



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:51 PM GMT

PDB ID : 4AQT  
Title : Laminin gamma1 LN-LE1-2 structure  
Authors : Carafoli, F.; Hussain, S.; Hohenester, E.  
Deposited on : 2012-04-19  
Resolution : 3.20 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) : 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

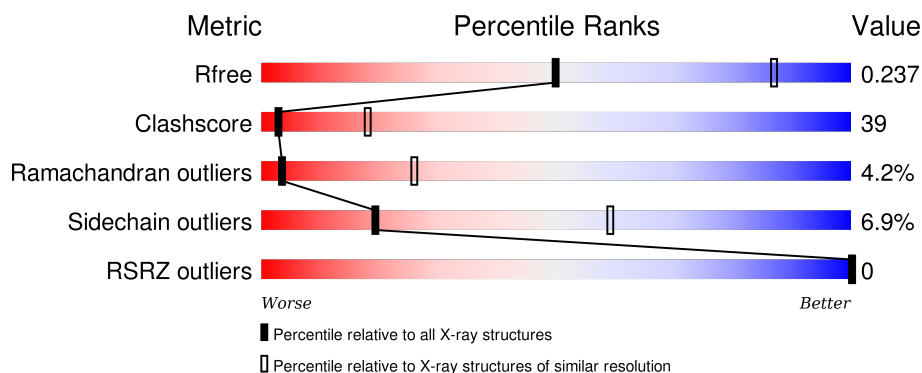
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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.

Mol	Chain	Length	Quality of chain
1	A	375	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2742 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 LAMININ SUBUNIT GAMMA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	357	2688	1668	467	526	27	0	0	1

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ALA	-	EXPRESSION TAG	UNP P02468
A	31	PRO	-	EXPRESSION TAG	UNP P02468
A	32	LEU	-	EXPRESSION TAG	UNP P02468
A	337	CYS	SER	CONFLICT	UNP P02468
A	396	ALA	-	EXPRESSION TAG	UNP P02468
A	397	ALA	-	EXPRESSION TAG	UNP P02468
A	398	ALA	-	EXPRESSION TAG	UNP P02468
A	399	HIS	-	EXPRESSION TAG	UNP P02468
A	400	HIS	-	EXPRESSION TAG	UNP P02468
A	401	HIS	-	EXPRESSION TAG	UNP P02468
A	402	HIS	-	EXPRESSION TAG	UNP P02468
A	403	HIS	-	EXPRESSION TAG	UNP P02468
A	404	HIS	-	EXPRESSION TAG	UNP P02468

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

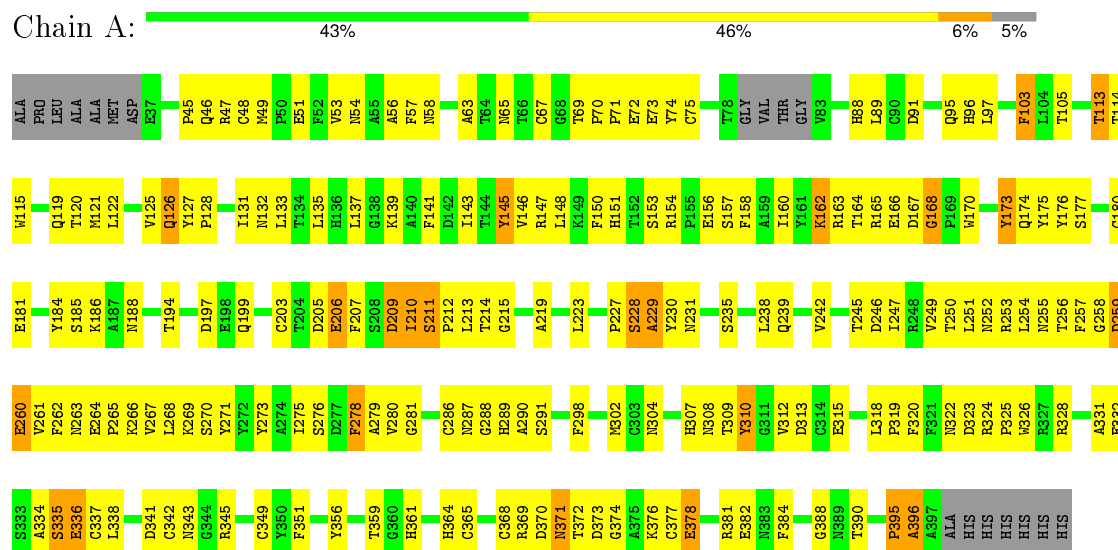
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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

