



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:22 am GMT

PDB ID : 4AY1  
Title : Human YKL-39 is a pseudo-chitinase with retained chitooligosaccharide binding properties  
Authors : Schimpl, M.; Rush, C.L.; Betou, M.; Eggleston, I.M.; Penman, G.A.; Recklies, A.D.; Van Aalten, D.M.F.  
Deposited on : 2012-06-17  
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

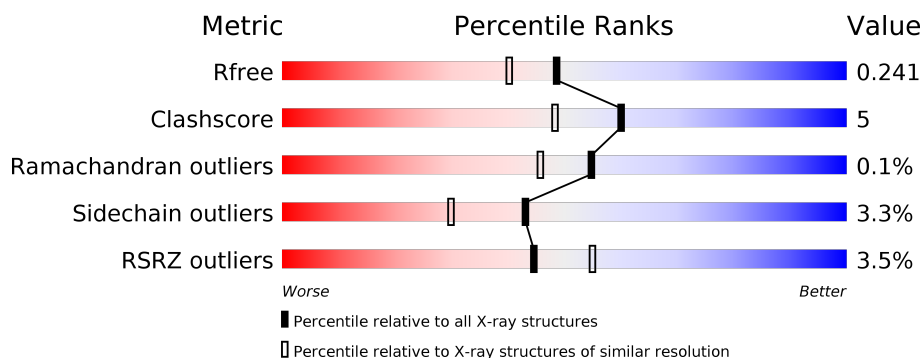
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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.



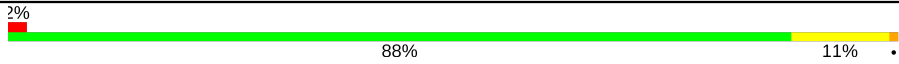
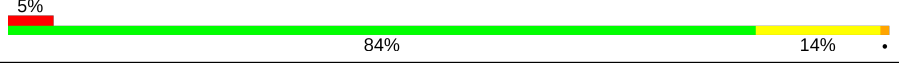
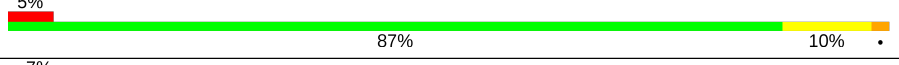

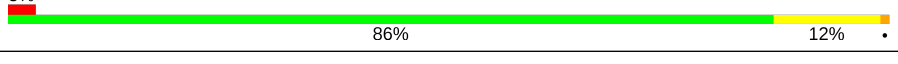
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	365	<div> <div>2%</div> <div>92%</div> <div>6%</div> </div>
1	B	365	<div> <div>4%</div> <div>85%</div> <div>13%</div> </div>
1	C	365	<div> <div>3%</div> <div>91%</div> <div>8%</div> </div>
1	D	365	<div> <div>3%</div> <div>86%</div> <div>12%</div> </div>
1	E	365	<div> <div>2%</div> <div>89%</div> <div>10%</div> </div>
1	F	365	<div> <div>3%</div> <div>92%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	365	 2% 88% 11% .
1	H	365	 4% 87% 12% .
1	I	365	 5% 84% 14% .
1	J	365	 5% 87% 10% .
1	K	365	 7% 83% 14% .
1	L	365	 3% 86% 12% .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 37104 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 CHITINASE-3-LIKE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2878	1853	474	539	12			
1	B	364	Total	C	N	O	S	0	0	0
			2869	1847	474	536	12			
1	C	364	Total	C	N	O	S	0	0	0
			2882	1856	475	539	12			
1	D	364	Total	C	N	O	S	0	0	0
			2882	1856	475	539	12			
1	E	364	Total	C	N	O	S	0	0	0
			2882	1856	475	539	12			
1	F	364	Total	C	N	O	S	0	0	0
			2878	1853	474	539	12			
1	G	364	Total	C	N	O	S	0	0	0
			2882	1856	475	539	12			
1	H	364	Total	C	N	O	S	0	0	0
			2874	1852	474	536	12			
1	I	364	Total	C	N	O	S	0	0	0
			2878	1853	474	539	12			
1	J	364	Total	C	N	O	S	0	0	0
			2866	1846	472	536	12			
1	K	364	Total	C	N	O	S	0	0	0
			2878	1853	474	539	12			
1	L	364	Total	C	N	O	S	0	0	0
			2878	1853	474	539	12			

