	0
4	C	67	Total 67	O 67	0	0

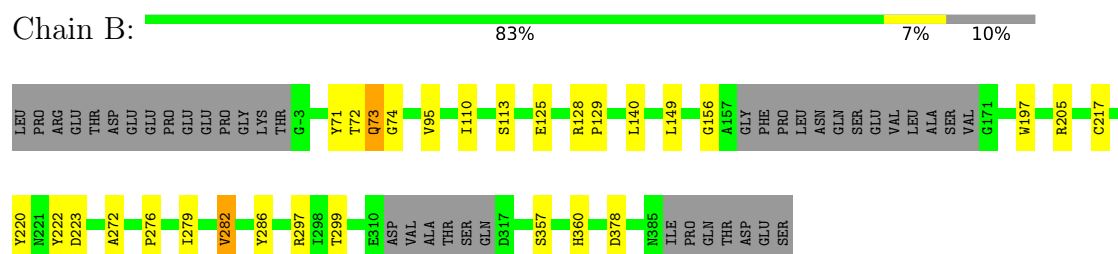
3 Residue-property plots [i](#)

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.

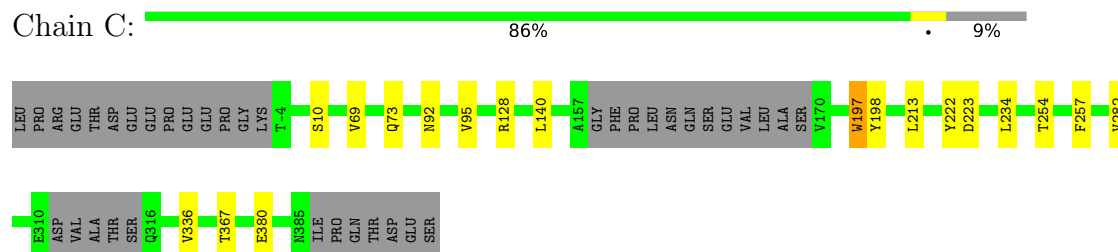
• Molecule 1: Beta-secretase 1



• Molecule 1: Beta-secretase 1



• Molecule 1: Beta-secretase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	232.55Å 100.13Å 64.78Å 90.00° 103.73° 90.00°	Depositor
Resolution (Å)	48.34 – 2.26 48.31 – 2.26	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.34-2.26) 98.5 (48.31-2.26)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.265 0.288 , 0.316	Depositor DCC
R_{free} test set	3318 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9063	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EV0, GOL

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	0.46	0/3052	0.58	0/4148
1	B	0.49	0/2995	0.57	0/4067
1	C	0.46	0/3023	0.61	0/4105
All	All	0.47	0/9070	0.59	0/12320

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	ASP	Peptide

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	2977	0	2888	18	0
1	B	2921	0	2832	17	0
1	C	2946	0	2865	7	0
2	A	11	0	11	1	0
2	B	22	0	22	0	0
3	C	6	0	8	1	0
4	A	46	0	0	0	0
4	B	67	0	0	0	0
4	C	67	0	0	0	0
All	All	9063	0	8626	42	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 2.

