W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 10:09 PM GMT

PDB ID	:	5C97
Title	:	Insulin regulated aminopeptidase
Authors	:	Mpakali, A.; Saridakis, E.; Harlos, K.; Zhao, Y.; Stratikos, E.
Deposited on	:	2015-06-26
Resolution	:	3.37 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
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)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 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	Percentile Ranks	Value
Rfree		0.297
Clashscore		34
Ramachandran outliers		2.4%
Sidechain outliers		3.8%
RSRZ outliers		4.2%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
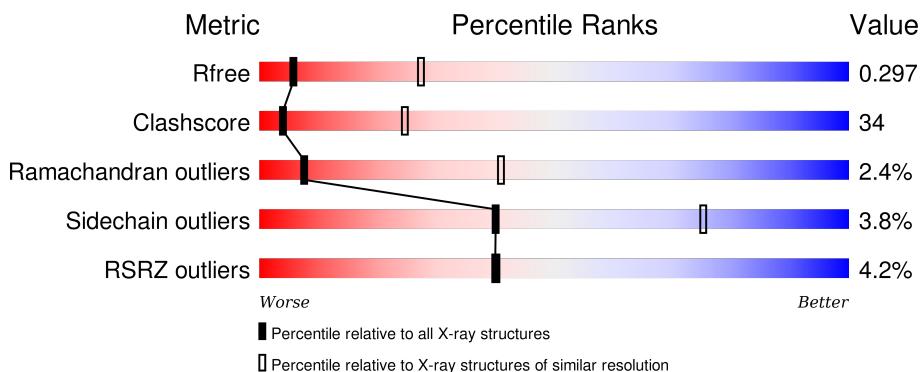
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1084 (3.46-3.30)
Clashscore	102246	1158 (3.46-3.30)
Ramachandran outliers	100387	1139 (3.46-3.30)
Sidechain outliers	100360	1138 (3.46-3.30)
RSRZ outliers	91569	1089 (3.46-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	912	3% / 51% / 39% / · · 6%
1	B	912	5% / 40% / 46% / · · 7%
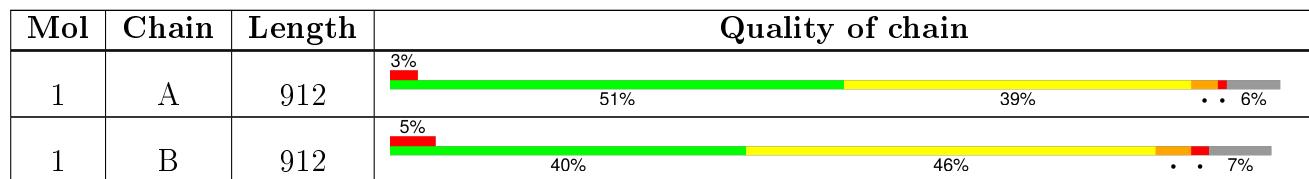
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1106	-	-	-	X
3	NAG	A	1113	-	-	X	-
3	NAG	B	1107	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14098 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 Leucyl-cystinyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	860	Total 6937	C 4487	N 1125	O 1298	S 27	0	2	0
1	B	851	Total 6808	C 4410	N 1097	O 1276	S 25	0	1	0

