



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:45 AM BST

PDB ID : 4EB1  
Title : Hyperstable in-frame insertion variant of antithrombin  
Authors : Martinez-Martinez, I.; Johnson, D.J.D.; Yamasaki, M.; Corral, J.; Huntington, J.A.  
Deposited on : 2012-03-23  
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

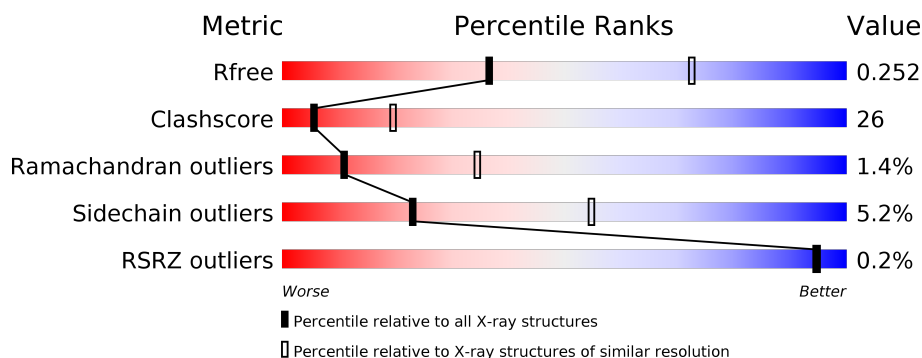
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*





The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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  $\leq 5\%$ . 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	I	440	
2	L	432	
3	A	2	
3	B	2	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	2	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6205 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 Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	I	411	3152	2023	518	593	18	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	137	ALA	SER	engineered mutation	UNP P01008
I	209	VAL	-	insertion	UNP P01008
I	210	LEU	-	insertion	UNP P01008
I	211	VAL	-	insertion	UNP P01008
I	212	LEU	-	insertion	UNP P01008
I	213	VAL	-	insertion	UNP P01008
I	214	ASN	-	insertion	UNP P01008
I	215	THR	-	insertion	UNP P01008
I	216	ARG	-	insertion	UNP P01008
I	217	THR	-	insertion	UNP P01008
I	218	SER	-	insertion	UNP P01008

- Molecule 2 is a protein called Antithrombin-III.

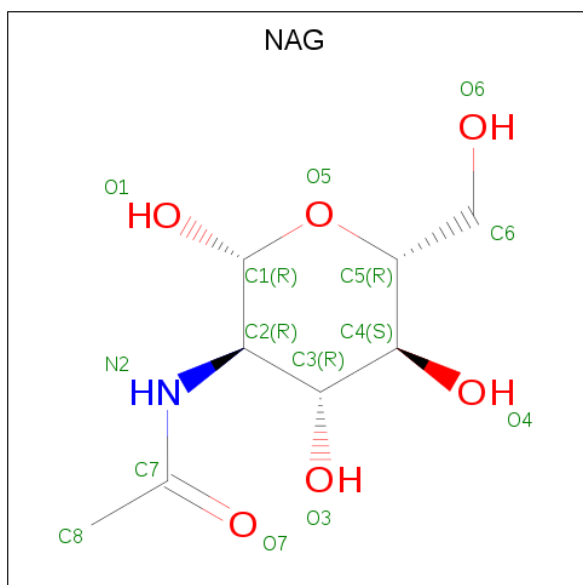
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	392	2942	1884	486	554	18	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		

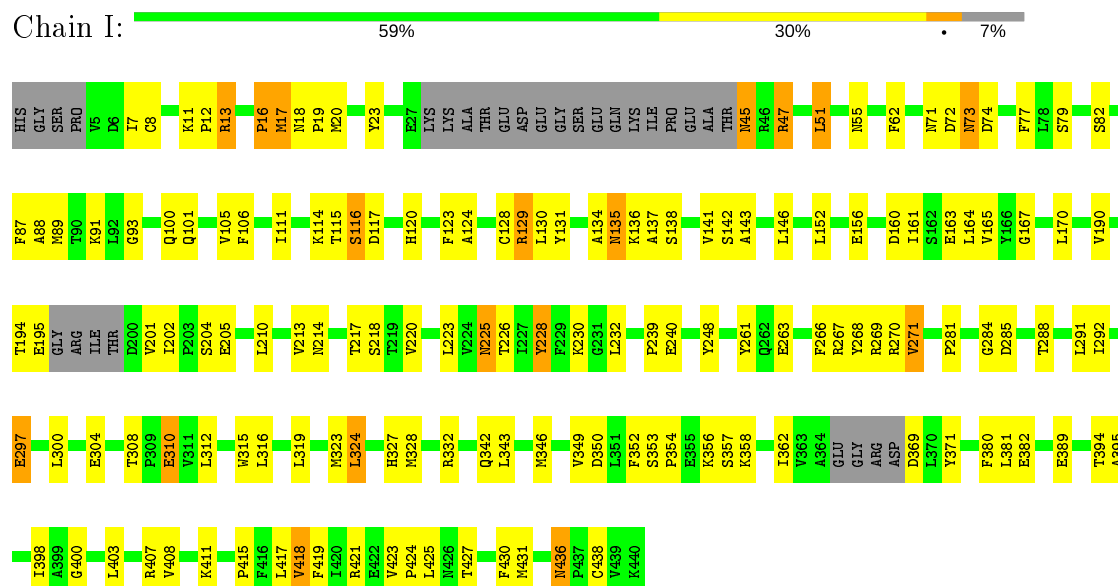
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	16	Total	O	0	0
			16	16		
5	L	11	Total	O	0	0
			11	11		

