



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:15 pm GMT

PDB ID : 2A91
Title : Crystal structure of ErbB2 domains 1-3
Authors : Garrett, T.P.J.; McKern, N.M.; Lou, M.; Elleman, T.C.; Adams, T.E.;
Lovrecz, G.O.; Kofler, M.; Jorissen, R.N.; Nice, E.C.; Burgess, A.W.
Deposited on : 2005-07-11
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

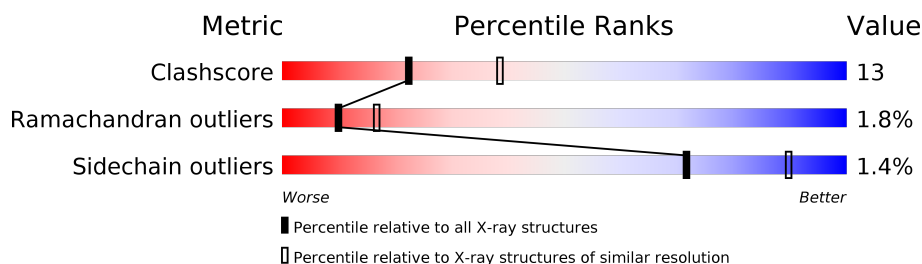
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	517	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4042 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 Receptor tyrosine-protein kinase erbB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	506	3852	2399	686	728	39	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	LYS	ARG	CONFLICT	UNP P04626
A	496	LYS	ARG	CONFLICT	UNP P04626
A	510	ASP	-	TAG	UNP P04626
A	511	TYR	-	TAG	UNP P04626
A	512	LYS	-	TAG	UNP P04626
A	513	ASP	-	TAG	UNP P04626
A	514	ASP	-	TAG	UNP P04626
A	515	ASP	-	TAG	UNP P04626
A	516	ASP	-	TAG	UNP P04626
A	517	LYS	-	TAG	UNP P04626

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is water.

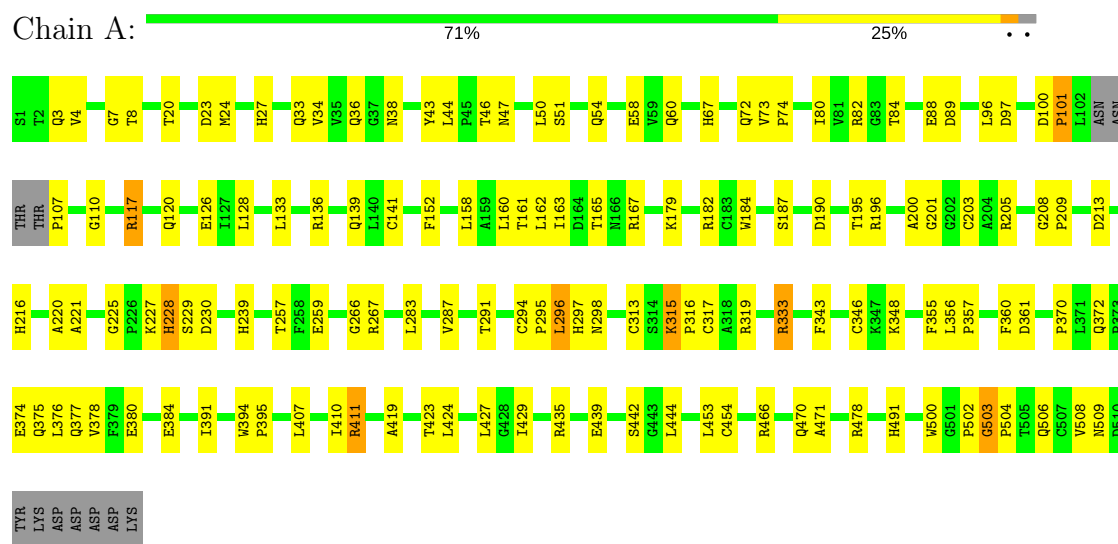
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	134	Total	O	0	0
			134	134		

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 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.

Note EDS was not executed.

- Molecule 1: Receptor tyrosine-protein kinase erbB-2



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	75.96Å 82.24Å 110.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50	Depositor
% Data completeness (in resolution range)	98.0 (25.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.226 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4042	wwPDB-VP
Average B, all atoms (Å ²)	56.0	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: 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	0.37	0/3938	0.66	1/5360 (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	107	PRO	N-CA-CB	5.50	109.90	103.30

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	3852	0	3672	98	0
2	A	28	0	26	1	0
3	A	28	0	25	1	0
4	A	134	0	0	6	0
All	All	4042	0	3723	99	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 13.