### 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.

#### • Molecule 1: LAMININ SUBUNIT GAMMA-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.01Å 203.01Å 93.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20 24.60 – 3.20	Depositor EDS
% Data completeness (in resolution range)	83.4 (50.00-3.20) 99.4 (24.60-3.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.95 (at 3.23Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.231 , 0.275 0.240 , 0.237	Depositor DCC
$R_{free}$ test set	1262 reflections (11.52%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.4	Xtriage
Anisotropy	0.792	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 20.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 12215 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2742	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BMA, 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	0.43	0/2757	0.71	0/3760

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	2688	0	2362	202	0
2	A	1	0	0	0	0
3	A	14	0	13	5	0
4	A	39	0	34	1	0
All	All	2742	0	2409	203	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 39.

All (203) 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:53:VAL:HG12	1:A:54:ASN:H	1.31	0.95
1:A:256:THR:HG21	1:A:260:GLU:CD	1.88	0.94
1:A:58:ASN:HA	3:A:2001:NAG:H82	1.50	0.92
1:A:48:CYS:O	1:A:288:GLY:HA2	1.74	0.88
1:A:342:CYS:O	1:A:377:CYS:HB2	1.76	0.86
1:A:113:THR:HG21	1:A:276:SER:HB2	1.58	0.81
1:A:345:ARG:HG3	1:A:377:CYS:HB3	1.60	0.81
1:A:369:ARG:O	1:A:372:THR:HG22	1.80	0.81
1:A:323:ASP:OD1	1:A:361:HIS:HB3	1.79	0.81
1:A:126:GLN:HG3	1:A:127:TYR:N	1.97	0.80
1:A:53:VAL:HG12	1:A:54:ASN:N	2.00	0.76
1:A:147:ARG:HG2	1:A:219:ALA:CB	2.16	0.74
1:A:121:MET:HG3	1:A:271:TYR:HB2	1.68	0.74
1:A:133:LEU:HB2	1:A:249:VAL:CG1	2.16	0.74
1:A:262:PHE:O	1:A:264:GLU:N	2.19	0.74
1:A:158:PHE:HB2	1:A:250:THR:O	1.87	0.74
1:A:235:SER:O	1:A:239:GLN:HG3	1.88	0.73
1:A:289:HIS:HA	1:A:307:HIS:HD2	1.51	0.73
1:A:258:GLY:O	1:A:261:VAL:HG23	1.88	0.72
1:A:126:GLN:HG3	1:A:127:TYR:H	1.54	0.72
