



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:59 pm GMT

PDB ID : 3D66
Title : Crystal structure of Thrombin-Activatable Fibrinolysis Inhibitor (TAFI)
Authors : Brondijk, T.H.C.; Huizinga, E.G.
Deposited on : 2008-05-19
Resolution : 3.10 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

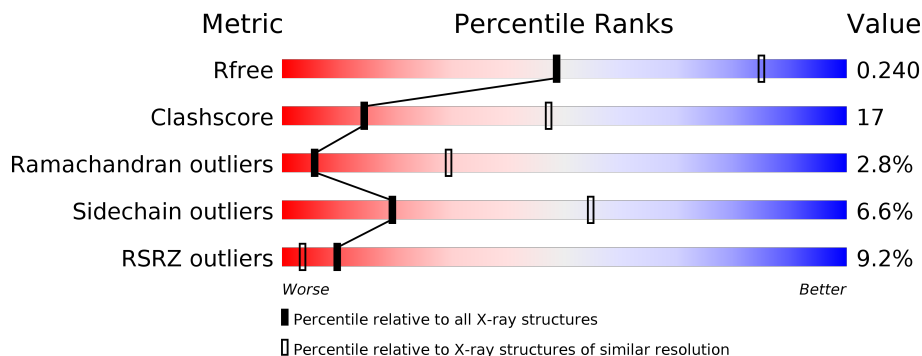
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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 $\leq 5\%$. 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	424	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>24%</div> <div>• 5%</div> </div> </div>
1	B	424	<div> <div>14%</div> <div> <div></div> <div>64%</div> <div>25%</div> <div>• • 5%</div> </div> </div>
1	C	424	<div> <div>11%</div> <div> <div></div> <div>63%</div> <div>26%</div> <div>5% • 5%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9864 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 Carboxypeptidase B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3245	2078	555	600	12			
1	B	401	Total	C	N	O	S	0	0	0
			3245	2078	555	600	12			
1	C	401	Total	C	N	O	S	0	0	0
			3245	2078	555	600	12			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	EXPRESSION TAG	UNP Q96IY4
A	-21	SER	-	EXPRESSION TAG	UNP Q96IY4
A	-20	HIS	-	EXPRESSION TAG	UNP Q96IY4
A	-19	HIS	-	EXPRESSION TAG	UNP Q96IY4
A	-18	HIS	-	EXPRESSION TAG	UNP Q96IY4
A	-17	HIS	-	EXPRESSION TAG	UNP Q96IY4
A	-16	HIS	-	EXPRESSION TAG	UNP Q96IY4
A	-15	HIS	-	EXPRESSION TAG	UNP Q96IY4
A	-14	ASP	-	EXPRESSION TAG	UNP Q96IY4
A	-13	TYR	-	EXPRESSION TAG	UNP Q96IY4
A	-12	ASP	-	EXPRESSION TAG	UNP Q96IY4
A	-11	ILE	-	EXPRESSION TAG	UNP Q96IY4
A	-10	PRO	-	EXPRESSION TAG	UNP Q96IY4
A	-9	SER	-	EXPRESSION TAG	UNP Q96IY4
A	-8	SER	-	EXPRESSION TAG	UNP Q96IY4
A	-7	GLU	-	EXPRESSION TAG	UNP Q96IY4
A	-6	ASN	-	EXPRESSION TAG	UNP Q96IY4
A	-5	LEU	-	EXPRESSION TAG	UNP Q96IY4
A	-4	TYR	-	EXPRESSION TAG	UNP Q96IY4
A	-3	PHE	-	EXPRESSION TAG	UNP Q96IY4
A	-2	GLN	-	EXPRESSION TAG	UNP Q96IY4
A	-1	GLY	-	EXPRESSION TAG	UNP Q96IY4
A	0	SER	-	EXPRESSION TAG	UNP Q96IY4

Continued on next page...

Continued from previous page...

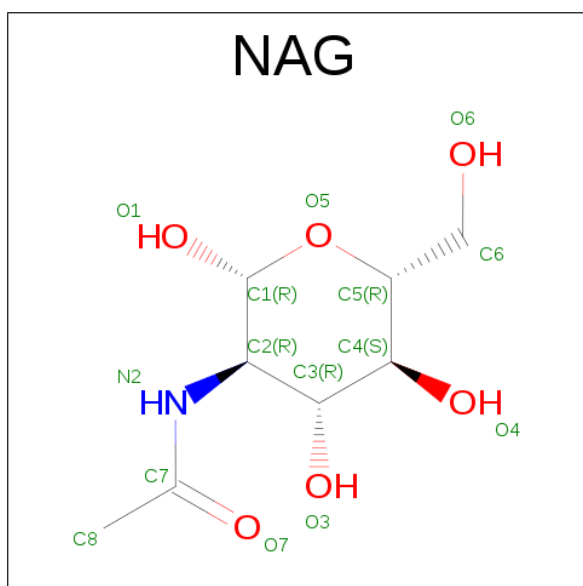
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	EXPRESSION TAG	UNP Q96IY4
A	147	THR	ALA	SEE REMARK 999	UNP Q96IY4
B	-22	GLY	-	EXPRESSION TAG	UNP Q96IY4
B	-21	SER	-	EXPRESSION TAG	UNP Q96IY4
B	-20	HIS	-	EXPRESSION TAG	UNP Q96IY4
B	-19	HIS	-	EXPRESSION TAG	UNP Q96IY4
B	-18	HIS	-	EXPRESSION TAG	UNP Q96IY4
B	-17	HIS	-	EXPRESSION TAG	UNP Q96IY4
B	-16	HIS	-	EXPRESSION TAG	UNP Q96IY4
B	-15	HIS	-	EXPRESSION TAG	UNP Q96IY4
B	-14	ASP	-	EXPRESSION TAG	UNP Q96IY4
B	-13	TYR	-	EXPRESSION TAG	UNP Q96IY4
B	-12	ASP	-	EXPRESSION TAG	UNP Q96IY4
B	-11	ILE	-	EXPRESSION TAG	UNP Q96IY4
B	-10	PRO	-	EXPRESSION TAG	UNP Q96IY4
B	-9	SER	-	EXPRESSION TAG	UNP Q96IY4
B	-8	SER	-	EXPRESSION TAG	UNP Q96IY4
B	-7	GLU	-	EXPRESSION TAG	UNP Q96IY4
B	-6	ASN	-	EXPRESSION TAG	UNP Q96IY4
B	-5	LEU	-	EXPRESSION TAG	UNP Q96IY4
B	-4	TYR	-	EXPRESSION TAG	UNP Q96IY4
B	-3	PHE	-	EXPRESSION TAG	UNP Q96IY4
B	-2	GLN	-	EXPRESSION TAG	UNP Q96IY4
B	-1	GLY	-	EXPRESSION TAG	UNP Q96IY4
B	0	SER	-	EXPRESSION TAG	UNP Q96IY4
B	1	ALA	-	EXPRESSION TAG	UNP Q96IY4
B	147	THR	ALA	SEE REMARK 999	UNP Q96IY4
C	-22	GLY	-	EXPRESSION TAG	UNP Q96IY4
C	-21	SER	-	EXPRESSION TAG	UNP Q96IY4
C	-20	HIS	-	EXPRESSION TAG	UNP Q96IY4
C	-19	HIS	-	EXPRESSION TAG	UNP Q96IY4
C	-18	HIS	-	EXPRESSION TAG	UNP Q96IY4
C	-17	HIS	-	EXPRESSION TAG	UNP Q96IY4
C	-16	HIS	-	EXPRESSION TAG	UNP Q96IY4
C	-15	HIS	-	EXPRESSION TAG	UNP Q96IY4
C	-14	ASP	-	EXPRESSION TAG	UNP Q96IY4
C	-13	TYR	-	EXPRESSION TAG	UNP Q96IY4
C	-12	ASP	-	EXPRESSION TAG	UNP Q96IY4
C	-11	ILE	-	EXPRESSION TAG	UNP Q96IY4
C	-10	PRO	-	EXPRESSION TAG	UNP Q96IY4
C	-9	SER	-	EXPRESSION TAG	UNP Q96IY4
C	-8	SER	-	EXPRESSION TAG	UNP Q96IY4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLU	-	EXPRESSION TAG	UNP Q96IY4
C	-6	ASN	-	EXPRESSION TAG	UNP Q96IY4
C	-5	LEU	-	EXPRESSION TAG	UNP Q96IY4
C	-4	TYR	-	EXPRESSION TAG	UNP Q96IY4
C	-3	PHE	-	EXPRESSION TAG	UNP Q96IY4
C	-2	GLN	-	EXPRESSION TAG	UNP Q96IY4
C	-1	GLY	-	EXPRESSION TAG	UNP Q96IY4
C	0	SER	-	EXPRESSION TAG	UNP Q96IY4
C	1	ALA	-	EXPRESSION TAG	UNP Q96IY4
C	147	THR	ALA	SEE REMARK 999	UNP Q96IY4