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MET	-	initiating methionine	UNP Q9UIQ6
A	125	GLY	-	expression tag	UNP Q9UIQ6
A	126	ILE	-	expression tag	UNP Q9UIQ6
A	127	LEU	-	expression tag	UNP Q9UIQ6
A	128	PRO	-	expression tag	UNP Q9UIQ6
A	129	SER	-	expression tag	UNP Q9UIQ6
A	130	PRO	-	expression tag	UNP Q9UIQ6
A	131	GLY	-	expression tag	UNP Q9UIQ6
A	132	ASN	-	expression tag	UNP Q9UIQ6
A	133	PRO	-	expression tag	UNP Q9UIQ6
A	134	ALA	-	expression tag	UNP Q9UIQ6
A	135	LEU	-	expression tag	UNP Q9UIQ6
A	136	LEU	-	expression tag	UNP Q9UIQ6
A	137	SER	-	expression tag	UNP Q9UIQ6
A	138	LEU	-	expression tag	UNP Q9UIQ6
A	139	VAL	-	expression tag	UNP Q9UIQ6
A	140	SER	-	expression tag	UNP Q9UIQ6
A	141	LEU	-	expression tag	UNP Q9UIQ6
A	142	LEU	-	expression tag	UNP Q9UIQ6
A	143	SER	-	expression tag	UNP Q9UIQ6
A	144	VAL	-	expression tag	UNP Q9UIQ6
A	145	LEU	-	expression tag	UNP Q9UIQ6
A	146	LEU	-	expression tag	UNP Q9UIQ6
A	147	MET	-	expression tag	UNP Q9UIQ6
A	148	GLY	-	expression tag	UNP Q9UIQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	149	CYS	-	expression tag	UNP Q9UIQ6
A	150	VAL	-	expression tag	UNP Q9UIQ6
A	151	ALA	-	expression tag	UNP Q9UIQ6
A	152	GLU	-	expression tag	UNP Q9UIQ6
A	153	THR	-	expression tag	UNP Q9UIQ6
A	154	GLY	-	expression tag	UNP Q9UIQ6
A	1026	ARG	-	expression tag	UNP Q9UIQ6
A	1027	THR	-	expression tag	UNP Q9UIQ6
A	1028	GLU	-	expression tag	UNP Q9UIQ6
A	1029	THR	-	expression tag	UNP Q9UIQ6
A	1030	SER	-	expression tag	UNP Q9UIQ6
A	1031	GLN	-	expression tag	UNP Q9UIQ6
A	1032	VAL	-	expression tag	UNP Q9UIQ6
A	1033	ALA	-	expression tag	UNP Q9UIQ6
A	1034	PRO	-	expression tag	UNP Q9UIQ6
A	1035	ALA	-	expression tag	UNP Q9UIQ6
B	124	MET	-	initiating methionine	UNP Q9UIQ6
B	125	GLY	-	expression tag	UNP Q9UIQ6
B	126	ILE	-	expression tag	UNP Q9UIQ6
B	127	LEU	-	expression tag	UNP Q9UIQ6
B	128	PRO	-	expression tag	UNP Q9UIQ6
B	129	SER	-	expression tag	UNP Q9UIQ6
B	130	PRO	-	expression tag	UNP Q9UIQ6
B	131	GLY	-	expression tag	UNP Q9UIQ6
B	132	ASN	-	expression tag	UNP Q9UIQ6
B	133	PRO	-	expression tag	UNP Q9UIQ6
B	134	ALA	-	expression tag	UNP Q9UIQ6
B	135	LEU	-	expression tag	UNP Q9UIQ6
B	136	LEU	-	expression tag	UNP Q9UIQ6
B	137	SER	-	expression tag	UNP Q9UIQ6
B	138	LEU	-	expression tag	UNP Q9UIQ6
B	139	VAL	-	expression tag	UNP Q9UIQ6
B	140	SER	-	expression tag	UNP Q9UIQ6
B	141	LEU	-	expression tag	UNP Q9UIQ6
B	142	LEU	-	expression tag	UNP Q9UIQ6
B	143	SER	-	expression tag	UNP Q9UIQ6
B	144	VAL	-	expression tag	UNP Q9UIQ6
B	145	LEU	-	expression tag	UNP Q9UIQ6
B	146	LEU	-	expression tag	UNP Q9UIQ6
B	147	MET	-	expression tag	UNP Q9UIQ6
B	148	GLY	-	expression tag	UNP Q9UIQ6
B	149	CYS	-	expression tag	UNP Q9UIQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	150	VAL	-	expression tag	UNP Q9UIQ6
B	151	ALA	-	expression tag	UNP Q9UIQ6
B	152	GLU	-	expression tag	UNP Q9UIQ6
B	153	THR	-	expression tag	UNP Q9UIQ6
B	154	GLY	-	expression tag	UNP Q9UIQ6
B	1026	ARG	-	expression tag	UNP Q9UIQ6
B	1027	THR	-	expression tag	UNP Q9UIQ6
B	1028	GLU	-	expression tag	UNP Q9UIQ6
B	1029	THR	-	expression tag	UNP Q9UIQ6
B	1030	SER	-	expression tag	UNP Q9UIQ6
B	1031	GLN	-	expression tag	UNP Q9UIQ6
B	1032	VAL	-	expression tag	UNP Q9UIQ6
B	1033	ALA	-	expression tag	UNP Q9UIQ6
B	1034	PRO	-	expression tag	UNP Q9UIQ6
B	1035	ALA	-	expression tag	UNP Q9UIQ6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Zn 1	0	0
2	A	1	Total 1	Zn 1	0	0