1:A:289:HIS:HA	1:A:307:HIS:CD2	2.24	0.72
1:A:341:ASP:HB3	1:A:376:LYS:HB2	1.72	0.71
1:A:162:LYS:HG2	1:A:173:TYR:CE2	2.26	0.71
1:A:210:ILE:HG12	1:A:255:ASN:HB3	1.71	0.71
1:A:143:ILE:HD12	1:A:247:ILE:HD11	1.73	0.71
1:A:127:TYR:CG	1:A:128:PRO:HA	2.27	0.70
1:A:368:CYS:HB2	1:A:372:THR:O	1.92	0.70
1:A:127:TYR:CD1	1:A:128:PRO:HA	2.27	0.69
1:A:121:MET:CG	1:A:271:TYR:HB2	2.22	0.69
1:A:56:ALA:HB2	1:A:280:VAL:HG12	1.72	0.69
1:A:230:TYR:CE1	1:A:231:ASN:HB2	2.30	0.66
1:A:63:ALA:HA	1:A:132:ASN:O	1.96	0.66
1:A:150:PHE:CD2	1:A:154:ARG:HG2	2.31	0.66
1:A:156:GLU:OE1	1:A:253:ARG:HD2	1.98	0.64
1:A:256:THR:HG22	1:A:258:GLY:H	1.63	0.64
1:A:146:VAL:HG11	1:A:160:ILE:HD11	1.79	0.63
1:A:148:LEU:HD21	1:A:278:PHE:CD1	2.34	0.63
1:A:322:ASN:HB3	1:A:351:PHE:HB2	1.80	0.63
1:A:257:PHE:HB2	1:A:271:TYR:OH	1.98	0.63
1:A:302:MET:CE	1:A:312:VAL:HG22	2.29	0.62
1:A:302:MET:HE3	1:A:312:VAL:HG22	1.81	0.62
1:A:223:LEU:HD12	1:A:229:ALA:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ARG:O	1:A:384:PHE:HB2	1.99	0.62
1:A:165:ARG:HE	1:A:168:GLY:H	1.48	0.62
1:A:58:ASN:HA	3:A:2001:NAG:C8	2.26	0.61
1:A:65:ASN:HD21	1:A:119:GLN:HG3	1.65	0.61
1:A:359:THR:HG23	1:A:361:HIS:O	1.99	0.61
1:A:53:VAL:CG1	1:A:54:ASN:H	2.10	0.61
1:A:239:GLN:NE2	1:A:328:ARG:HH11	1.97	0.61
1:A:163:ARG:HD2	1:A:170:TRP:CZ2	2.35	0.61
1:A:319:PRO:O	1:A:320:PHE:HB3	2.01	0.61
1:A:47:ARG:H	1:A:334:ALA:HB2	1.65	0.60
1:A:368:CYS:HB3	1:A:372:THR:HG23	1.83	0.60
1:A:121:MET:SD	1:A:126:GLN:HB2	2.41	0.60
1:A:345:ARG:CG	1:A:372:THR:HG21	2.32	0.59
1:A:259:ASP:HB2	1:A:267:VAL:HG11	1.85	0.59
1:A:188:ASN:ND2	1:A:188:ASN:O	2.35	0.59
1:A:223:LEU:HD12	1:A:229:ALA:CB	2.32	0.59
1:A:223:LEU:CD1	1:A:238:LEU:HD13	2.33	0.59
1:A:133:LEU:HB2	1:A:249:VAL:HG12	1.86	0.58
1:A:58:ASN:CA	3:A:2001:NAG:H82	2.27	0.58
1:A:137:LEU:HB2	1:A:245:THR:O	2.04	0.58
1:A:345:ARG:HD2	1:A:372:THR:HG21	1.85	0.58
1:A:153:SER:OG	1:A:210:ILE:HG23	2.04	0.58
1:A:139:LYS:NZ	1:A:313:ASP:OD1	2.37	0.57
1:A:309:THR:HG22	1:A:337:CYS:SG	2.44	0.57
1:A:210:ILE:O	1:A:211:SER:C	2.43	0.57
1:A:211:SER:HB2	1:A:212:PRO:CD	2.35	0.57