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

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

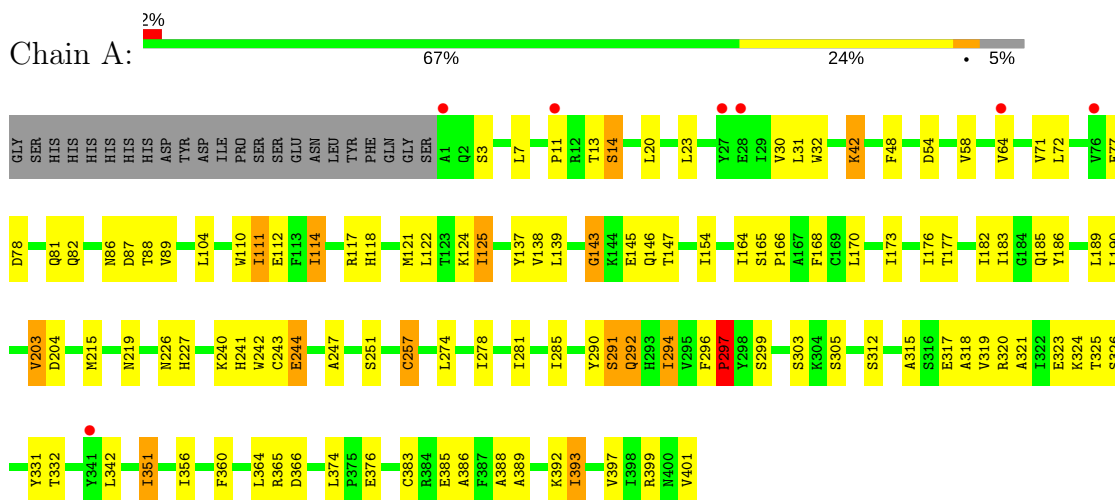
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

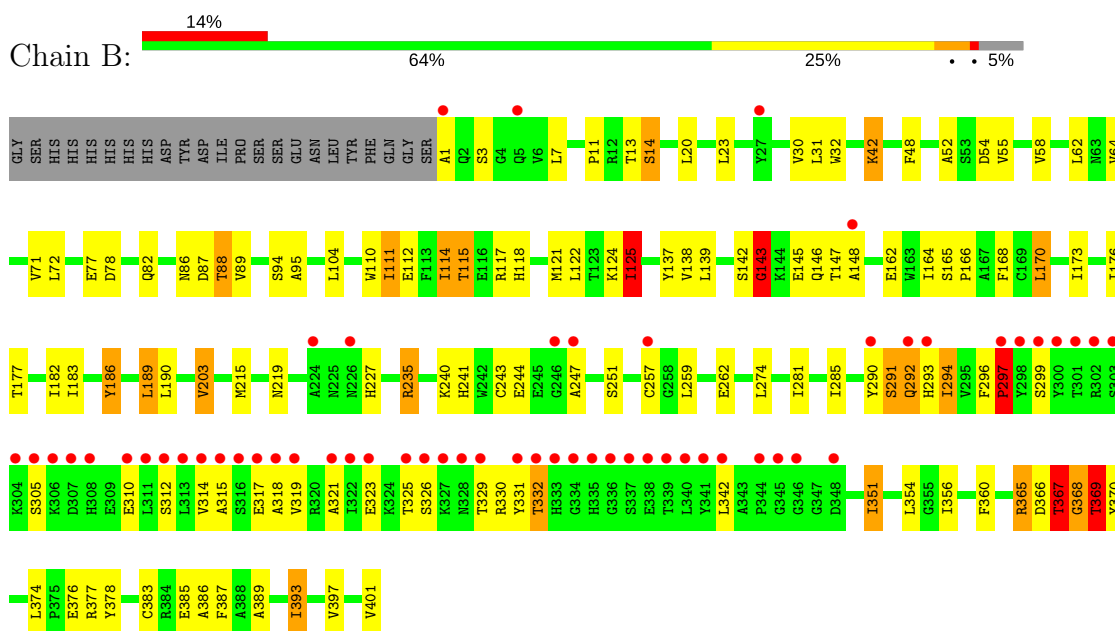
3 Residue-property plots

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

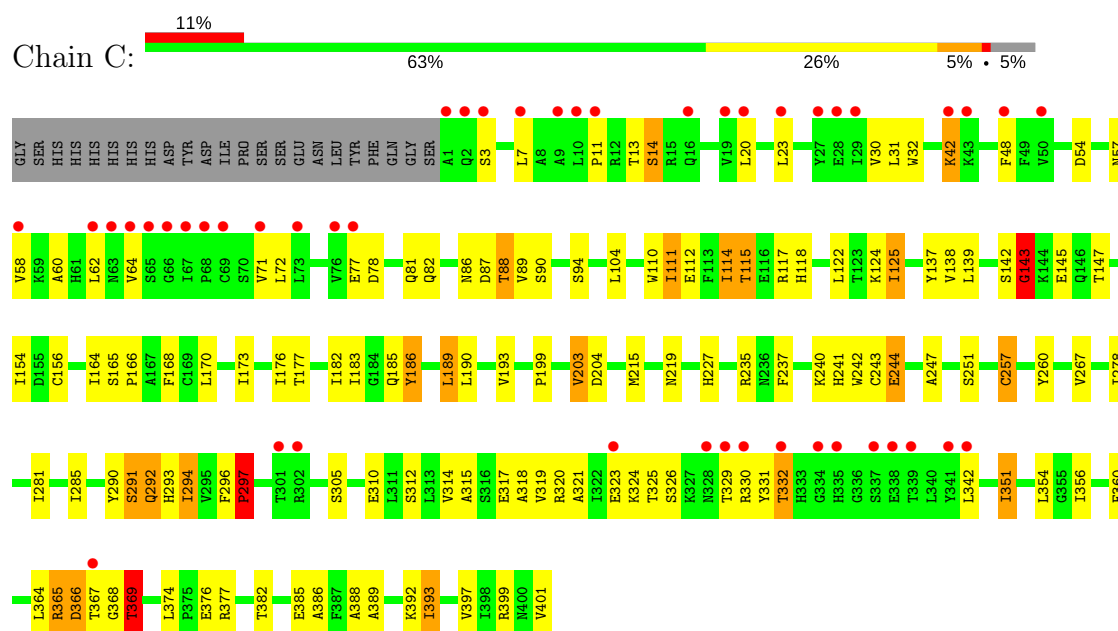
• Molecule 1: Carboxypeptidase B2



• Molecule 1: Carboxypeptidase B2



• Molecule 1: Carboxypeptidase B2



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.74Å 161.74Å 139.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.51 – 3.10 49.49 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.51-3.10) 100.0 (49.49-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.204 , 0.240 0.209 , 0.240	Depositor DCC
R_{free} test set	1953 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	91.1	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 101.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9864	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.85	4/3333 (0.1%)	0.85	4/4530 (0.1%)
1	B	0.91	3/3333 (0.1%)	0.88	4/4530 (0.1%)
1	C	0.83	4/3333 (0.1%)	0.84	6/4530 (0.1%)
All	All	0.87	11/9999 (0.1%)	0.86	14/13590 (0.1%)