All (99) 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:315:LYS:HB2	1:A:316:PRO:HD3	1.42	0.98
1:A:100:ASP:HB2	1:A:101:PRO:HD3	1.48	0.95
1:A:60:GLN:HE21	1:A:84:THR:HB	1.42	0.84
1:A:225:GLY:H	1:A:230:ASP:HB3	1.47	0.80
1:A:187:SER:HB3	1:A:190:ASP:OD2	1.83	0.77
1:A:160:LEU:HD23	1:A:161:THR:N	2.03	0.74
1:A:491:HIS:CD2	1:A:504:PRO:HG3	2.24	0.73
1:A:503:GLY:HA3	4:A:663:HOH:O	1.87	0.73
1:A:297:HIS:O	1:A:313:CYS:HB3	1.90	0.71
1:A:47:ASN:HB2	2:A:911:NAG:H82	1.76	0.66
1:A:203:CYS:HB2	4:A:718:HOH:O	1.96	0.66
1:A:266:GLY:O	1:A:267:ARG:HD3	1.96	0.66
1:A:377:GLN:O	1:A:380:GLU:HG3	1.97	0.65
1:A:141:CYS:HA	1:A:167:ARG:HE	1.62	0.65
1:A:73:VAL:O	1:A:73:VAL:HG23	1.95	0.64
1:A:454:CYS:SG	1:A:478:ARG:HD3	2.41	0.60
1:A:429:ILE:HG13	1:A:453:LEU:HD13	1.82	0.60
1:A:117:ARG:HA	1:A:139:GLN:O	2.02	0.58
1:A:375:GLN:O	1:A:378:VAL:HG23	2.03	0.58
1:A:444:LEU:HD23	1:A:471:ALA:N	2.20	0.57
1:A:444:LEU:HD23	1:A:471:ALA:H	1.69	0.57
1:A:4:VAL:HG22	1:A:34:VAL:HB	1.87	0.57
1:A:8:THR:HG22	1:A:419:ALA:HB2	1.87	0.56
1:A:315:LYS:HB2	1:A:316:PRO:CD	2.27	0.56
1:A:267:ARG:HG3	1:A:267:ARG:HH11	1.70	0.56
1:A:313:CYS:O	1:A:317:CYS:HB2	2.06	0.56
1:A:384:GLU:OE2	1:A:411:ARG:NE	2.38	0.55
1:A:44:LEU:HD13	1:A:50:LEU:HD21	1.87	0.55
1:A:506:GLN:HA	1:A:506:GLN:HE21	1.70	0.55
1:A:82:ARG:HG2	1:A:128:LEU:HD12	1.89	0.55
1:A:361:ASP:O	1:A:370:PRO:HG3	2.06	0.55
1:A:356:LEU:HB3	1:A:357:PRO:HD2	1.89	0.54
1:A:315:LYS:CB	1:A:316:PRO:HD3	2.26	0.54
1:A:216:HIS:CD2	1:A:228:HIS:HB3	2.42	0.54
1:A:58:GLU:HB3	1:A:80:ILE:HG23	1.91	0.54
1:A:51:SER:O	1:A:54:GLN:HG2	2.08	0.53
1:A:100:ASP:CB	1:A:101:PRO:HD3	2.31	0.53
1:A:60:GLN:HE21	1:A:84:THR:CB	2.17	0.53
1:A:24:MET:HG2	1:A:444:LEU:HD13	1.90	0.52
1:A:360:PHE:O	1:A:370:PRO:HB3	2.10	0.52
1:A:333:ARG:HD3	1:A:333:ARG:H	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ARG:HG3	1:A:267:ARG:NH1	2.26	0.51
1:A:423:THR:O	1:A:424:LEU:HD23	2.10	0.51
1:A:355:PHE:C	1:A:356:LEU:HD12	2.31	0.51
1:A:508:VAL:HG12	1:A:509:ASN:N	2.26	0.50
1:A:126:GLU:HB2	1:A:221:ALA:HA	1.92	0.50
1:A:200:ALA:HB2	1:A:209:PRO:O	2.12	0.50
1:A:225:GLY:H	1:A:230:ASP:CB	2.22	0.50
1:A:165:THR:O	1:A:167:ARG:HG3	2.12	0.49
1:A:43:TYR:HA	1:A:67:HIS:O	2.12	0.49
1:A:257:THR:HG21	1:A:259:GLU:OE1	2.11	0.49
1:A:20:THR:HG22	4:A:721:HOH:O	2.13	0.49
1:A:208:GLY:N	1:A:213:ASP:HB3	2.27	0.49
1:A:333:ARG:CD	1:A:333:ARG:H	2.26	0.48
1:A:161:THR:HG23	1:A:163:ILE:HG13	1.95	0.48
1:A:506:GLN:HA	1:A:506:GLN:NE2	2.28	0.48
1:A:72:GLN:HE22	1:A:120:GLN:HB2	1.78	0.48
1:A:343:PHE:HA	1:A:346:CYS:SG	2.54	0.48
1:A:372:GLN:HB2	1:A:375:GLN:HG3	1.96	0.47
1:A:36:GLN:NE2	4:A:660:HOH:O	2.44	0.47
1:A:200:ALA:O	1:A:201:GLY:C	2.53	0.47
1:A:283:LEU:HB2	1:A:291:THR:O	2.15	0.47
1:A:161:THR:CG2	1:A:163:ILE:HG13	2.45	0.46
1:A:394:TRP:CG	1:A:395:PRO:HD2	2.50	0.46
1:A:435:ARG:HA	1:A:500:TRP:CD1	2.51	0.46
1:A:72:GLN:NE2	1:A:120:GLN:NE2	2.65	0.45
1:A:506:GLN:CA	1:A:506:GLN:HE21	2.28	0.45
1:A:374:GLU:O	1:A:377:GLN:HG2	2.17	0.45
1:A:439:GLU:HB2	1:A:466:ARG:NH2	2.32	0.45
1:A:227:LYS:C	1:A:229:SER:H	2.19	0.45
1:A:356:LEU:HD12	1:A:356:LEU:N	2.32	0.45
1:A:7:GLY:HA3	1:A:38:ASN:O	2.17	0.45
1:A:195:THR:O	1:A:205:ARG:HA	2.16	0.44
1:A:158:LEU:O	1:A:160:LEU:N	2.48	0.44
1:A:333:ARG:HG3	1:A:333:ARG:HH11	1.81	0.44
1:A:182:ARG:HG2	1:A:182:ARG:HH11	1.82	0.43
1:A:88:GLU:O	1:A:89:ASP:HB2	2.18	0.43
1:A:295:PRO:O	1:A:296:LEU:C	2.55	0.43
1:A:97:ASP:HA	1:A:136:ARG:O	2.19	0.43
1:A:333:ARG:HG3	1:A:333:ARG:NH1	2.33	0.43
1:A:294:CYS:HB3	1:A:295:PRO:CD	2.49	0.42
1:A:239:HIS:HD2	4:A:602:HOH:O	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PHE:O	1:A:196:ARG:NH1	2.45	0.42
1:A:407:LEU:HD21	1:A:410:ILE:HD11	2.02	0.42
1:A:184:TRP:HA	4:A:664:HOH:O	2.20	0.41
1:A:295:PRO:HD2	1:A:298:ASN:HB2	2.02	0.41
1:A:356:LEU:HB3	1:A:357:PRO:CD	2.49	0.41
1:A:3:GLN:HB2	1:A:33:GLN:HE21	1.85	0.41
1:A:220:ALA:O	1:A:221:ALA:HB3	2.21	0.41
1:A:348:LYS:HE3	1:A:384:GLU:OE2	2.21	0.41
1:A:391:ILE:HG22	1:A:427:LEU:HD21	2.02	0.41
1:A:376:LEU:C	1:A:378:VAL:H	2.22	0.41
1:A:23:ASP:O	1:A:27:HIS:HD2	2.04	0.41
1:A:442:SER:HA	1:A:470:GLN:NE2	2.35	0.40
1:A:225:GLY:N	1:A:230:ASP:HB3	2.25	0.40
1:A:96:LEU:HD21	1:A:133:LEU:HG	2.02	0.40
1:A:84:THR:HG22	1:A:84:THR:O	2.21	0.40
1:A:162:LEU:HA	1:A:162:LEU:HD23	1.88	0.40
3:A:951:NAG:H62	3:A:952:NAG:N2	2.37	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	502/517 (97%)	451 (90%)	42 (8%)	9 (2%)	10 17