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
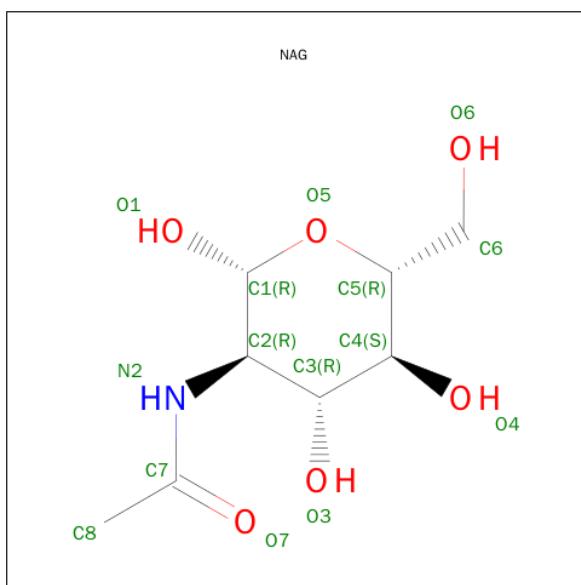
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		

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: Leucyl-cystinyl aminopeptidase
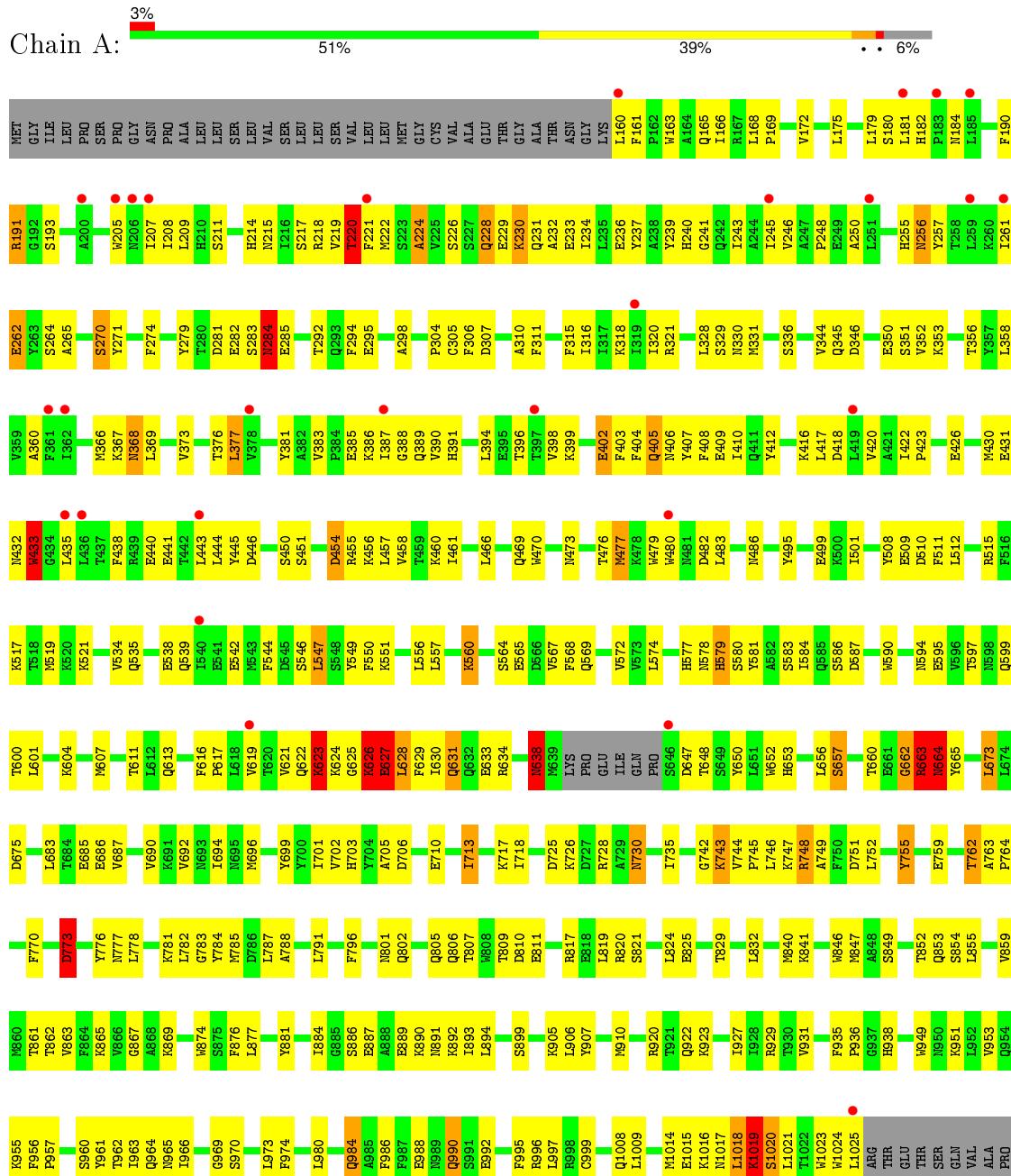
ALA

