



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:55 PM GMT

PDB ID : 1VSG  
Title : 2.9 ANGSTROMS RESOLUTION STRUCTURE OF THE N-TERMINAL  
DOMAIN OF A VARIANT SURFACE GLYCOPROTEIN FROM TRY-  
PANOSOMA BRUCEI  
Authors : Freymann, D.; Down, J.; Wiley, D.C.  
Deposited on : 1990-10-22  
Resolution : 2.90 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](mailto: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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

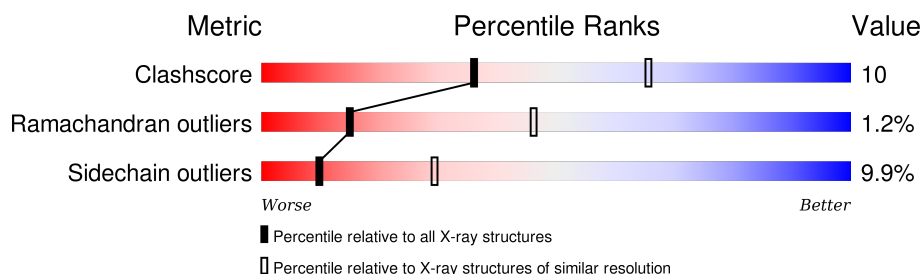
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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  $\geq 3$ , 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	364	
1	B	364	

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
3	MAN	B	368	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5508 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 VARIANT SURFACE GLYCOPROTEIN MITAT 1.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2706	1684	472	540	10			
1	B	362	Total	C	N	O	S	0	0	0
			2706	1684	472	540	10			

- 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
			39	22	2	15		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is water.

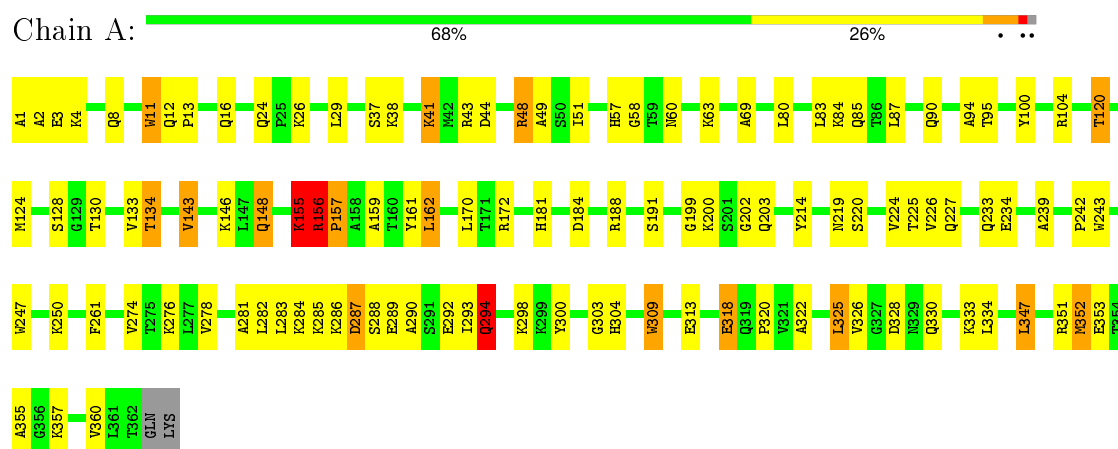
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	10	Total	O	0	0
			10	10		