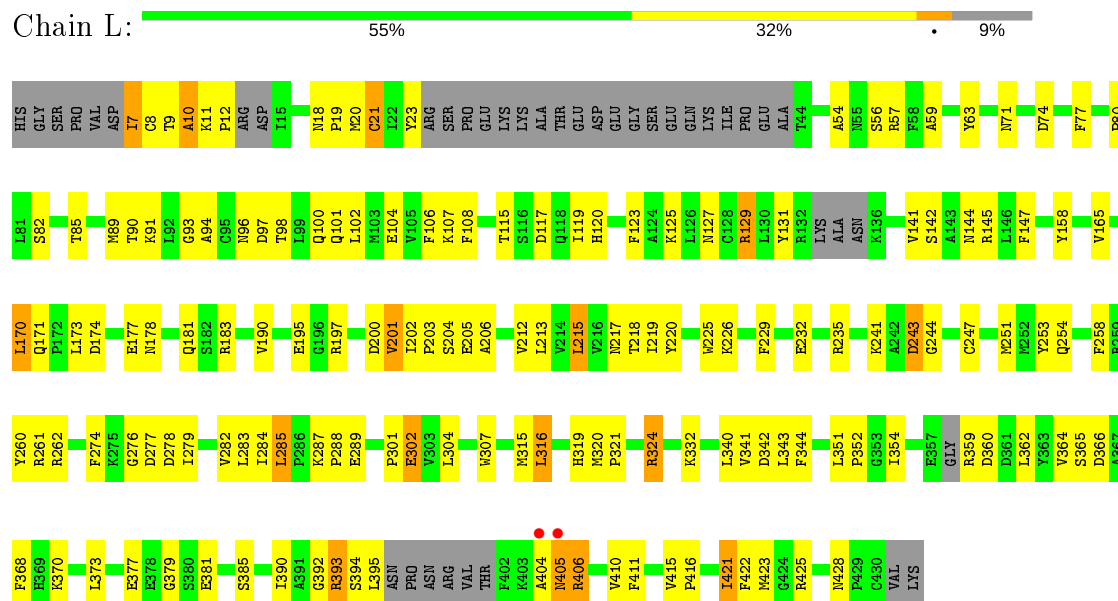
### 3 Residue-property plots

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 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: Antithrombin-III



#### • Molecule 2: Antithrombin-III



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:  50% 50%

MAG1  
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  50% 50%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.75Å 101.75Å 88.81Å 90.00° 105.42° 90.00°	Depositor
Resolution (Å)	61.40 – 2.80 61.40 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.7 (61.40-2.80) 95.7 (61.40-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0098	Depositor
R, $R_{free}$	0.198 , 0.255 0.197 , 0.252	Depositor DCC
$R_{free}$ test set	1426 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.2	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	I	0.24	0/3215	0.41	0/4362
2	L	0.23	0/2999	0.38	0/4078
All	All	0.24	0/6214	0.40	0/8440

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	I	3152	0	3010	159	1
2	L	2942	0	2721	150	0
3	A	28	0	25	3	0
3	B	28	0	25	3	0
4	I	28	0	26	1	0
5	I	16	0	0	0	0
5	L	11	0	0	0	0
All	All	6205	0	5807	307	1

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 26.