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			57	32	4	21		
2	B	4	Total	C	N	O	0	0
			57	32	4	21		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	4	Total	C	N	O	0	0
			57	32	4	21		
2	D	4	Total	C	N	O	0	0
			57	32	4	21		
2	E	4	Total	C	N	O	0	0
			57	32	4	21		
2	F	4	Total	C	N	O	0	0
			57	32	4	21		
2	G	4	Total	C	N	O	0	0
			57	32	4	21		
2	H	4	Total	C	N	O	0	0
			57	32	4	21		
2	I	4	Total	C	N	O	0	0
			57	32	4	21		
2	J	4	Total	C	N	O	0	0
			57	32	4	21		
2	K	4	Total	C	N	O	0	0
			57	32	4	21		
2	L	4	Total	C	N	O	0	0
			57	32	4	21		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	210	Total	O	0	0
			210	210		
3	B	147	Total	O	0	0
			147	147		
3	C	184	Total	O	0	0
			184	184		
3	D	170	Total	O	0	0
			170	170		
3	E	195	Total	O	0	0
			195	195		
3	F	179	Total	O	0	0
			179	179		
3	G	169	Total	O	0	0
			169	169		
3	H	166	Total	O	0	0
			166	166		
3	I	117	Total	O	0	0
			117	117		

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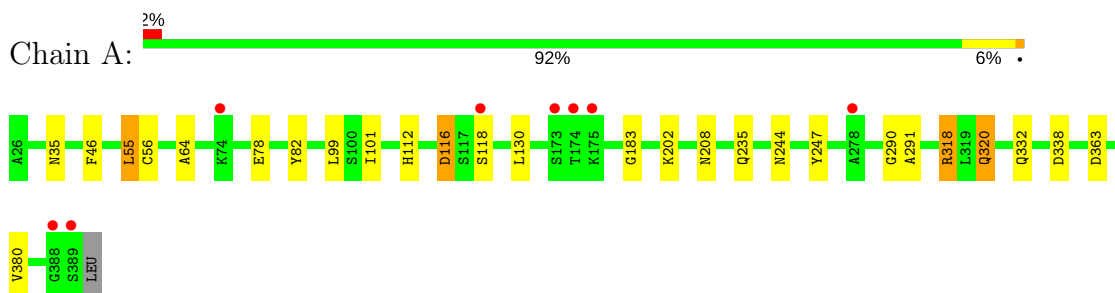
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	150	Total 150	O 150	0	0
3	K	83	Total 83	O 83	0	0
3	L	123	Total 123	O 123	0	0

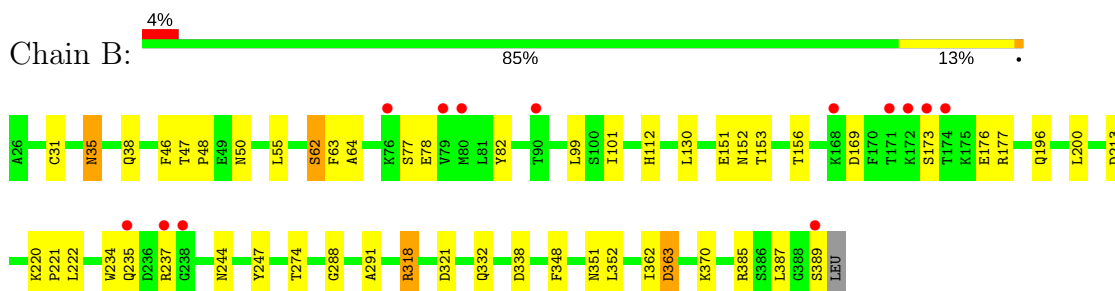
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

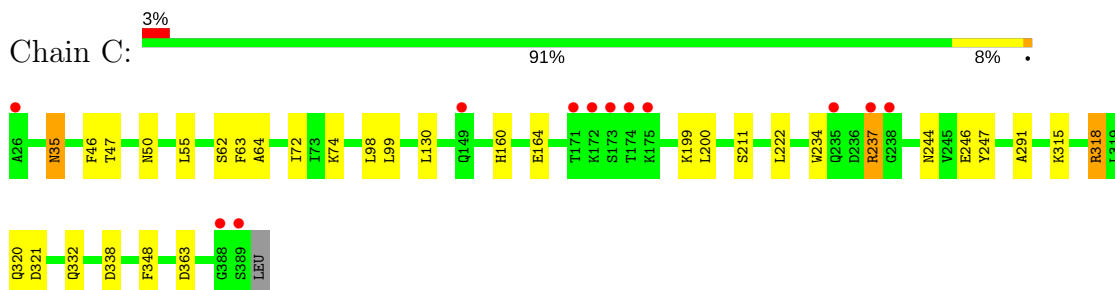
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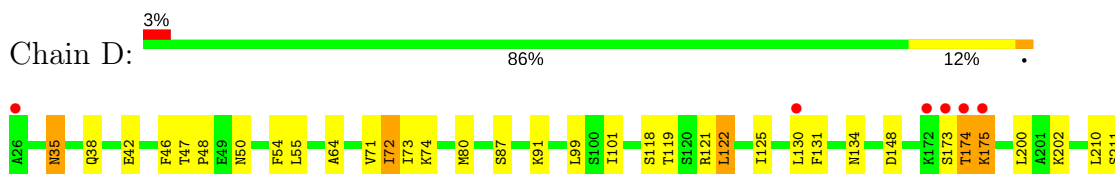
#### • Molecule 1: CHITINASE-3-LIKE PROTEIN 2