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	3
1	B	0	4
1	C	0	3
All	All	0	10

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	VAL	CB-CG1	-12.02	1.27	1.52
1	B	64	VAL	CB-CG2	-11.88	1.27	1.52
1	C	64	VAL	CB-CG1	-6.55	1.39	1.52
1	A	64	VAL	CB-CG1	-6.53	1.39	1.52
1	B	186	TYR	CE1-CZ	-6.21	1.30	1.38
1	A	383	CYS	CB-SG	-6.09	1.71	1.82
1	C	64	VAL	CB-CG2	-6.06	1.40	1.52
1	A	376	GLU	CD-OE1	5.65	1.31	1.25
1	C	186	TYR	CE2-CZ	-5.45	1.31	1.38
1	C	125	ILE	CB-CG2	5.30	1.69	1.52
1	A	64	VAL	CB-CG2	-5.26	1.41	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	VAL	CG1-CB-CG2	-16.11	85.12	110.90
1	C	125	ILE	CA-CB-CG1	-9.53	92.90	111.00
1	A	64	VAL	CG1-CB-CG2	-8.29	97.63	110.90
1	C	64	VAL	CG1-CB-CG2	-8.01	98.08	110.90
1	B	125	ILE	CG1-CB-CG2	-7.69	94.48	111.40
1	C	125	ILE	CB-CG1-CD1	6.55	132.24	113.90
1	C	365	ARG	N-CA-C	-6.52	93.41	111.00
1	A	125	ILE	CG1-CB-CG2	-5.96	98.28	111.40
1	B	162	GLU	OE1-CD-OE2	-5.83	116.31	123.30
1	B	235	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	204	ASP	CB-CG-OD2	-5.48	113.36	118.30
1	A	257	CYS	CA-CB-SG	-5.11	104.80	114.00
1	C	257	CYS	CA-CB-SG	-5.11	104.81	114.00
1	C	125	ILE	CG1-CB-CG2	-5.02	100.35	111.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	GLY	Peptide
1	A	145	GLU	Peptide
1	A	364	LEU	Peptide
1	B	143	GLY	Peptide
1	B	145	GLU	Peptide
1	B	148	ALA	Peptide
1	B	369	THR	Peptide
1	C	143	GLY	Peptide
1	C	145	GLU	Peptide
1	C	364	LEU	Peptide

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	3245	0	3156	97	0
1	B	3245	0	3156	119	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3245	0	3159	129	0
2	A	56	0	52	3	0
2	B	56	0	52	3	0
2	C	14	0	13	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
All	All	9864	0	9588	335	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 17.