All (42) 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:73:GLN:NE2	1:B:73:GLN:HA	1.41	1.16
1:B:73:GLN:HE21	1:B:73:GLN:CA	1.67	1.08
1:B:73:GLN:NE2	1:B:73:GLN:CA	2.30	0.89
1:B:73:GLN:HA	1:B:73:GLN:HE21	0.75	0.87
1:C:95:VAL:HG11	1:C:140:LEU:HD12	1.77	0.67
1:A:124:ALA:O	1:A:126:ILE:N	2.29	0.65
1:B:72:THR:O	1:B:73:GLN:NE2	2.30	0.65
1:A:69:VAL:HG23	1:A:128:ARG:CG	2.29	0.63
1:B:71:TYR:HB2	1:B:74:GLY:O	1.98	0.62
1:A:69:VAL:HG23	1:A:128:ARG:HG2	1.87	0.55
1:A:298:ILE:HB	1:A:341:PHE:CZ	2.45	0.52
1:A:42:ALA:CB	1:A:101:ALA:HB1	2.40	0.51
1:B:276:PRO:O	1:B:279:ILE:HG12	2.09	0.51
1:A:124:ALA:C	1:A:126:ILE:H	2.16	0.49
1:A:314:THR:HG22	1:A:315:SER:N	2.27	0.49
1:A:108:PHE:CE1	2:A:441:EV0:H10A	2.48	0.48
1:A:69:VAL:HG23	1:A:128:ARG:HG3	1.96	0.48
1:A:95:VAL:HG11	1:A:140:LEU:HD12	1.96	0.47
1:A:156:GLY:O	1:A:157:ALA:HB2	2.14	0.47
1:A:311:ASP:O	1:A:313:ALA:N	2.41	0.46
1:B:217:CYS:HA	1:B:220:TYR:CD1	2.52	0.45
1:B:357:SER:HB3	1:B:360:HIS:HB3	1.97	0.45
1:C:222:TYR:HA	1:C:223:ASP:HA	1.72	0.44
1:B:125:GLU:O	1:B:125:GLU:HG3	2.17	0.44
1:B:95:VAL:HG11	1:B:140:LEU:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:TYR:HA	1:A:223:ASP:HA	1.79	0.43
1:C:234:LEU:HB2	1:C:336:VAL:CG2	2.48	0.43
1:A:282:VAL:HG13	1:A:299:THR:HG23	2.00	0.43
1:B:282:VAL:HG13	1:B:299:THR:HG23	2.02	0.42
1:C:197:TRP:CG	1:C:198:TYR:N	2.87	0.42
1:A:124:ALA:C	1:A:126:ILE:N	2.72	0.42
1:B:149:LEU:C	1:B:149:LEU:HD23	2.41	0.42
1:B:205:ARG:HB3	1:B:286:TYR:HB2	2.02	0.41
1:A:199:TYR:HB3	1:A:352:ILE:HD11	2.02	0.41
1:A:349:ARG:O	1:A:350:LYS:C	2.59	0.41
1:C:69:VAL:HG22	1:C:128:ARG:HG3	2.03	0.41
1:C:213:LEU:HD12	1:C:213:LEU:HA	1.96	0.41
1:A:218:LYS:HD3	1:A:381:ASP:O	2.21	0.41
1:C:10:SER:HA	3:C:441:GOL:H11	2.03	0.41
1:B:222:TYR:HA	1:B:223:ASP:HA	1.78	0.41
1:B:110:ILE:HB	1:B:113:SER:HB3	2.04	0.40
1:B:128:ARG:HA	1:B:129:PRO:C	2.42	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	375/411 (91%)	356 (95%)	15 (4%)	4 (1%)	14	10
1	B	365/411 (89%)	348 (95%)	15 (4%)	2 (0%)	29	29
1	C	368/411 (90%)	355 (96%)	12 (3%)	1 (0%)	41	46
All	All	1108/1233 (90%)	1059 (96%)	42 (4%)	7 (1%)	25	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	GLU
1	A	312	VAL
1	C	73	GLN
1	A	315	SER
1	B	156	GLY
1	A	-3	GLY
1	B	272	ALA

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	323/352 (92%)	313 (97%)	10 (3%)	40	49
1	B	316/352 (90%)	311 (98%)	5 (2%)	62	73
1	C	319/352 (91%)	312 (98%)	7 (2%)	52	61
All	All	958/1056 (91%)	936 (98%)	22 (2%)	50	59