### 3 Residue-property plots

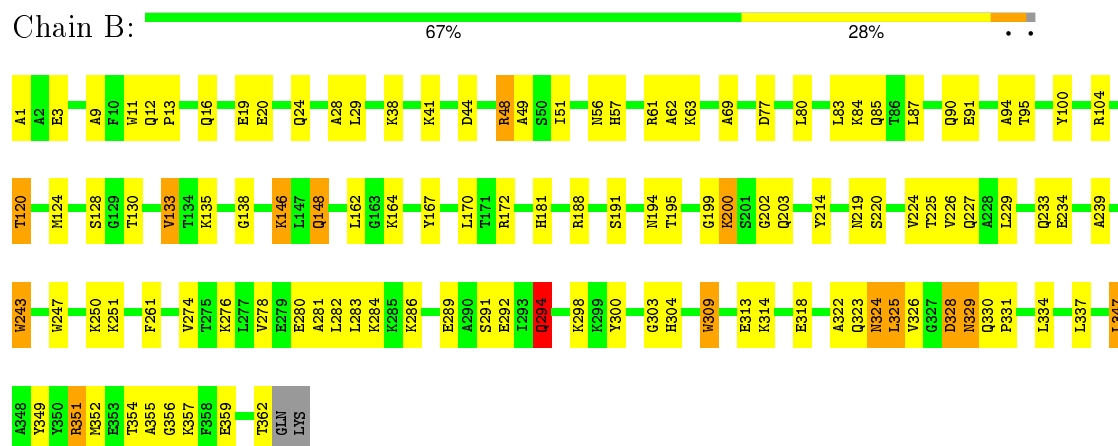
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: VARIANT SURFACE GLYCOPROTEIN MITAT 1.2



#### • Molecule 1: VARIANT SURFACE GLYCOPROTEIN MITAT 1.2



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.50Å 97.50Å 123.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5508	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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: BMA, NAG, MAN

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	0.87	1/2745 (0.0%)	1.44	30/3713 (0.8%)
1	B	0.86	1/2745 (0.0%)	1.41	28/3713 (0.8%)
All	All	0.87	2/5490 (0.0%)	1.42	58/7426 (0.8%)

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
3	B	1	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	19	GLU	C-O	5.76	1.34	1.23
1	A	143	VAL	CA-CB	5.08	1.65	1.54

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ARG	NE-CZ-NH1	-10.88	114.86	120.30
1	B	11	TRP	CD1-CG-CD2	9.41	113.83	106.30
1	A	48	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	B	48	ARG	NE-CZ-NH1	-9.23	115.68	120.30
1	A	11	TRP	CD1-CG-CD2	9.22	113.68	106.30
1	B	20	GLU	O-C-N	8.66	136.56	122.70
1	B	11	TRP	CE2-CD2-CG	-8.21	100.73	107.30
1	A	11	TRP	CE2-CD2-CG	-8.14	100.79	107.30
1	B	100	TYR	CB-CG-CD2	-8.08	116.15	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	TRP	CD1-CG-CD2	7.94	112.65	106.30
1	A	100	TYR	CB-CG-CD2	-7.85	116.29	121.00
1	A	309	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	A	243	TRP	CD1-CG-CD2	7.57	112.35	106.30
1	A	309	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	A	156	ARG	NE-CZ-NH2	7.47	124.03	120.30
1	B	48	ARG	NE-CZ-NH2	7.43	124.01	120.30
1	B	324	ASN	CA-CB-CG	7.13	129.09	113.40
1	B	309	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	A	243	TRP	CE2-CD2-CG	-6.90	101.78	107.30