• Molecule 1: Leucyl-cystinyl aminopeptidase

Chain B:
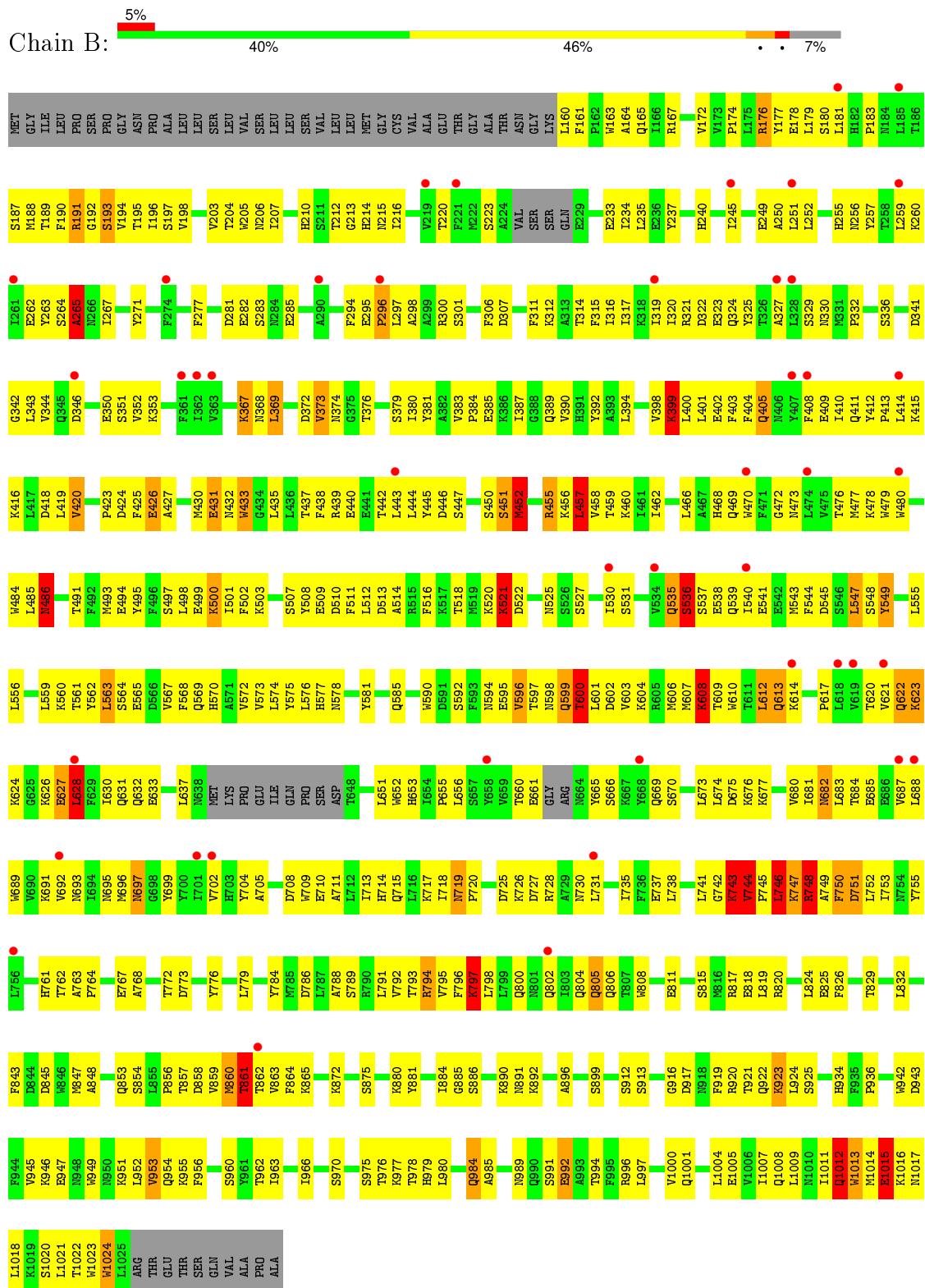
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.00Å 260.15Å 73.36Å 90.00° 111.61° 90.00°	Depositor
Resolution (Å)	68.20 – 3.37 68.20 – 3.37	Depositor EDS
% Data completeness (in resolution range)	99.6 (68.20-3.37) 99.7 (68.20-3.37)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.216 , 0.285 0.235 , 0.297	Depositor DCC
R_{free} test set	1615 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	131.8	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 75.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.30$	Xtriage
Outliers	0 of 33834 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14098	wwPDB-VP
Average B, all atoms (Å^2)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.65	3/7115 (0.0%)	0.96	17/9660 (0.2%)
1	B	0.66	4/6979 (0.1%)	1.06	36/9486 (0.4%)
All	All	0.66	7/14094 (0.0%)	1.01	53/19146 (0.3%)

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	A	0	11
1	B	0	16
All	All	0	27

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	627	GLU	CG-CD	-7.17	1.41	1.51
1	B	1024	TRP	CE3-CZ3	-6.41	1.27	1.38
1	B	797	LYS	CD-CE	6.17	1.66	1.51
1	A	433	TRP	CB-CG	-5.69	1.40	1.50
1	B	748	ARG	CB-CG	5.45	1.67	1.52

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	377	LEU	CA-CB-CG	11.58	141.94	115.30
1	A	663	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	A	663	ARG	NE-CZ-NH2	-9.93	115.33	120.30
1	B	369	LEU	CA-CB-CG	9.37	136.84	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	628	LEU	CA-CB-CG	9.24	136.55	115.30

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	THR	Peptide
1	A	230	LYS	Peptide
1	A	284	ASN	Peptide
1	A	404	PHE	Peptide
1	A	626	LYS	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	6937	0	6760	412	1
1	B	6808	0	6593	534	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	182	0	166	20	0
3	B	168	0	153	8	1
4	A	1	0	0	0	0
All	All	14098	0	13672	952	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 34.