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	69	VAL
1	A	126	ILE
1	A	138	ASP
1	A	197	TRP
1	A	259	ASP
1	A	282	VAL
1	A	292	THR
1	A	311	ASP
1	A	317	ASP
1	B	73	GLN
1	B	197	TRP
1	B	282	VAL
1	B	297	ARG
1	B	378	ASP
1	C	92	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	197	TRP
1	C	254	THR
1	C	257	PHE
1	C	282	VAL
1	C	367	THR
1	C	380	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	53	GLN
1	A	111	ASN
1	A	362	HIS
1	B	28	ASN
1	B	73	GLN
1	B	111	ASN
1	B	266	GLN
1	C	28	ASN
1	C	53	GLN
1	C	92	ASN
1	C	111	ASN
1	C	181	HIS
1	C	278	ASN
1	C	385	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

4 ligands 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	EV0	B	441	-	10,11,11	3.26	6 (60%)	12,14,14	2.98	6 (50%)
2	EV0	A	441	-	10,11,11	3.23	5 (50%)	12,14,14	2.65	5 (41%)
3	GOL	C	441	-	5,5,5	0.40	0	5,5,5	0.47	0
2	EV0	B	442	-	10,11,11	3.25	4 (40%)	12,14,14	2.87	6 (50%)

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	EV0	B	441	-	-	2/3/3/3	0/1/1/1
2	EV0	A	441	-	-	0/3/3/3	0/1/1/1
3	GOL	C	441	-	-	2/4/4/4	-
2	EV0	B	442	-	-	2/3/3/3	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	442	EV0	C2-N4	8.55	1.49	1.34
2	B	441	EV0	C2-N4	8.38	1.48	1.34
2	A	441	EV0	C2-N4	8.19	1.48	1.34
2	B	441	EV0	C3-N5	3.48	1.39	1.33
2	A	441	EV0	C3-N5	3.41	1.39	1.33
2	B	442	EV0	C3-N5	3.15	1.38	1.33
2	A	441	EV0	C1-C2	-2.90	1.34	1.39
2	B	442	EV0	C1-C2	-2.65	1.35	1.39
2	A	441	EV0	C6-N4	-2.54	1.30	1.35
2	B	441	EV0	C6-N4	-2.44	1.31	1.35
2	B	441	EV0	C1-C2	-2.38	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	442	EV0	C6-N4	-2.28	1.31	1.35
2	B	441	EV0	C6-N5	2.21	1.39	1.35
2	B	441	EV0	C6-N7	2.20	1.38	1.33
2	A	441	EV0	C6-N5	2.16	1.39	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	442	EV0	C6-N4-C2	5.70	122.00	117.07
2	B	441	EV0	C6-N4-C2	5.31	121.67	117.07
2	B	441	EV0	C3-N5-C6	4.80	121.35	115.67
2	A	441	EV0	C6-N4-C2	4.54	121.00	117.07
2	A	441	EV0	C3-N5-C6	4.47	120.97	115.67
2	B	441	EV0	C1-C3-N5	-4.42	118.92	124.08
2	B	442	EV0	C1-C2-N4	-4.37	118.27	122.90
2	A	441	EV0	C1-C3-N5	-4.06	119.34	124.08
2	B	442	EV0	C3-N5-C6	3.97	120.37	115.67
2	B	441	EV0	C1-C2-N4	-3.78	118.90	122.90
2	B	442	EV0	C1-C3-N5	-3.38	120.14	124.08
2	B	441	EV0	N5-C6-N4	-3.14	120.50	125.42
2	A	441	EV0	N5-C6-N4	-2.95	120.80	125.42
2	B	442	EV0	N5-C6-N4	-2.88	120.90	125.42
2	A	441	EV0	C1-C2-N4	-2.84	119.89	122.90
2	B	441	EV0	C8-C2-N4	2.45	119.60	115.95
2	B	442	EV0	N7-C6-N4	2.24	120.74	117.25

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	441	GOL	C1-C2-C3-O3
3	C	441	GOL	O2-C2-C3-O3
2	B	442	EV0	C1-C2-C8-C9
2	B	441	EV0	N4-C2-C8-C9
2	B	442	EV0	N4-C2-C8-C9
2	B	441	EV0	C1-C2-C8-C9

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	441	EV0	1	0
3	C	441	GOL	1	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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.