



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:40 AM GMT

PDB ID : 2I69
Title : Crystal structure of the West Nile virus envelope glycoprotein
Authors : Kanai, R.; Modis, Y.
Deposited on : 2006-08-28
Resolution : 3.11 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

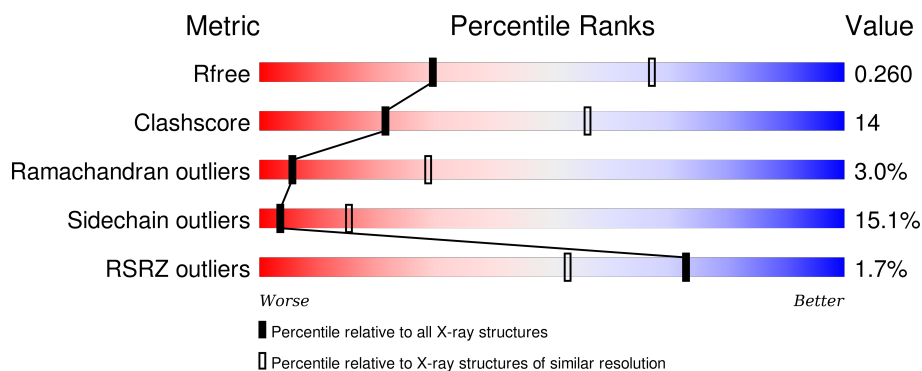
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

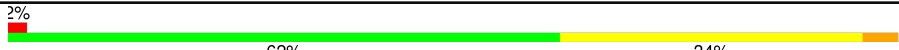
The reported resolution of this entry is 3.11 Å.

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}	91344	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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.

Mol	Chain	Length	Quality of chain
1	A	403	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3095 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 Polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3043	1914	522	585	22			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			38	22	2	14		

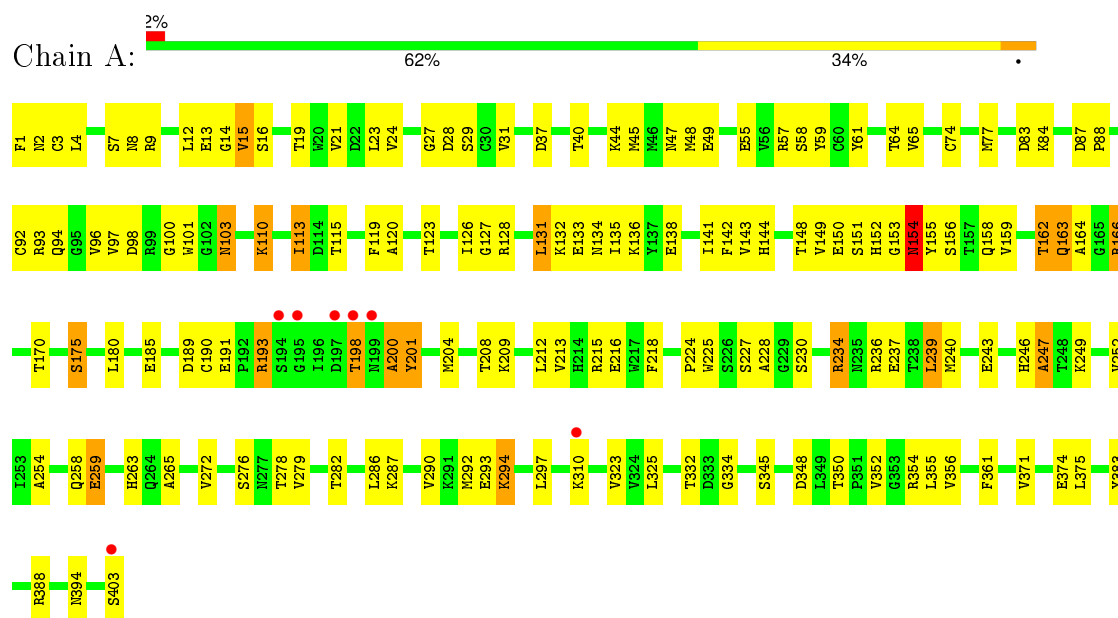
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		