1	B	243	TRP	CD1-CG-CD2	6.76	111.71	106.30
1	B	247	TRP	CE2-CD2-CG	-6.74	101.91	107.30
1	B	309	TRP	CG-CD2-CE3	6.71	139.94	133.90
1	A	247	TRP	CE2-CD2-CG	-6.67	101.97	107.30
1	B	234	GLU	CA-CB-CG	6.44	127.57	113.40
1	A	234	GLU	CA-CB-CG	6.43	127.55	113.40
1	B	294	GLN	CA-CB-CG	6.38	127.44	113.40
1	A	294	GLN	CA-CB-CG	6.34	127.36	113.40
1	B	243	TRP	CE2-CD2-CG	-6.31	102.25	107.30
1	A	11	TRP	CG-CD1-NE1	-6.24	103.86	110.10
1	B	104	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	A	134	THR	CA-CB-CG2	-6.19	103.73	112.40
1	B	11	TRP	CG-CD1-NE1	-6.14	103.96	110.10
1	B	300	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	A	11	TRP	CB-CG-CD1	-6.04	119.15	127.00
1	A	11	TRP	CG-CD2-CE3	6.04	139.33	133.90
1	A	170	LEU	CA-C-N	-5.86	104.31	117.20
1	A	43	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	309	TRP	CB-CG-CD1	-5.75	119.53	127.00
1	A	247	TRP	CD1-CG-CD2	5.74	110.89	106.30
1	A	243	TRP	CG-CD1-NE1	-5.70	104.40	110.10
1	B	11	TRP	CG-CD2-CE3	5.64	138.97	133.90
1	A	309	TRP	CG-CD2-CE3	5.63	138.96	133.90
1	B	172	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	B	11	TRP	CB-CG-CD1	-5.55	119.79	127.00
1	B	9	ALA	O-C-N	5.52	131.53	122.70
1	B	247	TRP	CD1-CG-CD2	5.34	110.58	106.30
1	B	77	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	351	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	A	170	LEU	CA-C-O	5.32	131.27	120.10
1	A	360	VAL	CA-CB-CG1	5.31	118.87	110.90
1	A	161	TYR	CB-CG-CD2	-5.28	117.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	155	LYS	CA-CB-CG	5.23	124.91	113.40
1	A	172	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	A	172	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	B	57	HIS	CB-CA-C	-5.06	100.28	110.40
1	B	95	THR	CA-CB-CG2	5.02	119.43	112.40
1	A	95	THR	CA-CB-CG2	5.02	119.42	112.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	368	MAN	C1