All (335) 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:C:125:ILE:HD11	1:C:138:VAL:C	1.14	1.44
1:C:125:ILE:HD12	1:C:138:VAL:CB	1.51	1.41
1:C:125:ILE:CD1	1:C:138:VAL:HB	1.54	1.37
1:C:125:ILE:CD1	1:C:138:VAL:C	2.10	1.20
1:C:125:ILE:CD1	1:C:138:VAL:CB	2.14	1.19
1:C:125:ILE:HD11	1:C:138:VAL:CA	1.72	1.18
1:C:87:ASP:O	1:C:88:THR:HG22	1.43	1.16
1:C:118:HIS:CE1	1:C:177:THR:HG23	1.80	1.15
1:A:32:TRP:HE1	1:A:215:MET:HE3	0.97	1.13
1:B:32:TRP:HE1	1:B:215:MET:HE3	1.01	1.12
1:A:118:HIS:CE1	1:A:177:THR:HG23	1.85	1.12
1:C:32:TRP:HE1	1:C:215:MET:HE3	0.97	1.09
1:B:32:TRP:HE1	1:B:215:MET:CE	1.65	1.08
1:B:118:HIS:CE1	1:B:177:THR:HG23	1.89	1.07
1:C:32:TRP:HE1	1:C:215:MET:CE	1.68	1.06
1:C:125:ILE:HD11	1:C:138:VAL:O	1.57	1.02
1:C:125:ILE:CD1	1:C:138:VAL:CA	2.36	0.99
1:C:87:ASP:O	1:C:88:THR:CG2	2.09	0.99
1:B:87:ASP:O	1:B:88:THR:HG22	1.63	0.98
1:A:32:TRP:NE1	1:A:215:MET:HE3	1.78	0.98
1:A:32:TRP:HE1	1:A:215:MET:CE	1.76	0.97
1:C:32:TRP:NE1	1:C:215:MET:HE3	1.80	0.95
1:B:292:GLN:HE22	1:B:365:ARG:HE	1.14	0.93
1:B:32:TRP:NE1	1:B:215:MET:HE3	1.82	0.93
1:C:365:ARG:HD3	1:C:382:THR:OG1	1.69	0.93
1:B:329:THR:HG23	1:B:365:ARG:HD2	1.50	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ASP:O	1:B:88:THR:CG2	2.18	0.92
1:B:292:GLN:OE1	1:B:365:ARG:HG3	1.71	0.90
1:A:112:GLU:OE2	1:A:124:LYS:NZ	2.04	0.89
1:B:112:GLU:OE2	1:B:124:LYS:NZ	2.06	0.88
1:C:125:ILE:O	1:C:125:ILE:HG13	1.72	0.88
1:B:329:THR:HG23	1:B:365:ARG:CD	2.03	0.88
1:C:112:GLU:OE2	1:C:124:LYS:NZ	2.05	0.88
1:B:292:GLN:HE22	1:B:365:ARG:NE	1.72	0.87
1:A:87:ASP:O	1:A:88:THR:HG22	1.74	0.87
2:A:604:NAG:H82	2:A:604:NAG:O3	1.73	0.87
1:C:125:ILE:CG1	1:C:138:VAL:O	2.23	0.86
1:C:125:ILE:CD1	1:C:138:VAL:O	2.21	0.84
1:B:368:GLY:HA3	1:B:370:TYR:H	1.42	0.83
1:A:185:GLN:HE21	1:C:399:ARG:NE	1.76	0.83
1:A:399:ARG:CZ	1:C:185:GLN:HE21	1.92	0.82
1:C:285:ILE:HD11	1:C:393:ILE:HD11	1.64	0.80
1:B:292:GLN:NE2	1:B:365:ARG:HE	1.80	0.79
1:A:86:ASN:HA	1:A:89:VAL:HG21	1.64	0.78
1:A:87:ASP:O	1:A:88:THR:CG2	2.32	0.78
1:C:88:THR:O	1:C:90:SER:N	2.16	0.78
1:B:117:ARG:HG2	1:B:118:HIS:CD2	2.18	0.78
1:C:285:ILE:CD1	1:C:393:ILE:HD11	2.13	0.77
1:A:118:HIS:CE1	1:A:177:THR:CG2	2.67	0.77
1:A:285:ILE:HD11	1:A:393:ILE:HD11	1.67	0.76
1:B:285:ILE:CD1	1:B:393:ILE:HD11	2.16	0.76
1:A:185:GLN:HE21	1:C:399:ARG:CZ	1.99	0.76
1:C:117:ARG:HG2	1:C:118:HIS:CD2	2.21	0.75
1:C:351:ILE:CG2	1:C:356:ILE:HB	2.16	0.75
1:A:117:ARG:HG2	1:A:118:HIS:CD2	2.22	0.74
1:A:399:ARG:NH2	1:C:185:GLN:HE21	1.86	0.74
1:B:139:LEU:HD12	1:B:173:ILE:CD1	2.18	0.73
1:A:351:ILE:CG2	1:A:356:ILE:HB	2.18	0.73
1:B:32:TRP:NE1	1:B:215:MET:CE	2.47	0.73
1:A:88:THR:O	1:A:89:VAL:HB	1.89	0.73
1:B:118:HIS:CE1	1:B:177:THR:CG2	2.71	0.73
1:C:142:SER:O	1:C:143:GLY:O	2.07	0.73
1:A:285:ILE:CD1	1:A:393:ILE:HD11	2.19	0.73
1:B:292:GLN:NE2	1:B:365:ARG:NE	2.37	0.73
1:B:117:ARG:HG2	1:B:118:HIS:HD2	1.52	0.72
1:C:118:HIS:CE1	1:C:177:THR:CG2	2.67	0.72
1:B:292:GLN:OE1	1:B:365:ARG:CG	2.38	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ILE:HD11	1:C:318:ALA:HB3	1.72	0.71
2:B:604:NAG:O3	2:B:604:NAG:H82	1.90	0.71
1:B:329:THR:CG2	1:B:365:ARG:HD2	2.20	0.71
1:C:368:GLY:O	1:C:369:THR:C	2.28	0.71
1:C:139:LEU:HD12	1:C:173:ILE:HD13	1.74	0.69
1:C:117:ARG:HG2	1:C:118:HIS:HD2	1.57	0.69
1:B:262:GLU:HG3	1:C:182:ILE:HD11	1.73	0.69
1:B:285:ILE:HD11	1:B:393:ILE:HD11	1.73	0.69
1:C:86:ASN:HA	1:C:89:VAL:HG21	1.75	0.68
1:B:351:ILE:CG2	1:B:356:ILE:HB	2.23	0.68
1:B:366:ASP:O	1:B:368:GLY:N	2.26	0.68
1:A:294:ILE:HD11	1:A:318:ALA:HB3	1.76	0.67
1:C:125:ILE:CD1	1:C:138:VAL:CG1	2.72	0.67
1:A:114:ILE:HG23	1:A:122:LEU:HD12	1.76	0.67
1:A:139:LEU:HD12	1:A:173:ILE:HD13	1.75	0.67
1:B:367:THR:HG21	1:B:378:TYR:CE2	2.30	0.67
1:C:365:ARG:O	1:C:366:ASP:HB3	1.95	0.67
1:C:114:ILE:HG23	1:C:122:LEU:HD12	1.76	0.66
1:C:125:ILE:HG12	1:C:138:VAL:O	1.95	0.66
1:B:294:ILE:CD1	1:B:318:ALA:HB3	2.26	0.66
1:B:114:ILE:HG23	1:B:122:LEU:HD12	1.78	0.65
1:C:164:ILE:HD13	1:C:374:LEU:HD23	1.79	0.65
1:A:78:ASP:OD2	1:A:82:GLN:NE2	2.21	0.64
2:C:604:NAG:H82	2:C:604:NAG:O3	1.95	0.64
1:C:114:ILE:HG23	1:C:122:LEU:CD1	2.28	0.64
1:A:139:LEU:HD12	1:A:173:ILE:CD1	2.27	0.64
1:A:117:ARG:HG2	1:A:118:HIS:HD2	1.63	0.64
1:C:294:ILE:CD1	1:C:318:ALA:HB3	2.28	0.64
1:A:54:ASP:O	1:A:58:VAL:HG23	1.98	0.63
1:B:86:ASN:HA	1:B:89:VAL:HG21	1.79	0.63
1:A:118:HIS:ND1	1:A:177:THR:HG23	2.14	0.62
1:C:11:PRO:O	1:C:42:LYS:O	2.17	0.62
1:A:86:ASN:HA	1:A:89:VAL:CG2	2.29	0.61
1:A:114:ILE:HG23	1:A:122:LEU:CD1	2.30	0.61
1:C:104:LEU:HD21	1:C:203:VAL:HG13	1.81	0.61
1:B:294:ILE:HD11	1:B:318:ALA:HB3	1.81	0.61
1:C:118:HIS:ND1	1:C:177:THR:HG23	2.16	0.61
1:A:164:ILE:HD13	1:A:374:LEU:HD23	1.83	0.61
1:B:54:ASP:O	1:B:58:VAL:HG23	2.01	0.61
1:C:125:ILE:HD11	1:C:139:LEU:N	2.05	0.60
1:C:376:GLU:OE1	2:C:604:NAG:H83	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LEU:HD13	1:B:351:ILE:HD11	1.83	0.60
1:A:110:TRP:CZ3	1:A:170:LEU:HD22	2.36	0.60
1:B:114:ILE:HG23	1:B:122:LEU:CD1	2.31	0.60