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	LYS
1	A	296	LEU
1	A	110	GLY
1	A	503	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	101	PRO
1	A	502	PRO
1	A	315	LYS
1	A	287	VAL
1	A	74	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	421/445 (95%)	415 (99%)	6 (1%)	71 90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	THR
1	A	117	ARG
1	A	228	HIS
1	A	319	ARG
1	A	333	ARG
1	A	411	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	33	GLN
1	A	60	GLN
1	A	120	GLN
1	A	228	HIS
1	A	372	GLN
1	A	377	GLN
1	A	506	GLN

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 ⓘ

2 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	$\# Z > 2$
3	NAG	A	951	1,3	14,14,15	0.58	0	15,19,21	0.77	1 (6%)
3	NAG	A	952	3	14,14,15	0.52	0	15,19,21	0.78	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
3	NAG	A	951	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	952	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	951	NAG	C2-N2-C7	-2.21	119.72	122.94
3	A	952	NAG	C2-N2-C7	-2.16	119.80	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	951	NAG	1	0
3	A	952	NAG	1	0

5.6 Ligand geometry

2 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	NAG	A	911	1	14,14,15	0.70	0	15,19,21	0.63	0
2	NAG	A	941	1	14,14,15	0.58	0	15,19,21	0.73	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	911	1	-	0/6/23/26	0/1/1/1
2	NAG	A	941	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	941	NAG	C2-N2-C7	-2.06	119.94	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	911	NAG	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

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.