#### • Molecule 1: CHITINASE-3-LIKE PROTEIN 2

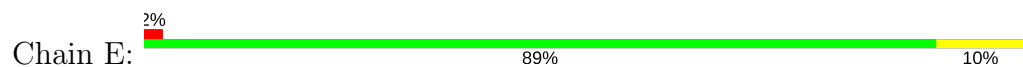


#### • Molecule 1: CHITINASE-3-LIKE PROTEIN 2

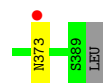
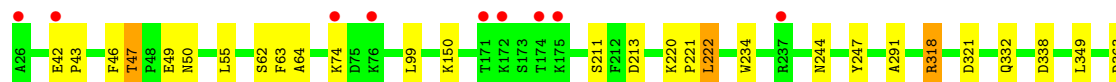




• Molecule 1: CHITINASE-3-LIKE PROTEIN 2



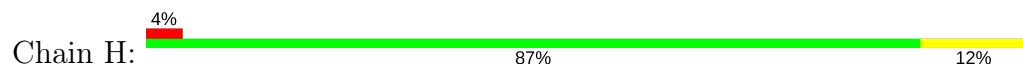
• Molecule 1: CHITINASE-3-LIKE PROTEIN 2



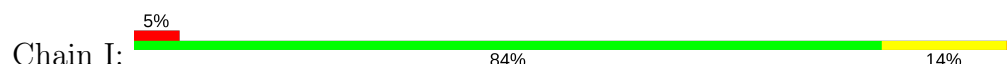
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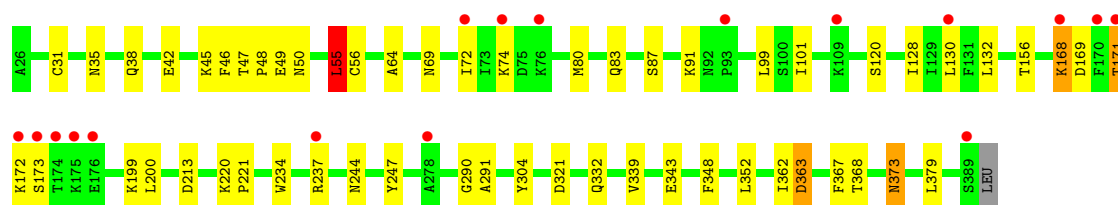
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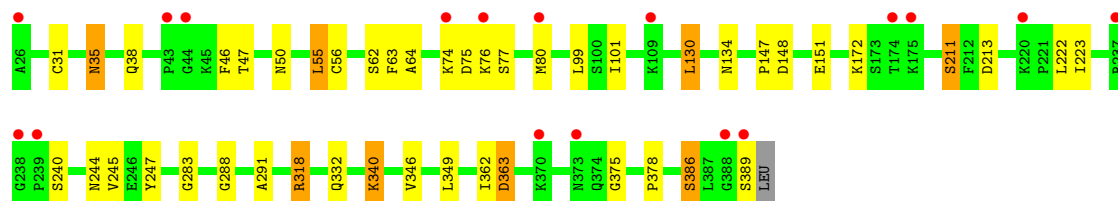
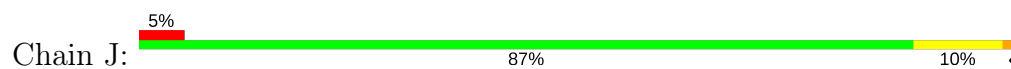
• Molecule 1: CHITINASE-3-LIKE PROTEIN 2



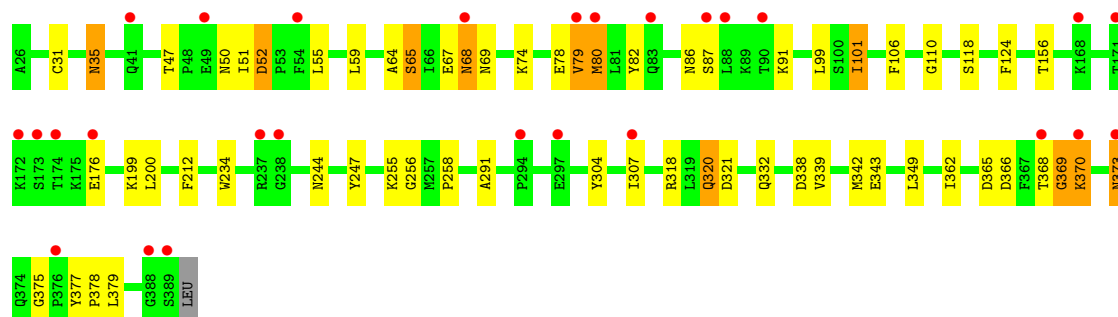
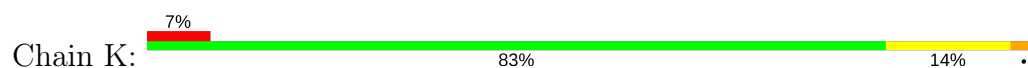