1:B:139:LEU:HD12	1:B:173:ILE:HD13	1.83	0.60
1:C:54:ASP:O	1:C:58:VAL:HG23	2.02	0.60
1:C:7:LEU:CD2	1:C:71:VAL:HG22	2.32	0.60
1:C:139:LEU:HD12	1:C:173:ILE:CD1	2.32	0.59
1:B:165:SER:HB3	1:B:166:PRO:HD3	1.84	0.59
1:C:32:TRP:NE1	1:C:215:MET:CE	2.50	0.59
1:C:365:ARG:HB2	1:C:382:THR:HG23	1.85	0.59
1:C:176:ILE:HG21	1:C:190:LEU:HD11	1.85	0.58
1:A:399:ARG:NH2	1:C:185:GLN:NE2	2.52	0.58
1:A:397:VAL:HG13	1:A:401:VAL:HG21	1.86	0.58
1:B:13:THR:HG22	1:B:14:SER:N	2.18	0.57
1:C:110:TRP:CZ3	1:C:170:LEU:HD22	2.39	0.57
1:B:319:VAL:HG13	1:B:331:TYR:HB2	1.85	0.57
1:B:368:GLY:HA3	1:B:370:TYR:N	2.16	0.57
1:C:111:ILE:HD11	1:C:137:TYR:CD2	2.39	0.57
1:A:243:CYS:HA	1:A:247:ALA:HB3	1.87	0.57
1:C:351:ILE:HG22	1:C:356:ILE:HB	1.87	0.56
1:B:11:PRO:O	1:B:42:LYS:O	2.24	0.56
1:C:165:SER:HB3	1:C:166:PRO:HD3	1.87	0.56
1:B:389:ALA:O	1:B:393:ILE:HG23	2.04	0.56
1:B:243:CYS:HA	1:B:247:ALA:HB3	1.87	0.56
1:B:259:LEU:O	1:C:94:SER:HA	2.05	0.56
1:B:118:HIS:ND1	1:B:177:THR:HG23	2.21	0.55
1:B:118:HIS:HE1	1:B:177:THR:HG23	1.61	0.55
1:C:243:CYS:HA	1:C:247:ALA:HB3	1.89	0.55
1:B:369:THR:HG22	1:B:370:TYR:HA	1.89	0.55
1:C:124:LYS:HE3	1:C:137:TYR:CE1	2.42	0.55
1:A:111:ILE:HD11	1:A:137:TYR:CD2	2.41	0.55
1:A:165:SER:HB3	1:A:166:PRO:HD3	1.89	0.55
1:C:31:LEU:HD23	1:C:48:PHE:HB3	1.89	0.55
1:B:329:THR:HG23	1:B:365:ARG:NE	2.22	0.55
1:A:294:ILE:CD1	1:A:318:ALA:HB3	2.37	0.54
1:B:326:SER:OG	1:B:385:GLU:OE1	2.20	0.54
1:B:125:ILE:HG13	1:B:138:VAL:HB	1.88	0.54
1:B:315:ALA:O	1:B:319:VAL:HG23	2.06	0.54
1:A:240:LYS:O	1:A:241:HIS:CG	2.61	0.54
1:B:87:ASP:O	1:B:88:THR:HG23	2.07	0.54
1:B:168:PHE:CE1	1:B:386:ALA:HB3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:ARG:CD	1:C:382:THR:OG1	2.50	0.54
1:B:369:THR:HG22	1:B:370:TYR:N	2.23	0.54
1:A:88:THR:O	1:A:89:VAL:CB	2.56	0.54
1:C:176:ILE:CG2	1:C:190:LEU:HD11	2.38	0.54
1:B:142:SER:O	1:B:143:GLY:O	2.25	0.53
1:B:7:LEU:HD22	1:B:71:VAL:HG22	1.91	0.53
1:C:20:LEU:HA	1:C:23:LEU:HD12	1.89	0.53
1:C:360:PHE:CD2	1:C:393:ILE:HD12	2.43	0.53
1:B:247:ALA:HB1	1:B:257:CYS:HB3	1.90	0.53
1:C:125:ILE:HD12	1:C:138:VAL:HB	0.65	0.53
1:C:7:LEU:HD22	1:C:71:VAL:HG22	1.88	0.53
1:A:32:TRP:NE1	1:A:215:MET:CE	2.53	0.53
1:C:319:VAL:HG13	1:C:331:TYR:HB2	1.91	0.53
1:C:78:ASP:OD2	1:C:82:GLN:NE2	2.33	0.53
1:A:183:ILE:HB	1:A:186:TYR:HD2	1.74	0.53
1:B:23:LEU:CD1	1:B:62:LEU:HD21	2.39	0.53
1:A:185:GLN:NE2	1:C:399:ARG:CZ	2.70	0.53
1:B:164:ILE:HD13	1:B:374:LEU:HD23	1.91	0.52
1:B:397:VAL:HG13	1:B:401:VAL:HG21	1.91	0.52
2:A:604:NAG:C8	2:A:604:NAG:O3	2.53	0.52
1:C:168:PHE:CE1	1:C:386:ALA:HB3	2.44	0.52
1:B:183:ILE:HB	1:B:186:TYR:HD2	1.74	0.52
1:C:182:ILE:HG22	1:C:183:ILE:HG13	1.92	0.52
1:A:7:LEU:CD2	1:A:71:VAL:HG22	2.40	0.52
1:B:376:GLU:OE1	2:B:604:NAG:H83	2.10	0.51
1:B:240:LYS:O	1:B:241:HIS:CG	2.63	0.51
1:C:125:ILE:CD1	1:C:138:VAL:HG12	2.40	0.51
1:A:274:LEU:HD13	1:A:351:ILE:HD11	1.92	0.51
1:C:247:ALA:HB1	1:C:257:CYS:HB3	1.93	0.50
1:C:118:HIS:HE1	1:C:177:THR:HG23	1.59	0.50
1:B:124:LYS:HE3	1:B:137:TYR:CE1	2.46	0.50
1:C:365:ARG:O	1:C:366:ASP:CB	2.60	0.50
1:C:315:ALA:O	1:C:319:VAL:HG23	2.12	0.50
1:A:321:ALA:O	1:A:325:THR:HG23	2.12	0.50
1:B:20:LEU:HA	1:B:23:LEU:HD12	1.94	0.50
1:C:86:ASN:HA	1:C:89:VAL:CG2	2.40	0.50
1:A:124:LYS:HE3	1:A:137:TYR:CE1	2.47	0.50
1:B:354:LEU:O	1:B:354:LEU:HG	2.12	0.50
1:C:117:ARG:CG	1:C:118:HIS:HD2	2.24	0.50
1:B:78:ASP:OD2	1:B:82:GLN:NE2	2.34	0.49
1:C:125:ILE:HG13	1:C:138:VAL:O	2.09	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD23	1:A:48:PHE:HB3	1.94	0.49
1:A:7:LEU:HD22	1:A:71:VAL:HG22	1.93	0.49
1:B:321:ALA:O	1:B:325:THR:HG23	2.11	0.49
1:B:290:TYR:CD2	1:B:366:ASP:OD2	2.65	0.49
1:C:183:ILE:HB	1:C:186:TYR:HD2	1.78	0.49
1:B:235:ARG:HD2	1:B:247:ALA:HB2	1.94	0.49
1:C:104:LEU:HD11	1:C:203:VAL:HG22	1.95	0.49
1:B:262:GLU:CG	1:C:182:ILE:HD11	2.42	0.49
1:A:168:PHE:CE1	1:A:386:ALA:HB3	2.49	0.48
1:A:3:SER:CB	1:A:77:GLU:HB2	2.42	0.48
1:C:326:SER:OG	1:C:385:GLU:OE1	2.21	0.48
1:A:319:VAL:HG13	1:A:331:TYR:HB2	1.95	0.48
1:B:329:THR:CG2	1:B:365:ARG:CD	2.81	0.48
1:C:11:PRO:HG3	1:C:20:LEU:HD12	1.95	0.48
1:A:351:ILE:HG22	1:A:356:ILE:HB	1.95	0.48
1:B:7:LEU:CD2	1:B:71:VAL:HG22	2.43	0.48
1:C:30:VAL:HG11	1:C:215:MET:HB3	1.94	0.48
1:A:182:ILE:HG22	1:A:183:ILE:HG13	1.96	0.48
1:A:104:LEU:HD21	1:A:203:VAL:HG13	1.95	0.48
1:A:389:ALA:O	1:A:393:ILE:HG23	2.14	0.48
1:C:321:ALA:O	1:C:325:THR:HG23	2.13	0.48
1:B:182:ILE:HG22	1:B:183:ILE:HG13	1.96	0.48
1:B:111:ILE:HD11	1:B:137:TYR:CD2	2.49	0.48
1:A:324:LYS:HZ3	1:C:320:ARG:NH2	2.11	0.47
1:A:351:ILE:HG23	1:A:356:ILE:HG12	1.96	0.47
1:B:104:LEU:HD21	1:B:203:VAL:HG13	1.94	0.47
1:C:351:ILE:HG23	1:C:356:ILE:HG12	1.96	0.47
1:B:31:LEU:HD23	1:B:48:PHE:HB3	1.95	0.47
1:A:324:LYS:NZ	1:C:320:ARG:NH2	2.62	0.47
1:C:241:HIS:HB3	1:C:244:GLU:OE1	2.14	0.47
1:C:57:ASN:O	1:C:60:ALA:HB3	2.14	0.47
1:A:86:ASN:O	1:A:88:THR:O	2.32	0.47
1:A:292:GLN:OE1	1:A:365:ARG:HG3	2.15	0.47
1:B:290:TYR:CG	1:B:366:ASP:OD2	2.67	0.47