All (307) 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)
2:L:20:MET:CE	2:L:352:PRO:HG2	1.49	1.42
1:I:17:MET:O	1:I:19:PRO:HD3	1.35	1.24
1:I:291:LEU:HD11	1:I:328:MET:CE	1.76	1.15
2:L:241:LYS:NZ	2:L:247:CYS:SG	2.21	1.14
2:L:20:MET:HE3	2:L:352:PRO:HG2	1.16	1.09
2:L:129:ARG:HH11	2:L:129:ARG:HG3	1.01	1.07
2:L:20:MET:CE	2:L:352:PRO:CG	2.35	1.04
2:L:20:MET:HE1	2:L:352:PRO:HG2	1.38	1.04
1:I:13:ARG:HH11	1:I:13:ARG:CG	1.71	1.03
2:L:129:ARG:HH11	2:L:129:ARG:CG	1.71	1.03
2:L:20:MET:HE1	2:L:352:PRO:CG	1.89	1.01
1:I:13:ARG:HH11	1:I:13:ARG:HG2	0.83	1.00
1:I:291:LEU:HD11	1:I:328:MET:HE1	1.42	0.97
2:L:174:ASP:OD2	2:L:177:GLU:HB3	1.64	0.96
2:L:283:LEU:HD11	2:L:320:MET:CE	1.97	0.95
1:I:91:LYS:HE2	1:I:120:HIS:NE2	1.82	0.94
2:L:283:LEU:HD11	2:L:320:MET:HE3	1.47	0.94
1:I:13:ARG:NH1	1:I:13:ARG:HG2	1.64	0.94
1:I:89:MET:CE	1:I:225:ASN:OD1	2.16	0.93
1:I:291:LEU:HD11	1:I:328:MET:HE3	1.49	0.93
2:L:20:MET:HE1	2:L:352:PRO:CB	2.00	0.91
1:I:91:LYS:CE	1:I:120:HIS:NE2	2.35	0.90
1:I:436:ASN:C	1:I:436:ASN:HD22	1.75	0.90
2:L:63:TYR:HB2	2:L:423:MET:HE1	1.55	0.88
2:L:129:ARG:HG3	2:L:129:ARG:NH1	1.81	0.87
2:L:20:MET:O	2:L:21:CYS:SG	2.32	0.87
1:I:19:PRO:O	3:A:2:NAG:H81	1.74	0.87
2:L:91:LYS:HE2	2:L:120:HIS:CE1	2.11	0.85
1:I:91:LYS:NZ	1:I:120:HIS:NE2	2.23	0.85
2:L:96:ASN:OD1	2:L:97:ASP:N	2.10	0.84
1:I:143:ALA:HB3	1:I:226:THR:OG1	1.77	0.83
1:I:201:VAL:O	1:I:230:LYS:HE2	1.79	0.82
2:L:203:PRO:HG3	2:L:368:PHE:CE1	2.16	0.81
2:L:178:ASN:ND2	2:L:181:GLN:OE1	2.13	0.81
2:L:63:TYR:HB2	2:L:423:MET:CE	2.10	0.80
1:I:89:MET:HE1	1:I:225:ASN:OD1	1.81	0.80
2:L:145:ARG:HG2	2:L:147:PHE:CE1	2.16	0.79
2:L:91:LYS:CE	2:L:120:HIS:NE2	2.46	0.79
2:L:215:LEU:N	2:L:215:LEU:HD12	1.98	0.79
1:I:263:GLU:OE2	1:I:403:LEU:HD12	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:332:LYS:HG3	2:L:344:PHE:CD1	2.19	0.78
2:L:205:GLU:O	2:L:393:ARG:HD2	1.84	0.77
1:I:17:MET:O	1:I:19:PRO:CD	2.27	0.77
1:I:91:LYS:HZ3	1:I:120:HIS:CD2	2.03	0.76
1:I:141:VAL:HG21	1:I:228:TYR:CE1	2.21	0.76
1:I:16:PRO:O	1:I:17:MET:HB2	1.86	0.75
3:B:2:NAG:O7	3:B:2:NAG:H3	1.85	0.74
1:I:205:GLU:HG2	1:I:380:PHE:CE2	2.22	0.74
2:L:284:ILE:C	2:L:285:LEU:HD23	2.07	0.74
2:L:96:ASN:CG	2:L:97:ASP:H	1.87	0.73
2:L:9:THR:O	2:L:10:ALA:HB2	1.89	0.72
2:L:74:ASP:O	2:L:425:ARG:HD2	1.89	0.72
2:L:201:VAL:HG11	2:L:385:SER:HB3	1.72	0.71
2:L:57:ARG:HG3	2:L:301:PRO:HG2	1.71	0.71
2:L:215:LEU:H	2:L:215:LEU:HD12	1.53	0.71
2:L:9:THR:O	2:L:10:ALA:CB	2.38	0.71
2:L:129:ARG:NH1	2:L:129:ARG:CG	2.42	0.71
2:L:341:VAL:HG23	2:L:342:ASP:H	1.54	0.70
1:I:134:ALA:O	1:I:135:ASN:CB	2.40	0.70
1:I:62:PHE:HD1	1:I:346:MET:CE	2.06	0.69
1:I:213:VAL:HG13	1:I:218:SER:O	1.92	0.69
2:L:91:LYS:HE2	2:L:120:HIS:NE2	2.06	0.69
1:I:91:LYS:NZ	1:I:120:HIS:CD2	2.61	0.68
2:L:285:LEU:HD23	2:L:285:LEU:N	2.09	0.67
2:L:203:PRO:CG	2:L:368:PHE:CE1	2.77	0.66
2:L:205:GLU:O	2:L:393:ARG:CD	2.43	0.66
1:I:141:VAL:CG2	1:I:228:TYR:CE1	2.78	0.66
1:I:136:LYS:O	1:I:137:ALA:HB3	1.96	0.66
1:I:323:MET:CE	1:I:403:LEU:CD1	2.75	0.65
1:I:62:PHE:HD1	1:I:346:MET:HE1	1.60	0.65
2:L:274:PHE:HD2	2:L:279:ILE:O	1.80	0.65
1:I:323:MET:CE	1:I:403:LEU:HD13	2.27	0.64
2:L:20:MET:HE1	2:L:352:PRO:HB2	1.80	0.64
1:I:436:ASN:C	1:I:436:ASN:ND2	2.46	0.64
1:I:111:ILE:O	1:I:114:LYS:HG2	1.98	0.64
2:L:115:THR:HB	2:L:117:ASP:OD1	1.96	0.64
2:L:23:TYR:CZ	2:L:100:GLN:HG3	2.32	0.64