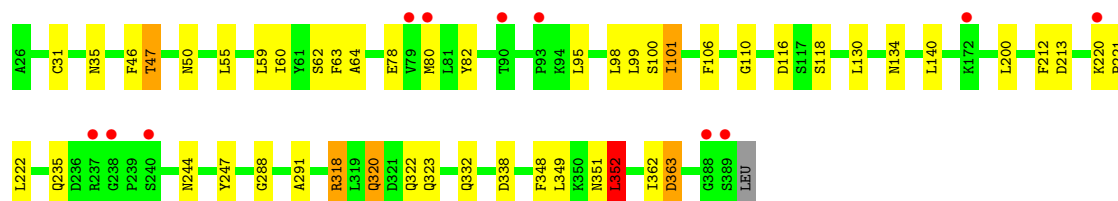
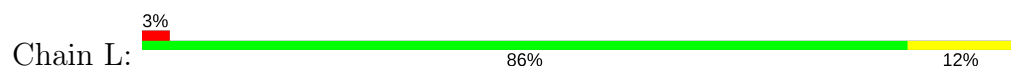
• Molecule 1: CHITINASE-3-LIKE PROTEIN 2



• Molecule 1: CHITINASE-3-LIKE PROTEIN 2



• Molecule 1: CHITINASE-3-LIKE PROTEIN 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	255.69Å 152.54Å 138.19Å 90.00° 94.62° 90.00°	Depositor
Resolution (Å)	137.36 – 1.95 19.99 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (137.36-1.95) 99.4 (19.99-1.95)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, $R_{free}$	0.191 , 0.239 0.191 , 0.241	Depositor DCC
$R_{free}$ test set	1897 reflections (0.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.1	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	37104	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.76% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.59	0/2954	0.67	2/4002 (0.0%)
1	B	0.50	0/2944	0.64	1/3985 (0.0%)
1	C	0.53	0/2958	0.65	2/4006 (0.0%)
1	D	0.55	0/2958	0.64	1/4006 (0.0%)
1	E	0.57	0/2958	0.67	4/4006 (0.1%)
1	F	0.57	0/2954	0.67	2/4002 (0.0%)
1	G	0.55	0/2958	0.63	0/4006
1	H	0.54	0/2950	0.64	1/3996 (0.0%)
1	I	0.49	0/2954	0.60	1/4002 (0.0%)
1	J	0.54	0/2942	0.64	0/3988
1	K	0.60	2/2954 (0.1%)	0.64	0/4002
1	L	0.50	0/2954	0.65	2/4002 (0.0%)
All	All	0.55	2/35438 (0.0%)	0.65	16/48003 (0.0%)

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
1	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	52	ASP	CG-OD2	12.61	1.54	1.25
1	K	86	ASN	C-O	7.66	1.37	1.23

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	318	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	A	318	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	A	318	ARG	CG-CD-NE	-7.20	96.68	111.80
1	D	342	MET	CA-CB-CG	-6.93	101.52	113.30
1	B	318	ARG	NE-CZ-NH2	-6.28	117.16	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	387	LEU	Peptide

## 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	2878	0	2819	19	0
1	B	2869	0	2811	34	0
1	C	2882	0	2830	18	1
1	D	2882	0	2830	43	1
1	E	2882	0	2830	25	1
1	F	2878	0	2819	20	0
1	G	2882	0	2830	31	0
1	H	2874	0	2820	33	0
1	I	2878	0	2819	48	0
1	J	2866	0	2798	29	0
1	K	2878	0	2819	49	0
1	L	2878	0	2819	28	0
2	A	57	0	51	0	0
2	B	57	0	51	1	0
2	C	57	0	51	0	0
2	D	57	0	51	2	0
2	E	57	0	51	0	0
2	F	57	0	51	1	0
2	G	57	0	51	0	0
2	H	57	0	51	1	0
2	I	57	0	51	1	0
2	J	57	0	51	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	57	0	51	1	0
2	L	57	0	51	1	0
3	A	210	0	0	0	0
3	B	147	0	0	3	0
3	C	184	0	0	0	0
3	D	170	0	0	1	0
3	E	195	0	0	0	0
3	F	179	0	0	3	1
3	G	169	0	0	2	0
3	H	166	0	0	1	0
3	I	117	0	0	1	0
3	J	150	0	0	2	0
3	K	83	0	0	2	0
3	L	123	0	0	2	0
All	All	37104	0	34456	370	2

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 5.