There are no planarity outliers.

## 5.2 Too-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 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	2706	0	2702	56	0
1	B	2706	0	2702	56	0
2	A	39	0	34	1	0
3	B	39	0	34	1	0
4	A	8	0	0	0	0
4	B	10	0	0	0	0
All	All	5508	0	5472	105	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 10.

All (105) 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:322:ALA:HB3	1:A:325:LEU:HD22	1.53	0.89
1:B:322:ALA:HB3	1:B:325:LEU:HD22	1.62	0.82
1:A:2:ALA:O	1:A:4:LYS:HG2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:LEU:HD13	1:B:250:LYS:HD3	1.74	0.69
1:A:326:VAL:HG13	1:A:330:GLN:HB2	1.75	0.68
1:A:159:ALA:HB1	1:A:162:LEU:O	1.96	0.65
1:A:3:GLU:HG2	1:A:191:SER:OG	1.97	0.65
1:A:289:GLU:O	1:A:292:GLU:HG2	1.97	0.64
1:B:356:GLY:O	1:B:359:GLU:HG2	1.98	0.64
1:A:352:MET:SD	1:B:63:LYS:HG2	2.38	0.64
1:A:1:ALA:O	1:A:181:HIS:HB3	1.99	0.62
1:A:3:GLU:HG2	1:A:191:SER:CB	2.29	0.62
1:B:146:LYS:O	1:B:148:GLN:HG3	1.98	0.62
1:B:331:PRO:O	1:B:337:LEU:HD21	2.00	0.61
1:B:38:LYS:HD2	1:B:261:PHE:HB3	1.82	0.61
1:A:3:GLU:HG2	1:A:191:SER:HB3	1.83	0.59
1:A:38:LYS:HD2	1:A:261:PHE:HB3	1.83	0.59
1:B:56:ASN:O	1:B:62:ALA:HB2	2.04	0.58
1:B:289:GLU:O	1:B:292:GLU:HG2	2.05	0.56
1:B:138:GLY:HA3	1:B:146:LYS:HD2	1.85	0.56
1:B:48:ARG:HD3	1:B:334:LEU:O	2.05	0.56
1:A:309:TRP:O	1:A:313:GLU:HG3	2.08	0.54
1:B:309:TRP:O	1:B:313:GLU:HG3	2.08	0.54
1:A:347:LEU:O	1:A:351:ARG:HG3	2.08	0.54
1:B:314:LYS:O	1:B:318:GLU:HG2	2.06	0.54
1:A:188:ARG:NH2	1:B:200:LYS:HA	2.23	0.54
1:B:120:THR:HG22	1:B:130:THR:O	2.09	0.53
1:A:48:ARG:HD3	1:A:334:LEU:O	2.08	0.52
1:A:200:LYS:HA	1:B:188:ARG:NH2	2.24	0.52
1:A:352:MET:O	1:A:355:ALA:HB3	2.11	0.51
1:A:155:LYS:HD2	1:A:157:PRO:HB3	1.91	0.51
1:A:41:LYS:HB2	2:A:366:NAG:H83	1.92	0.51
1:B:325:LEU:HD21	1:B:349:TYR:CD1	2.45	0.51
1:B:278:VAL:HG22	1:B:282:LEU:HD12	1.91	0.51
1:A:278:VAL:HG22	1:A:282:LEU:HD12	1.92	0.51
1:B:84:LYS:HE3	1:B:85:GLN:HE21	1.76	0.50
1:A:203:GLN:HB2	1:A:219:ASN:HB2	1.93	0.50
1:A:120:THR:HG22	1:A:130:THR:O	2.12	0.50
1:A:146:LYS:O	1:A:148:GLN:HG3	2.10	0.50
1:B:281:ALA:O	1:B:284:LYS:HG2	2.13	0.49
1:B:162:LEU:HG	1:B:167:TYR:CE1	2.48	0.49
1:B:44:ASP:HB3	1:B:48:ARG:NH1	2.27	0.49
1:B:203:GLN:HB2	1:B:219:ASN:HB2	1.95	0.49
1:B:347:LEU:O	1:B:351:ARG:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LYS:HD3	1:A:288:SER:OG	2.13	0.49
1:A:44:ASP:HB3	1:A:48:ARG:NH1	2.28	0.48
1:A:51:ILE:HG13	1:A:347:LEU:HG	1.96	0.48
1:A:188:ARG:HH21	1:B:200:LYS:HA	1.79	0.48
1:A:281:ALA:O	1:A:284:LYS:HG3	2.14	0.48
1:A:4:LYS:HE3	1:A:184:ASP:HA	1.96	0.48
1:B:3:GLU:HG2	1:B:191:SER:HB3	1.94	0.48