3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: Polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.26 Å 93.26 Å 159.32 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.06 – 3.11 23.70 – 3.11	Depositor EDS
% Data completeness (in resolution range)	94.8 (24.06-3.11) 94.5 (23.70-3.11)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.10 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.268 0.204 , 0.260	Depositor DCC
R_{free} test set	618 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	138.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 101.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 12476 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3095	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: FUL, 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	0.69	1/3108 (0.0%)	0.81	1/4217 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	GLU	CD-OE2	5.42	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	ASP	CB-CG-OD2	5.27	123.04	118.30

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	3043	0	2991	85	0
2	A	38	0	34	3	0
3	A	14	0	0	4	0
All	All	3095	0	3025	86	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 14.

All (86) 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:162:THR:HA	3:A:1161:HOH:O	1.45	1.14
1:A:246:HIS:HB3	1:A:249:LYS:O	1.74	0.88
1:A:12:LEU:HD12	1:A:31:VAL:HG11	1.71	0.73
1:A:132:LYS:HG3	1:A:198:THR:HG23	1.73	0.70
1:A:40:THR:HG22	1:A:144:HIS:CD2	2.27	0.70
1:A:14:GLY:HA2	1:A:21:VAL:HG22	1.78	0.65
1:A:1:PHE:HE2	1:A:153:GLY:O	1.81	0.63
1:A:148:THR:HG22	1:A:150:GLU:N	2.14	0.63
1:A:47:ASN:ND2	1:A:49:GLU:HG3	2.14	0.62
1:A:126:ILE:O	1:A:204:MET:HA	2.00	0.61
1:A:12:LEU:HD12	1:A:31:VAL:CG1	2.31	0.61
1:A:74:CYS:HB2	1:A:77:MET:HG3	1.82	0.60
1:A:191:GLU:HG3	1:A:193:ARG:CZ	2.33	0.59
1:A:2:ASN:ND2	1:A:152:HIS:O	2.37	0.58
1:A:15:VAL:O	1:A:16:SER:C	2.44	0.56
1:A:136:LYS:HA	1:A:170:THR:HG22	1.88	0.55
1:A:127:GLY:HA3	1:A:218:PHE:CZ	2.42	0.54
1:A:55:GLU:HA	1:A:128:ARG:HG2	1.89	0.54
1:A:97:VAL:HG12	1:A:98:ASP:O	2.08	0.53
1:A:272:VAL:CG1	1:A:279:VAL:HG23	2.38	0.53
1:A:325:LEU:C	1:A:325:LEU:HD12	2.28	0.53
1:A:272:VAL:HG11	1:A:279:VAL:HG23	1.90	0.53
1:A:23:LEU:HD21	1:A:290:VAL:CG2	2.40	0.52
1:A:65:VAL:HG22	1:A:240:MET:HE2	1.93	0.51
1:A:200:ALA:O	1:A:215:ARG:HB2	2.11	0.51
1:A:44:LYS:HG2	1:A:45:MET:N	2.23	0.51
1:A:143:VAL:CG2	1:A:180:LEU:HD13	2.41	0.51
1:A:383:TYR:HD1	1:A:394:ASN:HD22	1.59	0.51
1:A:65:VAL:HG11	1:A:252:VAL:HG12	1.93	0.50
1:A:224:PRO:CD	1:A:239:LEU:HD12	2.42	0.50