1:A:247:ALA:HB1	1:A:257:CYS:HB3	1.96	0.47
1:B:139:LEU:CD1	1:B:173:ILE:HD13	2.43	0.47
1:C:325:THR:HG21	1:C:388:ALA:HB2	1.96	0.47
1:C:285:ILE:HD11	1:C:393:ILE:CD1	2.40	0.47
1:B:104:LEU:HD11	1:B:203:VAL:HG22	1.97	0.47
1:A:78:ASP:O	1:A:81:GLN:HB2	2.15	0.47
1:A:176:ILE:CG2	1:A:190:LEU:HD11	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:THR:HG22	1:B:14:SER:H	1.80	0.46
1:B:86:ASN:HA	1:B:89:VAL:CG2	2.43	0.46
1:B:291:SER:O	1:B:292:GLN:HG3	2.15	0.46
1:C:240:LYS:O	1:C:241:HIS:CG	2.69	0.46
1:C:389:ALA:O	1:C:393:ILE:HG23	2.15	0.46
1:C:23:LEU:CD1	1:C:62:LEU:HD21	2.46	0.46
1:A:226:ASN:OD1	1:A:226:ASN:N	2.48	0.46
1:B:296:PHE:HB2	1:B:297:PRO:HD2	1.98	0.46
1:C:296:PHE:HB2	1:C:297:PRO:HD2	1.97	0.46
1:A:315:ALA:O	1:A:319:VAL:HG23	2.15	0.46
1:B:176:ILE:HG21	1:B:190:LEU:HD11	1.97	0.46
1:A:296:PHE:HB2	1:A:297:PRO:HD2	1.98	0.46
1:B:94:SER:O	1:B:95:ALA:C	2.54	0.46
1:C:397:VAL:HG13	1:C:401:VAL:HG21	1.98	0.46
1:A:125:ILE:HG21	1:A:125:ILE:HD13	1.54	0.45
1:A:125:ILE:HG13	1:A:138:VAL:HB	1.97	0.45
1:B:117:ARG:CG	1:B:118:HIS:HD2	2.25	0.45
1:B:23:LEU:HD11	1:B:62:LEU:HD21	1.97	0.45
1:A:117:ARG:CG	1:A:118:HIS:HD2	2.27	0.45
1:A:185:GLN:NE2	1:C:399:ARG:NH2	2.64	0.45
1:B:111:ILE:O	1:B:115:THR:HB	2.16	0.45
1:B:293:HIS:HA	1:B:332:THR:O	2.17	0.45
1:C:3:SER:CB	1:C:77:GLU:HB2	2.46	0.45
1:C:242:TRP:CH2	1:C:260:TYR:HA	2.51	0.45
1:B:310:GLU:O	1:B:314:VAL:HG23	2.17	0.45
1:B:3:SER:CB	1:B:77:GLU:HB2	2.46	0.45
1:C:13:THR:HG22	1:C:14:SER:N	2.32	0.45
1:C:237:PHE:CE2	1:C:267:VAL:HG13	2.52	0.45
1:A:121:MET:HE1	1:A:176:ILE:HG22	1.99	0.45
1:B:176:ILE:CG2	1:B:190:LEU:HD11	2.46	0.45
1:B:183:ILE:HD13	1:B:186:TYR:HE2	1.83	0.44
1:A:114:ILE:CG2	1:A:122:LEU:CD1	2.95	0.44
1:B:290:TYR:O	1:B:291:SER:OG	2.22	0.44
1:C:310:GLU:O	1:C:314:VAL:HG23	2.17	0.44
1:A:154:ILE:HA	1:A:285:ILE:O	2.17	0.44
1:A:11:PRO:O	1:A:42:LYS:O	2.35	0.44
1:C:124:LYS:HE3	1:C:137:TYR:CZ	2.52	0.44
1:A:294:ILE:HG21	1:A:294:ILE:HD13	1.59	0.44
1:C:290:TYR:O	1:C:291:SER:OG	2.29	0.44
1:B:168:PHE:HA	1:B:383:CYS:SG	2.58	0.43
1:A:121:MET:CE	1:A:176:ILE:HG22	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ILE:HB	1:A:186:TYR:CD2	2.52	0.43
1:A:290:TYR:O	1:A:291:SER:OG	2.30	0.43
1:C:110:TRP:CE3	1:C:111:ILE:HG22	2.54	0.43
1:A:399:ARG:NE	1:C:185:GLN:HE21	2.15	0.43
1:C:156:CYS:HB2	1:C:199:PRO:O	2.18	0.43
1:C:203:VAL:HG12	1:C:204:ASP:N	2.33	0.43
1:A:320:ARG:NH2	1:C:324:LYS:HZ3	2.15	0.43
1:B:30:VAL:HG11	1:B:215:MET:HB3	1.99	0.43
1:C:354:LEU:HG	1:C:354:LEU:O	2.18	0.43
1:A:285:ILE:HD11	1:A:393:ILE:CD1	2.44	0.43
1:B:290:TYR:O	1:B:291:SER:CB	2.66	0.43
1:A:185:GLN:HE21	1:C:399:ARG:HE	1.63	0.43
1:A:360:PHE:CD2	1:A:393:ILE:HD12	2.54	0.43
1:B:23:LEU:HD11	1:B:62:LEU:CD2	2.49	0.43
1:B:292:GLN:NE2	1:B:330:ARG:O	2.51	0.43
1:B:366:ASP:OD1	1:B:366:ASP:N	2.52	0.43
1:B:117:ARG:CG	1:B:118:HIS:CD2	2.97	0.43
1:A:11:PRO:HG3	1:A:20:LEU:HD12	2.01	0.43
1:B:11:PRO:HG3	1:B:20:LEU:HD12	2.01	0.43
1:A:30:VAL:HG11	1:A:215:MET:HB3	2.01	0.42
1:A:317:GLU:HG2	1:A:392:LYS:HG2	2.01	0.42
1:B:360:PHE:CD2	1:B:393:ILE:HD12	2.55	0.42
1:A:20:LEU:HA	1:A:23:LEU:HD12	2.01	0.42
1:C:78:ASP:O	1:C:81:GLN:HB2	2.19	0.42
1:B:125:ILE:HD13	1:B:125:ILE:HG21	1.54	0.42
1:A:176:ILE:HG21	1:A:190:LEU:HD11	2.00	0.42
1:B:369:THR:HG22	1:B:370:TYR:CA	2.49	0.42
1:B:52:ALA:O	1:B:55:VAL:HG23	2.19	0.42
1:C:293:HIS:HA	1:C:332:THR:O	2.18	0.42
1:B:290:TYR:HB2	1:B:366:ASP:OD2	2.19	0.42
1:C:190:LEU:HD23	1:C:190:LEU:HA	1.86	0.42
2:A:604:NAG:HO3	2:A:604:NAG:H82	1.79	0.41
1:B:20:LEU:HD23	1:B:23:LEU:HD12	2.02	0.41
1:C:292:GLN:NE2	1:C:330:ARG:O	2.51	0.41
1:B:1:ALA:CB	2:B:602:NAG:C8	2.98	0.41
1:C:154:ILE:HA	1:C:285:ILE:O	2.20	0.41
1:A:241:HIS:HB3	1:A:244:GLU:OE1	2.20	0.41
1:A:326:SER:OG	1:A:385:GLU:OE1	2.22	0.41
1:C:114:ILE:CG2	1:C:122:LEU:CD1	2.96	0.41
1:A:393:ILE:HG21	1:A:393:ILE:HD13	1.72	0.41
1:B:189:LEU:HD23	1:B:189:LEU:HA	1.76	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ARG:HD2	1:C:247:ALA:HB2	2.03	0.41
1:C:329:THR:CG2	1:C:330:ARG:N	2.83	0.41
1:A:124:LYS:HE3	1:A:137:TYR:CZ	2.54	0.41
1:B:186:TYR:HE1	1:B:387:PHE:CZ	2.38	0.41
1:C:351:ILE:HG23	1:C:356:ILE:CG1	2.50	0.41
1:A:325:THR:HG21	1:A:388:ALA:HB2	2.01	0.41
1:B:110:TRP:CZ3	1:B:170:LEU:HD22	2.56	0.41
1:B:121:MET:CE	1:B:176:ILE:HG22	2.51	0.41
1:C:111:ILE:O	1:C:115:THR:HB	2.20	0.41
1:B:331:TYR:CE2	1:B:365:ARG:HB2	2.56	0.41
1:A:13:THR:HG22	1:A:14:SER:N	2.36	0.41
1:A:356:ILE:HD13	1:A:356:ILE:N	2.35	0.41
1:B:114:ILE:CG2	1:B:122:LEU:CD1	2.99	0.41
1:C:290:TYR:O	1:C:291:SER:CB	2.69	0.41
1:A:242:TRP:CD2	1:A:243:CYS:HB2	2.56	0.40
1:C:189:LEU:HD22	1:C:193:VAL:HG12	2.03	0.40
1:B:190:LEU:HA	1:B:190:LEU:HD23	1.82	0.40
1:C:317:GLU:HG2	1:C:392:LYS:HG2	2.04	0.40
1:A:117:ARG:CG	1:A:118:HIS:CD2	2.98	0.40
1:B:88:THR:O	1:B:89:VAL:HB	2.20	0.40
1:A:20:LEU:HD23	1:A:23:LEU:HD12	2.02	0.40
1:B:117:ARG:C	1:B:118:HIS:HD2	2.25	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:B:317:GLU:OE2	1:B:317:GLU:OE2[5_555]	2.18	0.02