1:A:84:LYS:HE3	1:A:85:GLN:HE21	1.78	0.47
1:A:200:LYS:NZ	1:B:195:THR:O	2.47	0.47
1:B:1:ALA:O	1:B:181:HIS:HB3	2.14	0.47
1:A:12:GLN:O	1:A:16:GLN:HG3	2.15	0.47
1:B:181:HIS:NE2	1:B:224:VAL:HG22	2.29	0.46
1:B:51:ILE:HG13	1:B:347:LEU:HG	1.97	0.46
1:B:214:TYR:CE1	1:B:226:VAL:HB	2.50	0.46
1:A:353:GLU:O	1:A:357:LYS:HG2	2.16	0.46
1:A:156:ARG:HH21	1:A:156:ARG:H	1.64	0.46
1:B:294:GLN:HG2	1:B:304:HIS:CD2	2.50	0.46
1:B:298:LYS:HA	1:B:303:GLY:H	1.81	0.46
1:A:199:GLY:HA3	1:A:202:GLY:O	2.16	0.46
1:B:199:GLY:HA3	1:B:202:GLY:O	2.15	0.46
1:B:164:LYS:HE3	1:B:251:LYS:HZ2	1.80	0.46
1:A:330:GLN:HA	1:A:330:GLN:HE21	1.80	0.46
1:B:291:SER:O	1:B:294:GLN:HB3	2.16	0.46
1:B:325:LEU:HD11	1:B:349:TYR:CD2	2.50	0.45
1:A:294:GLN:HG2	1:A:304:HIS:CD2	2.50	0.45
1:A:162:LEU:HD13	1:A:250:LYS:HD3	1.99	0.45
1:A:318:GLU:O	1:A:333:LYS:HG2	2.17	0.45
1:B:326:VAL:O	1:B:330:GLN:HB2	2.17	0.45
1:A:200:LYS:HA	1:B:188:ARG:HH21	1.82	0.45
1:B:3:GLU:HG2	1:B:191:SER:CB	2.48	0.44
1:B:214:TYR:CZ	1:B:226:VAL:HB	2.53	0.44
1:A:298:LYS:HA	1:A:303:GLY:H	1.82	0.44
1:A:26:LYS:HD2	1:A:155:LYS:HG2	2.00	0.44
1:B:328:ASP:O	1:B:330:GLN:N	2.50	0.44
1:B:354:THR:HA	1:B:357:LYS:HD2	1.99	0.44
1:A:214:TYR:CE1	1:A:226:VAL:HB	2.53	0.43
1:B:41:LYS:HB2	3:B:366:NAG:H83	1.99	0.43
1:A:60:ASN:HB3	1:A:300:TYR:HD2	1.83	0.43
1:B:83:LEU:HA	1:B:87:LEU:HB2	1.99	0.43
1:A:124:MET:HB3	1:A:133:VAL:HG22	2.00	0.43
1:B:229:LEU:HD13	1:B:243:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HA	1:A:87:LEU:HB2	1.99	0.43
1:B:49:ALA:HB3	1:B:69:ALA:HB2	2.00	0.43
1:B:24:GLN:HE21	1:B:94:ALA:HB1	1.84	0.42
1:B:323:GLN:NE2	1:B:328:ASP:O	2.52	0.42
1:A:11:TRP:HZ2	1:A:133:VAL:HG11	1.85	0.42
1:B:24:GLN:NE2	1:B:94:ALA:HB1	2.34	0.42
1:B:12:GLN:O	1:B:16:GLN:HG3	2.18	0.42
1:A:286:LYS:O	1:A:287:ASP:HB2	2.20	0.42
1:B:124:MET:HB3	1:B:133:VAL:CG2	2.50	0.41
1:A:37:SER:O	1:A:41:LYS:HG3	2.20	0.41
1:B:28:ALA:HA	1:B:91:GLU:OE1	2.20	0.41
1:A:1:ALA:O	1:A:181:HIS:CB	2.67	0.41
1:A:290:ALA:HA	1:A:293:ILE:HG12	2.03	0.41
1:A:24:GLN:HE21	1:A:94:ALA:HB1	1.86	0.41
1:B:280:GLU:HB2	1:B:286:LYS:NZ	2.35	0.41
1:A:181:HIS:NE2	1:A:224:VAL:HG22	2.34	0.41
1:A:214:TYR:CZ	1:A:226:VAL:HB	2.55	0.41
1:A:49:ALA:HB3	1:A:69:ALA:HB2	2.02	0.40
1:B:194:ASN:HB3	1:B:202:GLY:O	2.21	0.40
1:A:58:GLY:HA2	1:B:355:ALA:O	2.22	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	360/364 (99%)	323 (90%)	32 (9%)	5 (1%)	14	44
1	B	360/364 (99%)	324 (90%)	32 (9%)	4 (1%)	17	51
All	All	720/728 (99%)	647 (90%)	64 (9%)	9 (1%)	15	46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	ASP
1	B	329	ASN
1	A	157	PRO
1	B	239	ALA
1	A	239	ALA
1	A	8	GLN
1	A	274	VAL
1	B	328	ASP
1	B	274	VAL