1:A:201:TYR:HA	1:A:215:ARG:HB2	1.92	0.49
1:A:375:LEU:C	1:A:375:LEU:HD12	2.33	0.49
1:A:65:VAL:HG22	1:A:240:MET:CE	2.42	0.49
1:A:259:GLU:HG2	1:A:263:HIS:CE1	2.47	0.48
1:A:23:LEU:HD23	1:A:23:LEU:N	2.28	0.48
1:A:97:VAL:HG21	1:A:113:ILE:HD13	1.95	0.48
1:A:47:ASN:HD21	1:A:49:GLU:HG3	1.78	0.48
1:A:65:VAL:HG23	1:A:254:ALA:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLN:HE21	1:A:163:GLN:HB3	1.79	0.48
1:A:154:ASN:OD1	2:A:1154:NAG:C2	2.60	0.47
1:A:138:GLU:CD	1:A:166:ARG:HH11	2.17	0.47
1:A:154:ASN:OD1	2:A:1154:NAG:H2	2.13	0.47
1:A:138:GLU:OE2	1:A:166:ARG:NH1	2.48	0.47
1:A:113:ILE:HD11	1:A:247:ALA:O	2.15	0.47
1:A:131:LEU:HD12	1:A:134:ASN:OD1	2.15	0.47
1:A:100:GLY:N	1:A:103:ASN:HD21	2.13	0.46
1:A:61:TYR:HB2	1:A:258:GLN:HB2	1.98	0.46
1:A:356:VAL:HB	1:A:374:GLU:HG2	1.98	0.46
1:A:131:LEU:H	1:A:131:LEU:HD12	1.79	0.46
1:A:185:GLU:HG2	1:A:294:LYS:HB3	1.98	0.46
1:A:191:GLU:HG2	1:A:191:GLU:O	2.15	0.45
1:A:23:LEU:HD21	1:A:290:VAL:HG23	1.97	0.45
1:A:94:GLN:HE21	1:A:94:GLN:HB3	1.57	0.45
1:A:148:THR:CG2	1:A:149:VAL:N	2.78	0.45
1:A:272:VAL:HG11	1:A:279:VAL:CG2	2.47	0.45
1:A:162:THR:HG23	3:A:1161:HOH:O	2.16	0.45
1:A:175:SER:OG	1:A:189:ASP:OD2	2.34	0.45
1:A:155:TYR:O	1:A:159:VAL:HG23	2.17	0.45
1:A:158:GLN:HB3	1:A:164:ALA:HB2	1.98	0.44
2:A:1154:NAG:H61	2:A:1155:NAG:O5	2.17	0.44
1:A:276:SER:O	1:A:278:THR:HG23	2.18	0.44
1:A:3:CYS:HB3	1:A:9:ARG:NE	2.32	0.44
1:A:64:THR:HB	1:A:120:ALA:HB3	2.00	0.44
1:A:100:GLY:H	1:A:103:ASN:HD21	1.66	0.44
1:A:27:GLY:O	1:A:28:ASP:C	2.57	0.43
1:A:21:VAL:HG23	1:A:292:MET:HE1	2.00	0.43
1:A:92:CYS:HA	1:A:115:THR:O	2.18	0.43
1:A:37:ASP:O	1:A:297:LEU:HD22	2.18	0.43
1:A:141:ILE:HG22	1:A:142:PHE:N	2.34	0.43
1:A:55:GLU:HG3	1:A:126:ILE:CG2	2.50	0.42
1:A:24:VAL:HA	1:A:286:LEU:O	2.19	0.42
1:A:190:CYS:N	3:A:1158:HOH:O	2.53	0.42
1:A:141:ILE:CG2	1:A:142:PHE:N	2.83	0.41
1:A:87:ASP:HA	1:A:88:PRO:HD2	1.96	0.41
1:A:96:VAL:HG13	1:A:110:LYS:HB3	2.02	0.41
1:A:2:ASN:N	1:A:44:LYS:HE3	2.35	0.41
1:A:143:VAL:HG23	1:A:180:LEU:HD13	2.03	0.41
1:A:375:LEU:O	1:A:375:LEU:HD12	2.21	0.41
1:A:234:ARG:HE	1:A:234:ARG:HB2	1.31	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LEU:HA	1:A:297:LEU:HD12	1.85	0.41
1:A:230:SER:HB3	3:A:1166:HOH:O	2.20	0.41
1:A:3:CYS:O	1:A:4:LEU:C	2.60	0.40
1:A:61:TYR:CE1	1:A:259:GLU:HG3	2.56	0.40
1:A:59:TYR:CD1	1:A:225:TRP:HB3	2.56	0.40
1:A:133:GLU:HG3	1:A:133:GLU:H	1.60	0.40
1:A:119:PHE:CD1	1:A:119:PHE:C	2.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	401/403 (100%)	357 (89%)	32 (8%)	12 (3%)	5 29