2:L:131:TYR:CE1	2:L:142:SER:HB2	2.33	0.64
1:I:101:GLN:O	1:I:105:VAL:HG23	1.97	0.63
1:I:7:ILE:CG2	1:I:164:LEU:HD11	2.29	0.63
2:L:20:MET:HE3	2:L:352:PRO:CG	2.08	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:327:HIS:HB2	1:I:411:LYS:HA	1.81	0.63
1:I:17:MET:HE1	1:I:120:HIS:HB2	1.80	0.63
2:L:71:ASN:HB3	2:L:74:ASP:HB2	1.81	0.63
1:I:7:ILE:CG2	1:I:164:LEU:CD1	2.78	0.62
2:L:284:ILE:HD13	2:L:307:TRP:HZ3	1.63	0.62
2:L:57:ARG:CG	2:L:301:PRO:HG2	2.29	0.62
2:L:20:MET:HE1	2:L:352:PRO:C	2.20	0.62
1:I:7:ILE:HG13	1:I:8:CYS:N	2.15	0.61
2:L:91:LYS:NZ	2:L:120:HIS:NE2	2.49	0.61
2:L:174:ASP:CG	2:L:177:GLU:HB3	2.22	0.60
2:L:283:LEU:CD1	2:L:320:MET:HE3	2.28	0.60
2:L:106:PHE:HB2	2:L:108:PHE:CE2	2.36	0.60
1:I:91:LYS:HE2	1:I:120:HIS:CE1	2.37	0.60
1:I:71:ASN:OD1	1:I:73:ASN:ND2	2.35	0.60
1:I:131:TYR:CE1	1:I:142:SER:HB2	2.37	0.59
2:L:283:LEU:HD11	2:L:320:MET:HE1	1.81	0.59
2:L:85:THR:O	2:L:89:MET:HG3	2.03	0.59
1:I:204:SER:HB2	1:I:381:LEU:HD12	1.84	0.59
1:I:194:THR:O	1:I:195:GLU:C	2.41	0.58
2:L:80:PRO:HD2	2:L:421:ILE:O	2.03	0.58
2:L:284:ILE:HD13	2:L:307:TRP:CZ3	2.39	0.58
1:I:436:ASN:ND2	1:I:438:CYS:H	2.02	0.58
1:I:291:LEU:CD1	1:I:328:MET:HE3	2.29	0.58
2:L:225:TRP:CD1	2:L:379:GLY:HA2	2.38	0.58
1:I:79:SER:HB2	1:I:430:PHE:CD1	2.39	0.58
1:I:101:GLN:HE22	1:I:349:VAL:HG23	1.69	0.57
2:L:7:ILE:HG23	2:L:8:CYS:H	1.70	0.57
2:L:404:ALA:HB2	2:L:428:ASN:HB2	1.86	0.57
2:L:201:VAL:CG1	2:L:385:SER:HB3	2.34	0.57
2:L:97:ASP:HB3	2:L:342:ASP:OD2	2.05	0.57
2:L:405:ASN:O	2:L:406:ARG:C	2.44	0.56
2:L:90:THR:OG1	2:L:215:LEU:HD22	2.05	0.56
1:I:271:VAL:HG11	1:I:315:TRP:CD1	2.40	0.56
1:I:316:LEU:HD13	1:I:421:ARG:CZ	2.36	0.56
2:L:171:GLN:HE21	2:L:173:LEU:HD21	1.71	0.56
2:L:183:ARG:CZ	2:L:204:SER:HA	2.36	0.56
2:L:102:LEU:HD23	2:L:340:LEU:HD11	1.87	0.56
2:L:183:ARG:NH1	2:L:202:ILE:O	2.38	0.55
2:L:332:LYS:HG3	2:L:344:PHE:CE1	2.42	0.55
1:I:356:LYS:O	1:I:358:LYS:HG2	2.05	0.55
1:I:423:VAL:HB	1:I:424:PRO:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:341:VAL:HG23	2:L:342:ASP:N	2.21	0.55
2:L:241:LYS:HD2	2:L:241:LYS:H	1.71	0.55
1:I:136:LYS:O	1:I:137:ALA:CB	2.54	0.54
2:L:19:PRO:O	3:B:2:NAG:H81	2.06	0.54
2:L:93:GLY:O	2:L:351:LEU:HA	2.07	0.54
1:I:436:ASN:ND2	1:I:438:CYS:N	2.56	0.54
2:L:243:ASP:OD1	2:L:243:ASP:C	2.45	0.54
1:I:213:VAL:HG13	1:I:218:SER:C	2.26	0.54
1:I:13:ARG:NH1	1:I:13:ARG:CG	2.42	0.54
2:L:302:GLU:CD	2:L:302:GLU:H	2.11	0.54
1:I:297:GLU:H	1:I:297:GLU:CD	2.11	0.54
1:I:308:THR:OG1	1:I:310:GLU:HG2	2.08	0.54
1:I:115:THR:O	1:I:116:SER:C	2.46	0.53
2:L:340:LEU:HD23	2:L:344:PHE:HE2	1.72	0.53
1:I:7:ILE:HG13	1:I:128:CYS:SG	2.49	0.53
1:I:111:ILE:HG22	1:I:114:LYS:CG	2.40	0.52
1:I:20:MET:HB2	3:A:1:NAG:H61	1.91	0.52
1:I:332:ARG:HD3	1:I:382:GLU:HB2	1.90	0.52
2:L:54:ALA:HB1	2:L:107:LYS:O	2.09	0.52
1:I:7:ILE:HG22	1:I:164:LEU:HD11	1.92	0.52
1:I:19:PRO:O	3:A:2:NAG:C8	2.54	0.52
1:I:213:VAL:HG12	1:I:214:ASN:N	2.25	0.52
2:L:145:ARG:HG2	2:L:147:PHE:CZ	2.44	0.52
1:I:23:TYR:CE1	1:I:100:GLN:HG3	2.45	0.52
2:L:287:LYS:O	2:L:289:GLU:N	2.43	0.51
2:L:20:MET:CE	2:L:352:PRO:CB	2.80	0.51
1:I:131:TYR:CZ	1:I:142:SER:HB2	2.45	0.51
1:I:228:TYR:C	1:I:228:TYR:CD2	2.84	0.51
1:I:93:GLY:HA3	1:I:362:ILE:HG13	1.93	0.51
1:I:323:MET:HE2	1:I:403:LEU:HD13	1.93	0.51
2:L:365:SER:HB3	2:L:392:GLY:H	1.76	0.51
1:I:146:LEU:CD2	1:I:223:LEU:HG	2.42	0.50