### 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	277/279 (99%)	248 (90%)	29 (10%)	8	25
1	B	277/279 (99%)	251 (91%)	26 (9%)	11	32
All	All	554/558 (99%)	499 (90%)	55 (10%)	10	29

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PRO
1	A	29	LEU
1	A	41	LYS
1	A	57	HIS
1	A	63	LYS
1	A	80	LEU
1	A	90	GLN
1	A	120	THR
1	A	128	SER
1	A	134	THR
1	A	143	VAL
1	A	148	GLN
1	A	155	LYS
1	A	156	ARG
1	A	162	LEU

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	220	SER
1	A	225	THR
1	A	227	GLN
1	A	233	GLN
1	A	242	PRO
1	A	276	LYS
1	A	283	LEU
1	A	294	GLN
1	A	318	GLU
1	A	320	PRO
1	A	325	LEU
1	A	328	ASP
1	A	347	LEU
1	A	352	MET
1	B	13	PRO
1	B	29	LEU
1	B	61	ARG
1	B	80	LEU
1	B	90	GLN
1	B	120	THR
1	B	128	SER
1	B	133	VAL
1	B	135	LYS
1	B	146	LYS
1	B	148	GLN
1	B	170	LEU
1	B	200	LYS
1	B	220	SER
1	B	225	THR
1	B	227	GLN
1	B	233	GLN
1	B	276	LYS
1	B	283	LEU
1	B	294	GLN
1	B	324	ASN
1	B	325	LEU
1	B	329	ASN
1	B	347	LEU
1	B	352	MET
1	B	362	THR

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	60	ASN
1	A	85	GLN
1	A	153	GLN
1	A	221	GLN
1	A	227	GLN
1	A	330	GLN
1	B	85	GLN
1	B	323	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 ⓘ

6 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	366	1,2	14,14,15	0.72	0	15,19,21	0.95	1 (6%)
2	NAG	A	367	2	14,14,15	1.10	1 (7%)	15,19,21	1.52	4 (26%)
2	BMA	A	368	2	11,11,12	1.02	1 (9%)	14,15,17	0.95	0
3	NAG	B	366	1,3	14,14,15	0.69	0	15,19,21	1.16	2 (13%)
3	NAG	B	367	3	14,14,15	0.95	0	15,19,21	1.50	3 (20%)
3	MAN	B	368	3	11,11,12	0.96	1 (9%)	14,15,17	0.93	0

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	366	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	367	2	-	0/6/23/26	0/1/1/1
2	BMA	A	368	2	-	0/2/19/22	0/1/1/1
3	NAG	B	366	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	367	3	-	0/6/23/26	0/1/1/1
3	MAN	B	368	3	1/1/4/5	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	368	BMA	C2-C3	2.23	1.55	1.52
3	B	368	MAN	C2-C3	2.23	1.55	1.52
2	A	367	NAG	C1-C2	2.27	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	367	NAG	O7-C7-C8	-2.68	117.15	122.06
2	A	367	NAG	O7-C7-C8	-2.43	117.61	122.06
2	A	366	NAG	C8-C7-N2	2.01	119.95	116.11
2	A	367	NAG	C8-C7-N2	2.06	120.05	116.11
3	B	366	NAG	C8-C7-N2	2.13	120.18	116.11
3	B	367	NAG	C1-O5-C5	2.31	115.19	112.25
3	B	367	NAG	C3-C4-C5	2.48	114.53	110.20
2	A	367	NAG	C1-O5-C5	2.55	115.48	112.25
3	B	366	NAG	C1-O5-C5	2.71	115.69	112.25
2	A	367	NAG	C3-C4-C5	2.82	115.12	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	368	MAN	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	366	NAG	1	0
3	B	366	NAG	1	0

## 5.6 Ligand geometry

There are no ligands in this entry.

## 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.