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	200	ALA
1	A	228	ALA
1	A	237	GLU
1	A	84	LYS
1	A	154	ASN
1	A	101	TRP
1	A	193	ARG
1	A	247	ALA
1	A	265	ALA
1	A	15	VAL
1	A	334	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	332/333 (100%)	282 (85%)	50 (15%)	3 15

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	8	ASN
1	A	13	GLU
1	A	19	THR
1	A	29	SER
1	A	48	MET
1	A	57	ARG
1	A	83	ASP
1	A	93	ARG
1	A	103	ASN
1	A	110	LYS
1	A	113	ILE
1	A	123	THR
1	A	131	LEU
1	A	135	ILE
1	A	151	SER
1	A	154	ASN
1	A	156	SER
1	A	162	THR
1	A	163	GLN
1	A	166	ARG
1	A	175	SER
1	A	198	THR
1	A	201	TYR
1	A	208	THR
1	A	209	LYS
1	A	212	LEU
1	A	213	VAL
1	A	216	GLU
1	A	227	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	234	ARG
1	A	236	ARG
1	A	239	LEU
1	A	243	GLU
1	A	282	THR
1	A	287	LYS
1	A	293	GLU
1	A	294	LYS
1	A	310	LYS
1	A	323	VAL
1	A	332	THR
1	A	345	SER
1	A	350	THR
1	A	352	VAL
1	A	354	ARG
1	A	355	LEU
1	A	361	PHE
1	A	371	VAL
1	A	388	ARG
1	A	403	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	94	GLN
1	A	103	ASN
1	A	158	GLN
1	A	163	GLN
1	A	264	GLN
1	A	394	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 ⓘ

3 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$
2	NAG	A	1154	1,2	14,14,15	0.48	0	15,19,21	1.44	3 (20%)
2	NAG	A	1155	2	14,14,15	0.62	0	15,19,21	1.68	3 (20%)
2	FUL	A	1156	2	10,10,11	0.82	0	14,14,16	1.47	4 (28%)

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	1154	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1155	2	-	0/6/23/26	0/1/1/1
2	FUL	A	1156	2	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1156	FUL	O5-C1-C2	-2.09	107.47	110.86
2	A	1155	NAG	O3-C3-C4	-2.08	105.65	110.34
2	A	1156	FUL	O4-C4-C5	2.03	114.59	109.84
2	A	1154	NAG	O5-C5-C6	2.25	112.23	107.35
2	A	1154	NAG	C3-C4-C5	2.29	114.18	110.20
2	A	1156	FUL	O5-C5-C6	2.29	109.91	106.13
2	A	1156	FUL	C1-C2-C3	2.73	112.77	109.54
2	A	1155	NAG	C3-C4-C5	2.85	115.17	110.20
2	A	1154	NAG	C4-C3-C2	3.19	116.19	111.23
2	A	1155	NAG	C4-C3-C2	4.66	118.47	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1154	NAG	3	0
2	A	1155	NAG	1	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	403/403 (100%)	-0.17	7 (1%) 73 53	88, 117, 137, 173	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	THR	4.2
1	A	199	ASN	3.5
1	A	195	GLY	3.5
1	A	310	LYS	2.4
1	A	403	SER	2.4
1	A	194	SER	2.2
1	A	197	ASP	2.0

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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	1155	14/15	0.87	0.55	-	190,196,205,206	0
2	FUL	A	1156	10/11	0.94	0.34	-	175,179,181,181	0
2	NAG	A	1154	14/15	0.93	0.31	-	165,171,178,188	0

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.