The worst 5 of 370 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:K:68:ASN:HB3	3:K:2004:HOH:O	1.47	1.14
1:I:168:LYS:O	1:I:171:THR:HG22	1.47	1.14
1:I:47:THR:HG21	1:I:80:MET:CE	1.81	1.09
1:I:47:THR:CG2	1:I:80:MET:CE	2.37	1.02
1:L:351:ASN:HB2	3:L:2111:HOH:O	1.60	1.01

All (2) 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:E:153:THR:OG1	3:F:2107:HOH:O[2_655]	1.96	0.24
1:C:320:GLN:NE2	1:D:347:GLN:OE1[4_546]	2.11	0.09

## 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	362/365 (99%)	357 (99%)	5 (1%)	0	100	100
1	B	362/365 (99%)	358 (99%)	4 (1%)	0	100	100
1	C	362/365 (99%)	360 (99%)	2 (1%)	0	100	100
1	D	362/365 (99%)	357 (99%)	3 (1%)	2 (1%)	28	15
1	E	362/365 (99%)	356 (98%)	6 (2%)	0	100	100
1	F	362/365 (99%)	357 (99%)	5 (1%)	0	100	100
1	G	362/365 (99%)	358 (99%)	4 (1%)	0	100	100
1	H	362/365 (99%)	357 (99%)	5 (1%)	0	100	100
1	I	362/365 (99%)	356 (98%)	6 (2%)	0	100	100
1	J	362/365 (99%)	359 (99%)	2 (1%)	1 (0%)	44	33
1	K	362/365 (99%)	351 (97%)	10 (3%)	1 (0%)	44	33
1	L	362/365 (99%)	358 (99%)	4 (1%)	0	100	100
All	All	4344/4380 (99%)	4284 (99%)	56 (1%)	4 (0%)	55	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	175	LYS
1	K	369	GLY
1	D	148	ASP
1	J	148	ASP

### 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	315/317 (99%)	308 (98%)	7 (2%)	57	49
1	B	313/317 (99%)	301 (96%)	12 (4%)	38	24
1	C	316/317 (100%)	307 (97%)	9 (3%)	49	37
1	D	316/317 (100%)	303 (96%)	13 (4%)	35	21
1	E	316/317 (100%)	309 (98%)	7 (2%)	57	49
1	F	315/317 (99%)	307 (98%)	8 (2%)	53	42
1	G	316/317 (100%)	306 (97%)	10 (3%)	44	31
1	H	314/317 (99%)	305 (97%)	9 (3%)	48	35
1	I	315/317 (99%)	306 (97%)	9 (3%)	48	35
1	J	312/317 (98%)	299 (96%)	13 (4%)	34	20
1	K	315/317 (99%)	301 (96%)	14 (4%)	33	18
1	L	315/317 (99%)	302 (96%)	13 (4%)	35	21
All	All	3778/3804 (99%)	3654 (97%)	124 (3%)	43	30

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	35	ASN
1	H	200	LEU
1	L	80	MET
1	G	55	LEU
1	G	235	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	332	GLN
1	G	373	ASN
1	L	50	ASN
1	F	373	ASN
1	G	244	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 ⓘ