The worst 5 of 952 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:574:LEU:CD1	3:A:1113:NAG:H81	1.57	1.33
1:A:574:LEU:HD11	3:A:1113:NAG:C8	1.65	1.26
1:A:367:LYS:HD2	1:A:368:ASN:H	1.02	1.17
1:B:518:THR:O	1:B:521:LYS:HB2	1.49	1.12
1:B:695:ASN:HB3	1:B:726:LYS:HD2	1.31	1.10

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:A:230:LYS:CD	3:B:1106:NAG:O7[1_554]	1.77	0.43

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	858/912 (94%)	760 (89%)	84 (10%)	14 (2%)	12	49
1	B	844/912 (92%)	743 (88%)	74 (9%)	27 (3%)	5	34
All	All	1702/1824 (93%)	1503 (88%)	158 (9%)	41 (2%)	7	41

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ALA
1	A	270	SER
1	A	284	ASN
1	A	626	LYS
1	A	627	GLU

5.3.2 Protein sidechains (i)

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	756/813 (93%)	728 (96%)	28 (4%)	41	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	736/813 (90%)	707 (96%)	29 (4%)	39	75
All	All	1492/1626 (92%)	1435 (96%)	57 (4%)	40	75

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	962	THR
1	B	399	LYS
1	B	861	THR
1	A	984	GLN
1	B	176	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	733	ASN
1	A	938	HIS
1	B	486	ASN
1	A	730	ASN
1	B	715	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 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	1102	1,3	14,14,15	1.07	1 (7%)	15,19,21	1.24	1 (6%)
3	NAG	A	1103	3	14,14,15	0.37	0	15,19,21	0.55	0
3	NAG	A	1104	1	14,14,15	0.78	1 (7%)	15,19,21	0.83	1 (6%)
3	NAG	A	1105	1	14,14,15	0.46	0	15,19,21	0.71	1 (6%)
3	NAG	A	1106	1	14,14,15	0.22	0	15,19,21	0.54	0
3	NAG	A	1107	1,3	14,14,15	1.19	1 (7%)	15,19,21	0.94	1 (6%)
3	NAG	A	1108	3	14,14,15	0.53	0	15,19,21	0.60	0
3	NAG	A	1109	1	14,14,15	0.45	0	15,19,21	1.00	1 (6%)
3	NAG	A	1110	1	14,14,15	0.75	1 (7%)	15,19,21	0.95	1 (6%)
3	NAG	A	1111	1	14,14,15	0.50	0	15,19,21	0.64	1 (6%)
3	NAG	A	1112	1	14,14,15	1.26	1 (7%)	15,19,21	1.43	1 (6%)
3	NAG	A	1113	1	14,14,15	0.55	0	15,19,21	0.64	1 (6%)
3	NAG	A	1114	-	14,14,15	0.68	0	15,19,21	0.62	0
3	NAG	B	1102	1,3	14,14,15	0.30	0	15,19,21	0.41	0
3	NAG	B	1103	3	14,14,15	0.25	0	15,19,21	0.43	0
3	NAG	B	1104	1	14,14,15	0.94	1 (7%)	15,19,21	0.61	0
3	NAG	B	1105	1,3	14,14,15	1.83	4 (28%)	15,19,21	1.76	2 (13%)
3	NAG	B	1106	3	14,14,15	0.32	0	15,19,21	0.48	0
3	NAG	B	1107	1	14,14,15	0.52	0	15,19,21	0.42	0
3	NAG	B	1108	1,3	14,14,15	0.92	2 (14%)	15,19,21	0.59	1 (6%)
3	NAG	B	1109	3	14,14,15	0.39	0	15,19,21	0.41	0
3	NAG	B	1110	1	14,14,15	0.66	1 (7%)	15,19,21	0.58	0
3	NAG	B	1111	1	14,14,15	0.49	0	15,19,21	0.47	0
3	NAG	B	1112	1	14,14,15	0.35	0	15,19,21	0.55	0