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	399/424 (94%)	355 (89%)	35 (9%)	9 (2%)	7	33
1	B	399/424 (94%)	354 (89%)	32 (8%)	13 (3%)	4	25
1	C	399/424 (94%)	354 (89%)	34 (8%)	11 (3%)	6	29
All	All	1197/1272 (94%)	1063 (89%)	101 (8%)	33 (3%)	6	29

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	ASN
1	A	366	ASP
1	B	219	ASN
1	C	143	GLY
1	C	219	ASN
1	A	42	LYS
1	A	291	SER
1	B	42	LYS
1	B	143	GLY
1	B	291	SER
1	B	297	PRO
1	B	369	THR
1	C	88	THR
1	C	291	SER
1	C	297	PRO
1	A	297	PRO
1	C	42	LYS
1	C	369	THR
1	C	377	ARG
1	A	146	GLN
1	B	88	THR
1	B	146	GLN
1	B	244	GLU
1	B	367	THR
1	C	203	VAL
1	C	244	GLU
1	A	203	VAL
1	A	244	GLU
1	C	366	ASP
1	B	203	VAL
1	B	377	ARG
1	B	368	GLY
1	A	143	GLY

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	354/375 (94%)	332 (94%)	22 (6%)	21	57
1	B	354/375 (94%)	329 (93%)	25 (7%)	17	52
1	C	354/375 (94%)	331 (94%)	23 (6%)	20	55
All	All	1062/1125 (94%)	992 (93%)	70 (7%)	19	54

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	72	LEU
1	A	111	ILE
1	A	114	ILE
1	A	147	THR
1	A	189	LEU
1	A	227	HIS
1	A	251	SER
1	A	278	ILE
1	A	281	ILE
1	A	292	GLN
1	A	294	ILE
1	A	297	PRO
1	A	299	SER
1	A	303	SER
1	A	305	SER
1	A	312	SER
1	A	323	GLU
1	A	332	THR
1	A	342	LEU
1	A	351	ILE
1	A	393	ILE
1	B	14	SER
1	B	72	LEU
1	B	111	ILE
1	B	114	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	115	THR
1	B	125	ILE
1	B	147	THR
1	B	170	LEU
1	B	189	LEU
1	B	227	HIS
1	B	251	SER
1	B	281	ILE
1	B	292	GLN
1	B	294	ILE
1	B	297	PRO
1	B	299	SER
1	B	305	SER
1	B	312	SER
1	B	323	GLU
1	B	332	THR
1	B	342	LEU
1	B	351	ILE
1	B	365	ARG
1	B	367	THR
1	B	393	ILE
1	C	14	SER
1	C	72	LEU
1	C	111	ILE
1	C	114	ILE
1	C	115	THR
1	C	147	THR
1	C	189	LEU
1	C	227	HIS
1	C	251	SER
1	C	278	ILE
1	C	281	ILE
1	C	292	GLN
1	C	294	ILE
1	C	297	PRO
1	C	305	SER
1	C	312	SER
1	C	323	GLU
1	C	332	THR
1	C	342	LEU
1	C	351	ILE
1	C	367	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	369	THR
1	C	393	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	57	ASN
1	A	100	GLN
1	A	118	HIS
1	A	185	GLN
1	A	279	ASN
1	A	308	HIS
1	B	45	GLN
1	B	57	ASN
1	B	100	GLN
1	B	118	HIS
1	B	279	ASN
1	B	308	HIS
1	C	45	GLN
1	C	57	ASN
1	C	100	GLN
1	C	118	HIS
1	C	185	GLN
1	C	279	ASN
1	C	308	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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$
2	NAG	A	601	1	14,14,15	0.94	0	15,19,21	1.45	2 (13%)
2	NAG	A	602	1	14,14,15	0.66	0	15,19,21	2.25	5 (33%)
2	NAG	A	603	1	14,14,15	0.46	0	15,19,21	2.96	4 (26%)
2	NAG	A	604	1	14,14,15	0.58	0	15,19,21	2.02	4 (26%)
2	NAG	B	601	1	14,14,15	0.63	0	15,19,21	1.95	4 (26%)
2	NAG	B	602	1	14,14,15	0.82	1 (7%)	15,19,21	1.68	2 (13%)
2	NAG	B	603	1	14,14,15	0.78	0	15,19,21	1.56	5 (33%)
2	NAG	B	604	1	14,14,15	0.56	0	15,19,21	1.97	3 (20%)
2	NAG	C	604	1	14,14,15	0.56	0	15,19,21	1.97	2 (13%)