1:I:195:GLU:N	1:I:202:ILE:HD12	2.27	0.50
1:I:323:MET:HE2	1:I:403:LEU:HD22	1.94	0.50
2:L:215:LEU:CD1	2:L:215:LEU:H	2.23	0.50
2:L:190:VAL:HG13	2:L:218:THR:HG22	1.94	0.50
2:L:260:TYR:CD2	2:L:261:ARG:N	2.80	0.50
2:L:215:LEU:CD1	2:L:215:LEU:N	2.70	0.50
2:L:97:ASP:CB	2:L:342:ASP:OD2	2.59	0.50
1:I:349:VAL:HG23	1:I:350:ASP:H	1.76	0.50
1:I:101:GLN:HE22	1:I:349:VAL:CG2	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:239:PRO:HD2	1:I:394:THR:O	2.13	0.49
2:L:276:GLY:C	2:L:278:ASP:H	2.16	0.49
2:L:106:PHE:CB	2:L:108:PHE:CE2	2.95	0.49
1:I:281:PRO:HB3	1:I:288:THR:HG22	1.95	0.48
1:I:7:ILE:HG23	1:I:164:LEU:CD1	2.42	0.48
1:I:16:PRO:O	1:I:17:MET:CB	2.56	0.48
1:I:213:VAL:HG11	1:I:217:THR:HA	1.95	0.48
1:I:349:VAL:HG23	1:I:350:ASP:N	2.28	0.48
1:I:136:LYS:C	1:I:138:SER:H	2.16	0.48
1:I:300:LEU:O	1:I:304:GLU:HG3	2.13	0.48
1:I:343:LEU:HA	1:I:346:MET:HE3	1.95	0.48
2:L:260:TYR:CG	2:L:261:ARG:N	2.82	0.48
2:L:282:VAL:HB	2:L:411:PHE:HB2	1.96	0.48
2:L:77:PHE:CE2	2:L:373:LEU:HB2	2.49	0.48
2:L:91:LYS:HZ1	2:L:120:HIS:CD2	2.31	0.48
1:I:111:ILE:HG22	1:I:114:LYS:HG3	1.96	0.48
1:I:267:ARG:NH2	1:I:319:LEU:O	2.45	0.48
2:L:20:MET:HE1	2:L:352:PRO:CA	2.42	0.48
1:I:310:GLU:CD	1:I:310:GLU:H	2.16	0.48
1:I:130:LEU:HD23	1:I:425:LEU:HD12	1.96	0.48
1:I:232:LEU:HD13	1:I:389:GLU:HG3	1.94	0.48
1:I:45:ASN:ND2	1:I:45:ASN:C	2.66	0.47
2:L:158:TYR:CE2	2:L:354:ILE:HG23	2.49	0.47
2:L:144:ASN:HD22	2:L:217:ASN:HA	1.79	0.47
2:L:226:LYS:HD2	2:L:277:ASP:OD1	2.14	0.47
2:L:63:TYR:HB2	2:L:423:MET:HE3	1.93	0.47
1:I:7:ILE:HG23	1:I:164:LEU:HD11	1.95	0.47
1:I:163:GLU:O	1:I:167:GLY:HA2	2.13	0.47
1:I:398:ILE:HA	2:L:319:HIS:HB2	1.95	0.47
1:I:240:GLU:HB3	2:L:262:ARG:NH1	2.29	0.47
1:I:51:LEU:O	1:I:51:LEU:HD23	2.15	0.47
2:L:241:LYS:CE	2:L:247:CYS:SG	3.02	0.47
1:I:323:MET:HE1	1:I:403:LEU:HD11	1.95	0.47
1:I:201:VAL:O	1:I:230:LYS:CE	2.58	0.47
2:L:147:PHE:O	2:L:213:LEU:HD12	2.14	0.47
1:I:195:GLU:HA	1:I:202:ILE:HD12	1.97	0.47
2:L:359:ARG:O	2:L:360:ASP:CB	2.62	0.47
1:I:124:ALA:HB2	1:I:165:VAL:HG13	1.95	0.46
1:I:62:PHE:HD1	1:I:346:MET:HE2	1.80	0.46
2:L:77:PHE:CZ	2:L:422:PHE:HB3	2.50	0.46
1:I:269:ARG:HG3	1:I:271:VAL:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:104:GLU:O	2:L:107:LYS:N	2.43	0.46
1:I:23:TYR:CD2	1:I:23:TYR:C	2.88	0.46
1:I:77:PHE:CZ	1:I:381:LEU:HB2	2.50	0.46
1:I:268:TYR:CG	1:I:269:ARG:N	2.84	0.46
1:I:400:GLY:H	2:L:321:PRO:HD3	1.81	0.46
1:I:266:PHE:HD2	1:I:324:LEU:HD21	1.80	0.46
1:I:214:ASN:HA	1:I:369:ASP:O	2.16	0.46
1:I:323:MET:CE	1:I:403:LEU:HD11	2.47	0.45
4:I:801:NAG:H3	4:I:801:NAG:O7	2.17	0.45
1:I:146:LEU:HD23	1:I:223:LEU:HG	1.98	0.45
2:L:229:PHE:HB2	2:L:377:GLU:HA	1.97	0.45
2:L:212:VAL:HG21	2:L:362:LEU:CD2	2.46	0.45
1:I:357:SER:OG	1:I:371:TYR:HA	2.16	0.45
2:L:232:GLU:O	2:L:235:ARG:NH1	2.49	0.45
2:L:102:LEU:HD21	2:L:343:LEU:HD22	1.98	0.45
2:L:190:VAL:HG13	2:L:218:THR:CG2	2.46	0.45
1:I:143:ALA:HB3	1:I:226:THR:HG1	1.81	0.45
2:L:217:ASN:HD21	2:L:219:ILE:HG13	1.82	0.45
1:I:423:VAL:HB	1:I:424:PRO:CD	2.47	0.44
2:L:203:PRO:HG2	2:L:206:ALA:HB2	1.99	0.44
1:I:352:PHE:O	1:I:354:PRO:HD3	2.18	0.44
1:I:129:ARG:HE	1:I:425:LEU:HD21	1.83	0.44
2:L:241:LYS:C	2:L:243:ASP:H	2.20	0.44
2:L:243:ASP:OD1	2:L:244:GLY:N	2.51	0.44
2:L:316:LEU:H	2:L:316:LEU:HD23	1.83	0.44
1:I:205:GLU:HG2	1:I:380:PHE:CZ	2.53	0.44
1:I:419:PHE:N	1:I:419:PHE:CD1	2.86	0.44