48 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	400	2	14,14,15	1.04	1 (7%)	15,19,21	0.84	0
2	NAG	A	401	2	14,14,15	0.94	0	15,19,21	1.75	3 (20%)
2	NAG	A	402	2	14,14,15	1.22	2 (14%)	15,19,21	0.95	0
2	NAG	A	403	2	15,15,15	1.19	1 (6%)	21,21,21	1.35	3 (14%)
2	NAG	B	400	2	14,14,15	0.75	1 (7%)	15,19,21	0.78	0
2	NAG	B	401	2	14,14,15	1.18	1 (7%)	15,19,21	1.43	2 (13%)
2	NAG	B	402	2	14,14,15	0.97	1 (7%)	15,19,21	1.07	1 (6%)
2	NAG	B	403	2	15,15,15	0.69	0	21,21,21	1.43	4 (19%)
2	NAG	C	400	2	14,14,15	0.80	0	15,19,21	0.89	0
2	NAG	C	401	2	14,14,15	1.22	1 (7%)	15,19,21	1.34	2 (13%)
2	NAG	C	402	2	14,14,15	0.93	0	15,19,21	1.02	1 (6%)
2	NAG	C	403	2	15,15,15	0.77	0	21,21,21	1.41	4 (19%)
2	NAG	D	400	2	14,14,15	0.85	0	15,19,21	0.93	0
2	NAG	D	401	2	14,14,15	0.99	1 (7%)	15,19,21	1.19	1 (6%)
2	NAG	D	402	2	14,14,15	1.01	1 (7%)	15,19,21	1.42	3 (20%)
2	NAG	D	403	2	15,15,15	0.72	0	21,21,21	1.45	4 (19%)
2	NAG	E	400	2	14,14,15	0.91	0	15,19,21	0.85	1 (6%)
2	NAG	E	401	2	14,14,15	0.90	0	15,19,21	1.16	2 (13%)
2	NAG	E	402	2	14,14,15	0.82	0	15,19,21	1.40	2 (13%)
2	NAG	E	403	2	15,15,15	1.04	2 (13%)	21,21,21	1.65	5 (23%)
2	NAG	F	400	2	14,14,15	0.77	1 (7%)	15,19,21	1.27	1 (6%)
2	NAG	F	401	2	14,14,15	1.30	2 (14%)	15,19,21	1.31	4 (26%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	F	402	2	14,14,15	0.99	2 (14%)	15,19,21	1.04	1 (6%)
2	NAG	F	403	2	15,15,15	0.86	1 (6%)	21,21,21	1.51	4 (19%)
2	NAG	G	400	2	14,14,15	0.94	0	15,19,21	0.97	0
2	NAG	G	401	2	14,14,15	1.40	3 (21%)	15,19,21	1.43	2 (13%)
2	NAG	G	402	2	14,14,15	0.90	1 (7%)	15,19,21	1.06	2 (13%)
2	NAG	G	403	2	15,15,15	0.93	1 (6%)	21,21,21	1.28	2 (9%)
2	NAG	H	400	2	14,14,15	0.83	0	15,19,21	0.87	1 (6%)
2	NAG	H	401	2	14,14,15	0.87	0	15,19,21	1.37	2 (13%)
2	NAG	H	402	2	14,14,15	0.92	1 (7%)	15,19,21	1.22	1 (6%)
2	NAG	H	403	2	15,15,15	0.75	0	21,21,21	1.18	2 (9%)
2	NAG	I	400	2	14,14,15	0.39	0	15,19,21	1.07	0
2	NAG	I	401	2	14,14,15	0.88	0	15,19,21	1.34	3 (20%)
2	NAG	I	402	2	14,14,15	0.70	0	15,19,21	1.03	1 (6%)
2	NAG	I	403	2	15,15,15	0.92	0	21,21,21	1.09	2 (9%)
2	NAG	J	400	2	14,14,15	0.92	0	15,19,21	1.05	1 (6%)
2	NAG	J	401	2	14,14,15	1.06	1 (7%)	15,19,21	1.47	3 (20%)
2	NAG	J	402	2	14,14,15	0.85	0	15,19,21	0.96	0
2	NAG	J	403	2	15,15,15	0.84	0	21,21,21	1.51	3 (14%)
2	NAG	K	400	2	14,14,15	0.95	1 (7%)	15,19,21	0.75	0
2	NAG	K	401	2	14,14,15	1.02	1 (7%)	15,19,21	1.66	5 (33%)
2	NAG	K	402	2	14,14,15	0.59	0	15,19,21	0.99	1 (6%)
2	NAG	K	403	2	15,15,15	0.98	0	21,21,21	1.38	4 (19%)
2	NAG	L	400	2	14,14,15	0.71	0	15,19,21	1.13	1 (6%)
2	NAG	L	401	2	14,14,15	0.98	0	15,19,21	1.34	3 (20%)
2	NAG	L	402	2	14,14,15	0.88	0	15,19,21	1.31	3 (20%)
2	NAG	L	403	2	15,15,15	1.00	1 (6%)	21,21,21	1.16	2 (9%)