1:A:256:THR:HG22	1:A:258:GLY:N	2.20	0.57
1:A:373:ASP:O	1:A:377:CYS:HA	2.04	0.57
1:A:256:THR:HG21	1:A:260:GLU:OE1	2.03	0.56
1:A:150:PHE:HD2	1:A:154:ARG:HG2	1.71	0.56
1:A:184:TYR:OH	1:A:252:ASN:ND2	2.36	0.56
1:A:256:THR:CG2	1:A:257:PHE:N	2.68	0.56
1:A:72:GLU:HG2	1:A:73:GLU:N	2.21	0.56
1:A:147:ARG:HG2	1:A:219:ALA:HB1	1.85	0.56
1:A:256:THR:HG22	1:A:257:PHE:N	2.20	0.55
1:A:238:LEU:O	1:A:242:VAL:HG13	2.07	0.55
1:A:374:GLY:HA3	1:A:378:GLU:OE1	2.07	0.55
1:A:373:ASP:CG	1:A:374:GLY:H	2.08	0.55
1:A:75:CYS:N	1:A:269:LYS:O	2.40	0.55
1:A:342:CYS:H	1:A:376:LYS:HB2	1.72	0.54
1:A:165:ARG:C	1:A:245:THR:HG21	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:THR:HG22	1:A:114:THR:H	1.73	0.54
1:A:47:ARG:NH1	1:A:331:ALA:HB2	2.23	0.54
1:A:115:TRP:HB2	1:A:275:ILE:O	2.07	0.54
1:A:223:LEU:HD12	1:A:229:ALA:CA	2.38	0.54
1:A:324:ARG:HB2	1:A:325:PRO:HD2	1.89	0.53
1:A:125:VAL:O	1:A:126:GLN:C	2.46	0.53
1:A:71:PRO:HG3	1:A:91:ASP:OD1	2.09	0.53
1:A:184:TYR:O	1:A:185:SER:C	2.46	0.53
1:A:67:CYS:HA	1:A:119:GLN:HG2	1.90	0.52
1:A:126:GLN:CG	1:A:127:TYR:N	2.64	0.52
1:A:211:SER:CB	1:A:212:PRO:CD	2.88	0.52
1:A:156:GLU:HB3	1:A:253:ARG:HG2	1.92	0.52
1:A:197:ASP:C	1:A:197:ASP:OD1	2.48	0.52
1:A:174:GLN:HG2	1:A:176:TYR:CZ	2.44	0.52
1:A:125:VAL:HG12	1:A:126:GLN:N	2.23	0.52
1:A:349:CYS:HB2	1:A:364:HIS:O	2.10	0.52
1:A:113:THR:CG2	1:A:276:SER:HB2	2.36	0.51
1:A:162:LYS:HG2	1:A:173:TYR:CZ	2.45	0.51
1:A:162:LYS:HG2	1:A:173:TYR:CD2	2.46	0.51
1:A:345:ARG:CD	1:A:372:THR:HG21	2.40	0.51
1:A:57:PHE:O	1:A:58:ASN:HB3	2.10	0.51
1:A:167:ASP:O	1:A:168:GLY:O	2.28	0.51
1:A:47:ARG:HH12	1:A:331:ALA:HB2	1.75	0.50
1:A:147:ARG:HG2	1:A:219:ALA:HB2	1.92	0.50
1:A:145:TYR:CD1	1:A:145:TYR:C	2.84	0.50
1:A:223:LEU:HD11	1:A:238:LEU:HD13	1.94	0.50
1:A:315:GLU:HA	1:A:326:TRP:CZ2	2.47	0.50
1:A:211:SER:HB2	1:A:212:PRO:HD3	1.93	0.50
1:A:156:GLU:O	1:A:177:SER:HA	2.12	0.50
1:A:206:GLU:OE1	1:A:207:PHE:HE1	1.94	0.49
1:A:368:CYS:CB	1:A:372:THR:O	2.61	0.49
1:A:160:ILE:CG2	1:A:174:GLN:HB3	2.42	0.49
1:A:160:ILE:O	1:A:173:TYR:HB2	2.12	0.49