2:L:91:LYS:HE2	2:L:91:LYS:HB3	1.90	0.44
1:I:114:LYS:HA	1:I:114:LYS:HD3	1.78	0.43
1:I:324:LEU:HB2	1:I:408:VAL:O	2.19	0.43
1:I:7:ILE:HG13	1:I:8:CYS:H	1.83	0.43
2:L:56:SER:O	2:L:59:ALA:HB3	2.18	0.43
1:I:23:TYR:O	1:I:115:THR:HA	2.19	0.43
2:L:82:SER:OG	2:L:217:ASN:ND2	2.52	0.43
1:I:268:TYR:CD2	1:I:269:ARG:N	2.86	0.43
2:L:119:ILE:HD12	2:L:119:ILE:N	2.34	0.43
2:L:324:ARG:HG3	2:L:324:ARG:O	2.19	0.43
2:L:170:LEU:C	2:L:170:LEU:CD2	2.87	0.43
1:I:51:LEU:CD2	1:I:51:LEU:O	2.66	0.43
1:I:71:ASN:OD1	1:I:72:ASP:N	2.52	0.42
2:L:18:ASN:C	3:B:2:NAG:H83	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:201:VAL:HG11	2:L:385:SER:CB	2.47	0.42
2:L:415:VAL:N	2:L:416:PRO:HD2	2.35	0.42
2:L:7:ILE:O	2:L:8:CYS:C	2.56	0.42
2:L:97:ASP:O	2:L:101:GLN:HG3	2.19	0.42
1:I:225:ASN:HD22	1:I:225:ASN:N	2.17	0.42
2:L:332:LYS:HB2	2:L:366:ASP:OD1	2.19	0.42
1:I:156:GLU:H	1:I:156:GLU:HG2	1.67	0.42
1:I:190:VAL:O	1:I:194:THR:N	2.52	0.42
1:I:292:ILE:HB	1:I:417:LEU:HB2	2.00	0.42
2:L:71:ASN:O	2:L:425:ARG:NH1	2.53	0.42
1:I:419:PHE:CE2	1:I:431:MET:HE3	2.55	0.42
2:L:258:PHE:HB2	2:L:316:LEU:HD21	2.01	0.42
1:I:284:GLY:O	1:I:285:ASP:HB2	2.20	0.42
2:L:127:ASN:O	2:L:131:TYR:HD2	2.02	0.42
2:L:195:GLU:HG3	2:L:220:TYR:CZ	2.55	0.42
1:I:194:THR:CB	1:I:205:GLU:OE1	2.68	0.42
1:I:261:TYR:HD2	1:I:327:HIS:NE2	2.17	0.42
1:I:266:PHE:HD2	1:I:324:LEU:CD2	2.33	0.42
1:I:418:VAL:CG2	1:I:418:VAL:O	2.68	0.42
1:I:141:VAL:HG21	1:I:228:TYR:CZ	2.54	0.42
1:I:195:GLU:H	1:I:202:ILE:HD12	1.85	0.42
2:L:125:LYS:O	2:L:129:ARG:HG2	2.20	0.42
2:L:120:HIS:HB3	2:L:165:VAL:HG11	2.02	0.42
1:I:111:ILE:CG2	1:I:114:LYS:HG3	2.49	0.41
1:I:111:ILE:HG22	1:I:114:LYS:HG2	2.02	0.41
1:I:11:LYS:CB	1:I:12:PRO:CD	2.98	0.41
1:I:152:LEU:HD12	1:I:220:VAL:HG13	2.01	0.41
1:I:17:MET:HA	1:I:161:ILE:HD11	2.02	0.41
1:I:342:GLN:NE2	1:I:342:GLN:H	2.17	0.41
2:L:253:TYR:O	2:L:254:GLN:HB3	2.20	0.41
1:I:55:ASN:HD22	1:I:55:ASN:HA	1.68	0.41
2:L:200:ASP:OD1	2:L:370:LYS:HE2	2.19	0.41
1:I:323:MET:HE1	1:I:403:LEU:CD1	2.49	0.41
2:L:364:VAL:HG22	2:L:390:ILE:HD13	2.03	0.41
2:L:394:SER:O	2:L:395:LEU:CB	2.67	0.41
2:L:96:ASN:CG	2:L:97:ASP:N	2.55	0.41
1:I:62:PHE:CD1	1:I:346:MET:HE2	2.56	0.41
1:I:88:ALA:O	1:I:120:HIS:HE1	2.04	0.41
2:L:304:LEU:HD11	2:L:411:PHE:CE2	2.56	0.41
2:L:94:ALA:HB1	2:L:98:THR:HG22	2.02	0.41
1:I:248:TYR:O	1:I:415:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:395:ALA:O	2:L:316:LEU:HB2	2.21	0.41
2:L:170:LEU:HD23	2:L:170:LEU:C	2.42	0.41
1:I:87:PHE:CG	1:I:106:PHE:CZ	3.09	0.40
1:I:210:LEU:HB2	1:I:223:LEU:HB2	2.03	0.40
1:I:263:GLU:OE2	1:I:407:ARG:NE	2.54	0.40
1:I:350:ASP:O	1:I:353:SER:N	2.52	0.40
1:I:47:ARG:HD2	1:I:47:ARG:N	2.36	0.40
2:L:147:PHE:C	2:L:213:LEU:HD12	2.41	0.40
2:L:251:MET:CE	2:L:319:HIS:HB3	2.52	0.40
1:I:195:GLU:CA	1:I:202:ILE:HD12	2.51	0.40
1:I:423:VAL:O	1:I:424:PRO:C	2.60	0.40
1:I:79:SER:O	1:I:82:SER:HB3	2.22	0.40
2:L:141:VAL:HG22	2:L:220:TYR:HB3	2.04	0.40
2:L:94:ALA:HA	2:L:351:LEU:HD23	2.03	0.40
2:L:197:ARG:NH2	2:L:381:GLU:OE1	2.53	0.40
1:I:17:MET:HE2	1:I:117:ASP:O	2.22	0.40
2:L:11:LYS:CB	2:L:12:PRO:CD	2.99	0.40
2:L:59:ALA:O	2:L:423:MET:HE1	2.22	0.40
1:I:152:LEU:CD1	1:I:220:VAL:HG13	2.52	0.40
1:I:71:ASN:HB3	1:I:74:ASP:OD2	2.22	0.40
2:L:304:LEU:HD23	2:L:304:LEU:HA	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:160:ASP:OD1	1:I:270:ARG:NH1[2_756]	2.13	0.07