3	NAG	B	1113	1	14,14,15	0.86	1 (7%)	15,19,21	0.53	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	1102	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1103	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1104	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1105	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1106	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1107	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1108	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1109	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1110	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1111	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1112	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1113	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1114	-	-	0/6/23/26	0/1/1/1
3	NAG	B	1102	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1103	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1104	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1105	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1106	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1107	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1108	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1109	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1110	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1111	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1112	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1113	1	-	0/6/23/26	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1107	NAG	O5-C1	-3.75	1.37	1.43
3	B	1105	NAG	O5-C1	-2.91	1.39	1.43
3	B	1105	NAG	C2-N2	2.08	1.50	1.46
3	B	1110	NAG	O5-C1	2.13	1.47	1.43
3	B	1105	NAG	C3-C2	2.16	1.57	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1105	NAG	C1-O5-C5	-5.14	104.58	112.14
3	A	1107	NAG	C1-O5-C5	-3.05	107.65	112.14
3	B	1105	NAG	O5-C5-C4	-2.67	105.70	110.13
3	A	1113	NAG	C1-O5-C5	-2.03	109.16	112.14
3	B	1108	NAG	C1-O5-C5	2.11	115.25	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	NAG	3	0
3	A	1104	NAG	1	0
3	A	1106	NAG	2	0
3	A	1107	NAG	2	0
3	A	1113	NAG	11	0
3	A	1114	NAG	6	0
3	B	1103	NAG	1	0
3	B	1105	NAG	1	0
3	B	1106	NAG	1	1
3	B	1107	NAG	1	0
3	B	1112	NAG	2	0
3	B	1113	NAG	3	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	860/912 (94%)	0.10	28 (3%)	50	51	77, 117, 159, 184	0
1	B	851/912 (93%)	0.11	44 (5%)	31	31	83, 141, 167, 189	0
All	All	1711/1824 (93%)	0.10	72 (4%)	40	40	77, 131, 162, 189	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	LEU	5.9
1	B	221	PHE	5.2
1	B	621	VAL	5.0
1	B	658	TYR	4.2
1	B	619	VAL	3.9