1:A:365:CYS:SG	1:A:376:LYS:HA	2.52	0.49
1:A:126:GLN:HA	1:A:254:LEU:HD12	1.92	0.49
1:A:175:TYR:O	1:A:203:CYS:HA	2.12	0.49
1:A:268:LEU:C	1:A:270:SER:H	2.15	0.49
1:A:103:PHE:CD1	1:A:103:PHE:N	2.81	0.49
1:A:49:MET:C	1:A:291:SER:HA	2.34	0.48
1:A:209:ASP:O	1:A:210:ILE:HB	2.13	0.48
1:A:320:PHE:HA	1:A:349:CYS:SG	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LYS:O	1:A:141:PHE:HD1	1.96	0.48
1:A:157:SER:HA	1:A:176:TYR:O	2.14	0.48
1:A:209:ASP:O	1:A:210:ILE:CB	2.62	0.48
1:A:56:ALA:HB1	1:A:105:THR:HG22	1.95	0.48
1:A:210:ILE:CG1	1:A:255:ASN:HB3	2.40	0.48
1:A:334:ALA:O	1:A:335:SER:C	2.51	0.48
1:A:188:ASN:ND2	1:A:188:ASN:C	2.66	0.48
1:A:345:ARG:HG3	1:A:377:CYS:CB	2.37	0.47
1:A:310:TYR:HB3	1:A:318:LEU:CD2	2.44	0.47
1:A:54:ASN:HD21	1:A:279:ALA:HA	1.78	0.47
1:A:96:HIS:O	1:A:97:LEU:HD23	2.14	0.47
1:A:251:LEU:HD13	1:A:273:TYR:CG	2.50	0.47
1:A:319:PRO:O	1:A:320:PHE:CB	2.62	0.47
1:A:280:VAL:HG13	1:A:280:VAL:O	2.15	0.47
1:A:345:ARG:CG	1:A:377:CYS:HB3	2.39	0.47
1:A:345:ARG:HG3	1:A:372:THR:HG21	1.97	0.46
1:A:46:GLN:HA	1:A:334:ALA:CB	2.45	0.46
1:A:45:PRO:HG3	1:A:336:GLU:OE1	2.15	0.46
1:A:166:GLU:N	1:A:245:THR:HG21	2.30	0.46
1:A:214:THR:HG22	1:A:215:GLY:N	2.31	0.46
1:A:72:GLU:CG	1:A:73:GLU:N	2.79	0.46
1:A:121:MET:HG2	1:A:271:TYR:HB2	1.97	0.46
1:A:49:MET:HA	1:A:290:ALA:O	2.15	0.46
1:A:180:CYS:HB3	1:A:186:LYS:O	2.14	0.46
1:A:135:LEU:CD2	1:A:280:VAL:HG11	2.46	0.46
1:A:74:TYR:CZ	1:A:88:HIS:HB2	2.51	0.45
1:A:181:GLU:CD	1:A:181:GLU:H	2.19	0.45
1:A:47:ARG:N	1:A:334:ALA:HB2	2.31	0.45
1:A:197:ASP:OD1	1:A:199:GLN:N	2.38	0.45
1:A:51:GLU:O	1:A:53:VAL:HG23	2.17	0.45
1:A:147:ARG:O	1:A:148:LEU:HD23	2.16	0.45
1:A:223:LEU:HD21	1:A:242:VAL:CG1	2.47	0.45
1:A:131:ILE:HD12	1:A:273:TYR:CD2	2.52	0.45
1:A:57:PHE:CE1	3:A:2001:NAG:O7	2.70	0.45
1:A:47:ARG:N	1:A:334:ALA:CB	2.81	0.44
1:A:342:CYS:O	1:A:343:ASN:HB2	2.17	0.44
1:A:211:SER:CB	1:A:212:PRO:HD3	2.48	0.44
1:A:356:TYR:O	1:A:359:THR:O	2.36	0.44
1:A:122:LEU:N	1:A:268:LEU:HB3	2.33	0.44
1:A:323:ASP:HB3	1:A:338:LEU:HB2	1.99	0.44
1:A:265:PRO:HG2	1:A:266:LYS:H	1.83	0.44