## 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	I	403/440 (92%)	368 (91%)	29 (7%)	6 (2%)	10	33
2	L	380/432 (88%)	343 (90%)	32 (8%)	5 (1%)	12	36
All	All	783/872 (90%)	711 (91%)	61 (8%)	11 (1%)	11	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	18	ASN
1	I	135	ASN
2	L	10	ALA
1	I	17	MET
1	I	116	SER
2	L	21	CYS
1	I	16	PRO
2	L	406	ARG
2	L	288	PRO
2	L	421	ILE
1	I	271	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	I	327/390 (84%)	310 (95%)	17 (5%)	23	55
2	L	292/383 (76%)	277 (95%)	15 (5%)	24	55
All	All	619/773 (80%)	587 (95%)	32 (5%)	23	55

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	13	ARG
1	I	45	ASN
1	I	47	ARG
1	I	51	LEU
1	I	73	ASN

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Mol	Chain	Res	Type
1	I	123	PHE
1	I	129	ARG
1	I	170	LEU
1	I	225	ASN
1	I	228	TYR
1	I	297	GLU
1	I	310	GLU
1	I	312	LEU
1	I	324	LEU
1	I	418	VAL
1	I	427	THR
1	I	436	ASN
2	L	7	ILE
2	L	123	PHE
2	L	129	ARG
2	L	170	LEU
2	L	201	VAL
2	L	215	LEU
2	L	243	ASP
2	L	285	LEU
2	L	302	GLU
2	L	315	MET
2	L	316	LEU
2	L	324	ARG
2	L	393	ARG
2	L	405	ASN
2	L	410	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	45	ASN
1	I	55	ASN
1	I	73	ASN
1	I	342	GLN
1	I	344	GLN
1	I	426	ASN
1	I	436	ASN
2	L	55	ASN
2	L	71	ASN
2	L	100	GLN
2	L	144	ASN