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	400	2	-	0/6/23/26	0/1/1/1
2	NAG	A	401	2	-	0/6/23/26	0/1/1/1
2	NAG	A	402	2	-	0/6/23/26	0/1/1/1
2	NAG	A	403	2	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	400	2	-	0/6/23/26	0/1/1/1
2	NAG	B	401	2	-	0/6/23/26	0/1/1/1
2	NAG	B	402	2	-	0/6/23/26	0/1/1/1
2	NAG	B	403	2	-	0/6/26/26	0/1/1/1
2	NAG	C	400	2	-	0/6/23/26	0/1/1/1
2	NAG	C	401	2	-	0/6/23/26	0/1/1/1
2	NAG	C	402	2	-	0/6/23/26	0/1/1/1
2	NAG	C	403	2	-	0/6/26/26	0/1/1/1
2	NAG	D	400	2	-	0/6/23/26	0/1/1/1
2	NAG	D	401	2	-	0/6/23/26	0/1/1/1
2	NAG	D	402	2	-	0/6/23/26	0/1/1/1
2	NAG	D	403	2	-	0/6/26/26	0/1/1/1
2	NAG	E	400	2	-	0/6/23/26	0/1/1/1
2	NAG	E	401	2	-	0/6/23/26	0/1/1/1
2	NAG	E	402	2	-	0/6/23/26	0/1/1/1
2	NAG	E	403	2	-	0/6/26/26	0/1/1/1
2	NAG	F	400	2	-	0/6/23/26	0/1/1/1
2	NAG	F	401	2	-	0/6/23/26	0/1/1/1
2	NAG	F	402	2	-	0/6/23/26	0/1/1/1
2	NAG	F	403	2	-	0/6/26/26	0/1/1/1
2	NAG	G	400	2	-	0/6/23/26	0/1/1/1
2	NAG	G	401	2	-	0/6/23/26	0/1/1/1
2	NAG	G	402	2	-	0/6/23/26	0/1/1/1
2	NAG	G	403	2	-	0/6/26/26	0/1/1/1
2	NAG	H	400	2	-	0/6/23/26	0/1/1/1
2	NAG	H	401	2	-	0/6/23/26	0/1/1/1
2	NAG	H	402	2	-	0/6/23/26	0/1/1/1
2	NAG	H	403	2	-	0/6/26/26	0/1/1/1
2	NAG	I	400	2	-	0/6/23/26	0/1/1/1
2	NAG	I	401	2	-	0/6/23/26	0/1/1/1
2	NAG	I	402	2	-	0/6/23/26	0/1/1/1
2	NAG	I	403	2	-	0/6/26/26	0/1/1/1
2	NAG	J	400	2	-	0/6/23/26	0/1/1/1
2	NAG	J	401	2	-	0/6/23/26	0/1/1/1
2	NAG	J	402	2	-	0/6/23/26	0/1/1/1
2	NAG	J	403	2	-	0/6/26/26	0/1/1/1
2	NAG	K	400	2	-	0/6/23/26	0/1/1/1
2	NAG	K	401	2	-	0/6/23/26	0/1/1/1
2	NAG	K	402	2	-	0/6/23/26	0/1/1/1
2	NAG	K	403	2	-	0/6/26/26	0/1/1/1
2	NAG	L	400	2	-	0/6/23/26	0/1/1/1
2	NAG	L	401	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	L	402	2	-	0/6/23/26	0/1/1/1
2	NAG	L	403	2	-	0/6/26/26	0/1/1/1

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	402	NAG	O5-C1	-2.59	1.39	1.43
2	F	402	NAG	C8-C7	2.01	1.54	1.50
2	F	403	NAG	C8-C7	2.04	1.55	1.50
2	D	402	NAG	C8-C7	2.07	1.55	1.50
2	B	402	NAG	C8-C7	2.08	1.55	1.50

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	402	NAG	O4-C4-C3	-3.85	101.98	110.36
2	F	400	NAG	O5-C1-C2	-3.84	106.13	111.47
2	D	403	NAG	O1-C1-O5	-3.63	99.45	110.20
2	C	403	NAG	C1-O5-C5	-3.56	106.98	113.39
2	F	403	NAG	O4-C4-C3	-3.50	102.75	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	NAG	1	0
2	D	401	NAG	2	0
2	D	402	NAG	1	0
2	F	402	NAG	1	0
2	H	402	NAG	1	0
2	I	402	NAG	1	0
2	J	402	NAG	1	0
2	K	401	NAG	1	0
2	K	402	NAG	1	0
2	L	402	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

### 6.1 Protein, DNA and RNA chains

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	364/365 (99%)	-0.13	8 (2%) 62 72	12, 22, 33, 50	0
1	B	364/365 (99%)	0.05	13 (3%) 43 54	17, 27, 43, 57	0
1	C	364/365 (99%)	-0.02	12 (3%) 47 58	15, 24, 38, 57	0
1	D	364/365 (99%)	0.03	10 (2%) 55 65	14, 25, 42, 59	0
1	E	364/365 (99%)	-0.09	7 (1%) 67 76	13, 23, 36, 50	0
1	F	364/365 (99%)	-0.10	10 (2%) 55 65	14, 23, 38, 52	0
1	G	364/365 (99%)	-0.09	9 (2%) 58 67	15, 24, 37, 53	0
1	H	364/365 (99%)	-0.00	13 (3%) 43 54	15, 24, 37, 51	0
1	I	364/365 (99%)	0.17	17 (4%) 32 43	17, 30, 48, 58	0
1	J	364/365 (99%)	0.08	17 (4%) 32 43	16, 27, 40, 50	0
1	K	364/365 (99%)	0.37	27 (7%) 15 24	21, 33, 56, 65	0
1	L	364/365 (99%)	0.09	11 (3%) 51 61	15, 29, 45, 57	0
All	All	4368/4380 (99%)	0.03	154 (3%) 44 55	12, 26, 43, 65	0