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)

There are no carbohydrates in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
3	NAG	A	1106	14/15	0.30	0.34	4.65	146,164,179,183	0
3	NAG	B	1107	14/15	0.78	0.24	3.90	144,155,160,163	0
2	ZN	A	1101	1/1	0.96	0.28	1.67	83,83,83,83	1
3	NAG	A	1113	14/15	0.66	0.28	0.77	121,136,145,146	0
2	ZN	B	1101	1/1	0.95	0.20	0.21	143,143,143,143	0
3	NAG	B	1102	14/15	0.84	0.20	-0.02	157,163,171,173	0
3	NAG	B	1113	14/15	0.77	0.19	-0.07	143,153,171,182	0
3	NAG	A	1102	14/15	0.81	0.18	-0.71	135,147,158,159	0
3	NAG	A	1105	14/15	0.90	0.15	-1.11	147,162,165,170	0
3	NAG	B	1105	14/15	0.91	0.09	-1.29	151,163,175,181	0
3	NAG	B	1109	14/15	0.84	0.26	-	155,181,185,185	0
3	NAG	B	1103	14/15	0.82	0.22	-	169,174,178,178	0
3	NAG	A	1112	14/15	0.84	0.23	-	157,172,178,180	0
3	NAG	B	1112	14/15	0.82	0.18	-	166,184,188,195	0
3	NAG	A	1110	14/15	0.84	0.25	-	127,139,149,152	0
3	NAG	A	1103	14/15	0.89	0.17	-	160,168,175,176	0
3	NAG	A	1109	14/15	0.80	0.20	-	144,166,176,184	0
3	NAG	A	1104	14/15	0.79	0.20	-	160,165,175,176	0
3	NAG	A	1108	14/15	0.90	0.12	-	166,182,196,202	0
3	NAG	B	1106	14/15	0.78	0.17	-	158,165,174,176	0
3	NAG	B	1110	14/15	0.78	0.30	-	166,174,187,189	0
3	NAG	A	1107	14/15	0.93	0.15	-	146,153,162,173	0
3	NAG	A	1114	14/15	0.72	0.21	-	123,136,144,170	0
3	NAG	B	1108	14/15	0.88	0.13	-	145,160,172,173	0
3	NAG	B	1111	14/15	0.74	0.31	-	150,163,166,167	0
3	NAG	A	1111	14/15	0.87	0.26	-	114,132,145,145	0
3	NAG	B	1104	14/15	0.75	0.22	-	162,180,186,189	0

6.5 Other polymers (i)

There are no such residues in this entry.