*Continued on next page...*

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:TYR:CG	1:A:231:ASN:N	2.86	0.43
1:A:167:ASP:HB2	1:A:168:GLY:H	1.58	0.43
1:A:223:LEU:HD21	1:A:242:VAL:HG11	2.01	0.43
1:A:69:THR:HA	1:A:70:PRO:HA	1.80	0.43
1:A:135:LEU:HD21	1:A:280:VAL:HG11	2.01	0.43
1:A:154:ARG:NH1	1:A:207:PHE:HA	2.34	0.43
1:A:131:ILE:HD12	1:A:273:TYR:HD2	1.83	0.43
1:A:156:GLU:HA	1:A:255:ASN:ND2	2.34	0.43
1:A:228:SER:O	1:A:230:TYR:N	2.52	0.43
1:A:181:GLU:O	1:A:185:SER:HA	2.18	0.43
1:A:341:ASP:CB	1:A:376:LYS:HD2	2.49	0.42
1:A:143:ILE:CD1	1:A:247:ILE:HD11	2.47	0.42
1:A:395:PRO:O	1:A:396:ALA:O	2.36	0.42
1:A:289:HIS:CA	1:A:307:HIS:HD2	2.26	0.42
1:A:151:HIS:O	1:A:214:THR:HG23	2.18	0.42
1:A:95:GLN:O	1:A:95:GLN:HG2	2.19	0.42
1:A:381:ARG:O	1:A:382:GLU:C	2.57	0.42
1:A:53:VAL:O	1:A:281:GLY:HA2	2.20	0.42
1:A:146:VAL:HG22	1:A:280:VAL:HG23	2.02	0.42
1:A:251:LEU:HB3	1:A:273:TYR:CE1	2.55	0.42
1:A:163:ARG:HD3	1:A:246:ASP:HB2	2.02	0.41
4:A:3001:NAG:C7	4:A:3001:NAG:O3	2.68	0.41
1:A:63:ALA:HB2	1:A:133:LEU:HD23	2.01	0.41
1:A:286:CYS:O	1:A:287:ASN:HB2	2.21	0.41
1:A:54:ASN:ND2	1:A:280:VAL:H	2.18	0.41
1:A:120:THR:O	1:A:121:MET:C	2.58	0.41
1:A:48:CYS:O	1:A:49:MET:HB3	2.21	0.41
1:A:205:ASP:O	1:A:207:PHE:N	2.54	0.41
1:A:126:GLN:CG	1:A:127:TYR:H	2.22	0.41
1:A:210:ILE:HG12	1:A:255:ASN:CB	2.44	0.41
1:A:370:ASP:O	1:A:371:ASN:C	2.58	0.41
1:A:158:PHE:CD1	1:A:176:TYR:HB2	2.55	0.41
1:A:57:PHE:CE1	3:A:2001:NAG:H81	2.56	0.41
1:A:145:TYR:C	1:A:145:TYR:HD1	2.24	0.41
1:A:342:CYS:O	1:A:345:ARG:HG2	2.21	0.41
1:A:307:HIS:O	1:A:308:ASN:HB2	2.22	0.40
1:A:207:PHE:N	1:A:207:PHE:CD1	2.90	0.40
1:A:139:LYS:C	1:A:139:LYS:HD3	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	353/375 (94%)	283 (80%)	55 (16%)	15 (4%)	3	26

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	GLY
1	A	263	ASN
1	A	396	ALA
1	A	126	GLN
1	A	206	GLU
1	A	210	ILE
1	A	211	SER
1	A	229	ALA
1	A	388	GLY
1	A	332	GLU
1	A	335	SER
1	A	213	LEU
1	A	371	ASN
1	A	227	PRO
1	A	395	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	277/317 (87%)	258 (93%)	19 (7%)	19	59

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	103	PHE
1	A	113	THR
1	A	145	TYR
1	A	162	LYS
1	A	164	THR
1	A	173	TYR
1	A	194	THR
1	A	209	ASP
1	A	228	SER
1	A	259	ASP
1	A	260	GLU
1	A	278	PHE
1	A	298	PHE
1	A	304	ASN
1	A	310	TYR
1	A	336	GLU
1	A	378	GLU
1	A	390	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	GLN
1	A	252	ASN
1	A	304	ASN
1	A	307	HIS

### 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	$\# Z  > 2$
4	NAG	A	3001	1,4	14,14,15	0.53	0	15,19,21	0.79	0
4	NAG	A	3002	4	14,14,15	0.56	0	15,19,21	0.93	1 (6%)
4	BMA	A	3003	4	11,11,12	0.71	0	14,15,17	0.68	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
4	NAG	A	3001	1,4	-	1/6/23/26	0/1/1/1
4	NAG	A	3002	4	-	0/6/23/26	0/1/1/1
4	BMA	A	3003	4	-	0/2/19/22	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(°)
4	A	3002	NAG	C2-N2-C7	-2.58	119.72	123.04

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3001	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3001	NAG	1	0

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	2001	1	14,14,15	0.68	0	15,19,21	1.10	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	2001	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( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	2001	NAG	C2-N2-C7	-3.74	118.23	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	NAG	5	0

## 5.7 Other polymers [i](#)

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	357/375 (95%)	-0.30	0 100 100	34, 62, 94, 105	0

There are no RSRZ outliers to report.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	A	3001	14/15	0.93	0.19	-0.35	61,65,69,69	0
4	NAG	A	3002	14/15	0.88	0.17	-	71,76,82,88	0
4	BMA	A	3003	11/12	0.85	0.31	-	93,94,95,95	0

### 6.4 Ligands [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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	CA	A	1001	1/1	0.97	0.10	-2.21	59,59,59,59	0
3	NAG	A	2001	14/15	0.80	0.23	-	91,96,97,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.