The worst 5 of 154 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	174	THR	10.3
1	E	388	GLY	7.4
1	B	174	THR	7.4
1	J	389	SER	6.7
1	H	389	SER	6.6

### 6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

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
2	NAG	E	403	15/15	0.94	0.09	0.26	17,22,28,30	0
2	NAG	B	403	15/15	0.94	0.10	0.14	20,23,28,30	0
2	NAG	B	402	14/15	0.96	0.09	-0.36	19,20,23,24	0
2	NAG	H	403	15/15	0.95	0.08	-0.52	18,21,28,28	0
2	NAG	C	403	15/15	0.96	0.07	-0.53	16,21,28,29	0
2	NAG	I	401	14/15	0.96	0.07	-0.61	23,24,26,26	0
2	NAG	K	403	15/15	0.94	0.08	-0.62	20,23,30,33	0
2	NAG	L	403	15/15	0.95	0.09	-0.66	21,24,29,33	0
2	NAG	D	400	14/15	0.97	0.07	-0.66	18,19,21,22	0
2	NAG	B	401	14/15	0.98	0.07	-0.67	16,19,21,21	0
2	NAG	D	403	15/15	0.96	0.07	-0.67	17,22,26,29	0
2	NAG	G	403	15/15	0.96	0.08	-0.69	15,18,23,23	0
2	NAG	F	401	14/15	0.97	0.07	-0.70	13,16,18,19	0
2	NAG	H	401	14/15	0.98	0.07	-0.71	13,15,17,17	0
2	NAG	K	400	14/15	0.95	0.09	-0.71	27,31,34,35	0
2	NAG	I	403	15/15	0.96	0.08	-0.75	24,26,35,39	0
2	NAG	K	402	14/15	0.97	0.07	-0.84	21,22,27,28	0
2	NAG	H	402	14/15	0.97	0.07	-0.84	14,16,20,21	0
2	NAG	K	401	14/15	0.97	0.07	-0.89	22,24,26,27	0
2	NAG	J	400	14/15	0.97	0.07	-0.95	19,22,25,25	0
2	NAG	B	400	14/15	0.97	0.07	-0.98	21,23,26,27	0
2	NAG	D	401	14/15	0.97	0.06	-1.02	16,17,19,21	0
2	NAG	I	400	14/15	0.96	0.07	-1.07	25,30,33,35	0
2	NAG	D	402	14/15	0.97	0.07	-1.14	17,18,21,23	0
2	NAG	J	402	14/15	0.97	0.07	-1.18	19,21,23,23	0
2	NAG	C	400	14/15	0.97	0.07	-1.22	14,17,19,20	0
2	NAG	F	400	14/15	0.97	0.06	-1.23	15,17,18,20	0
2	NAG	J	401	14/15	0.97	0.06	-1.24	18,20,21,21	0
2	NAG	G	401	14/15	0.98	0.07	-1.29	13,15,18,21	0
2	NAG	A	403	15/15	0.97	0.07	-1.33	12,19,23,26	0
2	NAG	G	402	14/15	0.97	0.06	-1.34	15,17,19,20	0
2	NAG	A	402	14/15	0.98	0.07	-1.35	12,15,20,23	0
2	NAG	F	402	14/15	0.98	0.06	-1.37	13,15,19,21	0
2	NAG	H	400	14/15	0.98	0.06	-1.40	15,17,18,18	0
2	NAG	I	402	14/15	0.98	0.06	-1.40	22,24,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	E	402	14/15	0.96	0.07	-1.40	15,17,21,21	0
2	NAG	E	400	14/15	0.99	0.05	-1.46	14,17,22,22	0
2	NAG	A	401	14/15	0.98	0.06	-1.47	11,13,15,18	0
2	NAG	C	402	14/15	0.99	0.06	-1.48	15,17,21,24	0
2	NAG	C	401	14/15	0.98	0.07	-1.56	13,15,17,19	0
2	NAG	G	400	14/15	0.98	0.05	-1.72	15,17,18,18	0
2	NAG	A	400	14/15	0.98	0.06	-1.74	14,16,19,19	0
2	NAG	F	403	15/15	0.98	0.06	-1.76	13,17,23,24	0
2	NAG	J	403	15/15	0.96	0.06	-1.80	19,22,29,31	0
2	NAG	L	402	14/15	0.98	0.06	-1.94	19,20,24,28	0
2	NAG	E	401	14/15	0.98	0.06	-1.96	13,15,17,18	0
2	NAG	L	400	14/15	0.98	0.05	-2.26	20,22,24,25	0
2	NAG	L	401	14/15	0.98	0.06	-2.45	18,19,22,23	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.