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Mol	Chain	Res	Type
2	L	178	ASN
2	L	217	ASN
2	L	254	GLN
2	L	336	GLN
2	L	405	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 ⓘ

4 monosaccharides 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	1	1,3	14,14,15	0.63	0	17,19,21	1.24	3 (17%)
3	NAG	A	2	3	14,14,15	0.57	0	17,19,21	0.66	0
3	NAG	B	1	3,2	14,14,15	0.59	0	17,19,21	0.68	0
3	NAG	B	2	3	14,14,15	0.59	0	17,19,21	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
3	NAG	A	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	NAG	C4-C3-C2	2.61	114.85	111.02
3	A	1	NAG	C1-O5-C5	-2.10	109.35	112.19
3	A	1	NAG	C3-C4-C5	2.05	113.90	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2	NAG	C3-C2-N2-C7
3	A	2	NAG	O5-C5-C6-O6
3	A	2	NAG	C4-C5-C6-O6
3	A	2	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2	NAG	3	0
3	A	1	NAG	1	0
3	A	2	NAG	2	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
4	NAG	I	801	1	14,14,15	0.57	0	17,19,21	0.66	0
4	NAG	I	804	1	14,14,15	0.56	0	17,19,21	0.62	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	I	801	1	-	3/6/23/26	0/1/1/1
4	NAG	I	804	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	801	NAG	O5-C5-C6-O6
4	I	801	NAG	C4-C5-C6-O6
4	I	804	NAG	C4-C5-C6-O6
4	I	804	NAG	O5-C5-C6-O6
4	I	801	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	801	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 [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	I	411/440 (93%)	-0.27	0 <span>100</span> <span>100</span>	44, 64, 107, 138	0
2	L	392/432 (90%)	-0.27	2 (0%) <span>91</span> <span>88</span>	52, 81, 127, 178	0
All	All	803/872 (92%)	-0.27	2 (0%) <span>95</span> <span>94</span>	44, 72, 119, 178	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	404	ALA	3.8
2	L	405	ASN	2.1

### 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	B	2	14/15	<span>0.71</span>	<span>0.52</span>	163,176,197,202	0
3	NAG	A	2	14/15	0.88	0.23	126,152,190,193	0
3	NAG	B	1	14/15	0.89	0.37	84,111,159,178	0
3	NAG	A	1	14/15	0.92	0.12	78,102,117,139	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	I	804	14/15	0.74	0.17	144,155,169,173	0
4	NAG	I	801	14/15	0.88	0.18	125,142,161,164	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.