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	601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1	-	0/6/23/26	0/1/1/1
2	NAG	A	603	1	-	0/6/23/26	0/1/1/1
2	NAG	A	604	1	-	0/6/23/26	0/1/1/1
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	602	1	-	0/6/23/26	0/1/1/1
2	NAG	B	603	1	-	0/6/23/26	0/1/1/1
2	NAG	B	604	1	-	0/6/23/26	0/1/1/1
2	NAG	C	604	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	NAG	C1-C2	2.49	1.55	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	NAG	O5-C1-C2	-5.62	103.65	111.47
2	C	604	NAG	O5-C1-C2	-4.91	104.64	111.47
2	A	604	NAG	O5-C1-C2	-4.57	105.12	111.47
2	B	604	NAG	O5-C1-C2	-4.05	105.84	111.47
2	A	602	NAG	O3-C3-C2	-3.25	102.42	109.39
2	B	603	NAG	O5-C1-C2	-3.00	107.30	111.47
2	B	601	NAG	C2-N2-C7	-2.61	119.14	122.94
2	B	601	NAG	O7-C7-C8	-2.39	117.71	122.06
2	A	604	NAG	O7-C7-C8	-2.33	117.81	122.06
2	B	603	NAG	C3-C4-C5	-2.32	106.13	110.22
2	A	601	NAG	C1-C2-N2	-2.29	106.58	110.49
2	A	603	NAG	O3-C3-C2	-2.27	104.52	109.39
2	A	602	NAG	C6-C5-C4	-2.21	107.83	113.00
2	B	603	NAG	O6-C6-C5	-2.20	103.93	111.34
2	B	603	NAG	C8-C7-N2	2.09	119.88	116.11
2	A	604	NAG	C4-C3-C2	2.13	114.14	111.02
2	B	603	NAG	C4-C3-C2	2.43	114.57	111.02
2	B	604	NAG	C4-C3-C2	2.61	114.84	111.02
2	A	602	NAG	O5-C1-C2	2.69	115.21	111.47
2	B	602	NAG	C2-N2-C7	2.71	126.90	122.94
2	A	603	NAG	C1-C2-N2	2.75	115.19	110.49
2	A	602	NAG	C4-C3-C2	2.99	115.40	111.02
2	B	601	NAG	C8-C7-N2	3.20	121.89	116.11
2	A	601	NAG	C4-C3-C2	3.59	116.27	111.02
2	B	604	NAG	C1-O5-C5	4.13	117.85	112.17
2	C	604	NAG	C1-O5-C5	4.29	118.08	112.17
2	A	604	NAG	C1-O5-C5	4.53	118.41	112.17
2	B	602	NAG	C1-O5-C5	4.75	118.71	112.17
2	B	601	NAG	C1-O5-C5	5.23	119.37	112.17
2	A	602	NAG	C1-O5-C5	6.13	120.62	112.17
2	A	603	NAG	C1-O5-C5	8.42	123.77	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	NAG	3	0
2	B	602	NAG	1	0
2	B	604	NAG	2	0
2	C	604	NAG	2	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

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, 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(Å ²)	Q<0.9
1	A	401/424 (94%)	0.16	7 (1%) 70 49	64, 91, 115, 122	0
1	B	401/424 (94%)	0.73	58 (14%) 3 1	65, 92, 130, 138	0
1	C	401/424 (94%)	0.57	46 (11%) 5 2	60, 92, 120, 130	0
All	All	1203/1272 (94%)	0.49	111 (9%) 10 3	60, 92, 125, 138	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	ALA	10.2
1	B	335	HIS	8.0
1	B	345	GLY	7.8
1	B	341	TYR	7.3
1	B	346	GLY	6.2
1	B	337	SER	6.1
1	B	338	GLU	6.1
1	B	334	GLY	5.8
1	B	333	HIS	5.7
1	B	342	LEU	5.7
1	C	339	THR	5.4
1	B	332	THR	5.1
1	B	339	THR	4.9
1	B	325	THR	4.9
1	B	301	THR	4.7
1	B	308	HIS	4.5
1	B	315	ALA	4.4
1	C	338	GLU	4.4
1	C	334	GLY	4.4
1	C	68	PRO	4.3
1	B	300	TYR	4.2
1	B	316	SER	4.1
1	B	298	TYR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	344	PRO	4.0
1	B	313	LEU	3.9
1	B	336	GLY	3.9
1	B	302	ARG	3.9
1	C	9	ALA	3.9
1	B	326	SER	3.9
1	B	312	SER	3.8
1	C	67	ILE	3.8
1	B	314	VAL	3.8
1	B	340	LEU	3.8
1	C	3	SER	3.8
1	C	2	GLN	3.7
1	B	303	SER	3.6
1	B	304	LYS	3.6
1	B	1	ALA	3.6
1	C	335	HIS	3.6
1	C	302	ARG	3.5
1	B	322	ILE	3.5
1	B	329	THR	3.5
1	C	58	VAL	3.4
1	C	28	GLU	3.4
1	B	323	GLU	3.4
1	C	301	THR	3.4
1	B	311	LEU	3.3
1	C	29	ILE	3.3
1	C	19	VAL	3.3
1	B	292	GLN	3.2
1	C	7	LEU	3.2
1	C	330	ARG	3.2
1	C	332	THR	3.2
1	C	328	ASN	3.2
1	B	331	TYR	3.1
1	B	318	ALA	3.1
1	B	327	LYS	3.1
1	C	27	TYR	3.1
1	B	224	ALA	3.1
1	B	27	TYR	2.9
1	C	323	GLU	2.9
1	B	310	GLU	2.9
1	C	11	PRO	2.9
1	C	66	GLY	2.9
1	C	76	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	20	LEU	2.9
1	B	317	GLU	2.9
1	C	69	CYS	2.9
1	C	10	LEU	2.8
1	B	246	GLY	2.8
1	C	42	LYS	2.8
1	C	64	VAL	2.8
1	C	23	LEU	2.8
1	C	65	SER	2.8
1	B	226	ASN	2.7
1	B	321	ALA	2.7
1	B	305	SER	2.6
1	B	5	GLN	2.6
1	C	337	SER	2.5
1	A	341	TYR	2.5
1	C	63	ASN	2.5
1	B	293	HIS	2.5
1	B	348	ASP	2.5
1	A	27	TYR	2.4
1	C	329	THR	2.4
1	C	50	VAL	2.4
1	C	71	VAL	2.4
1	B	148	ALA	2.4
1	B	247	ALA	2.4
1	B	319	VAL	2.3
1	C	341	TYR	2.3
1	C	73	LEU	2.3
1	C	62	LEU	2.3
1	A	11	PRO	2.3
1	C	16	GLN	2.3
1	A	76	VAL	2.2
1	A	64	VAL	2.2
1	B	328	ASN	2.2
1	A	1	ALA	2.1
1	C	342	LEU	2.1
1	B	290	TYR	2.1
1	B	297	PRO	2.1
1	C	367	THR	2.1
1	B	307	ASP	2.1
1	C	43	LYS	2.1
1	C	77	GLU	2.1
1	B	306	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	48	PHE	2.0
1	B	257	CYS	2.0
1	A	28	GLU	2.0
1	B	299	SER	2.0

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(Å ²)	Q<0.9
2	NAG	C	604	14/15	0.81	0.21	-0.72	87,90,97,97	0
2	NAG	B	602	14/15	0.77	0.20	-0.87	103,106,107,107	0
2	NAG	A	601	14/15	0.74	0.41	-	101,105,108,109	0
3	ZN	B	501	1/1	0.87	0.13	-	102,102,102,102	0
2	NAG	A	604	14/15	0.71	0.28	-	89,92,98,98	0
2	NAG	A	603	14/15	0.84	0.28	-	90,91,93,93	0
2	NAG	B	603	14/15	0.72	0.20	-	103,105,110,111	0
3	ZN	C	501	1/1	0.93	0.20	-	106,106,106,106	0
2	NAG	A	602	14/15	0.83	0.46	-	99,101,106,106	0
2	NAG	B	604	14/15	0.86	0.17	-	89,93,94,96	0
3	ZN	A	501	1/1	0.93	0.22	-	99,99,99,99	0
2	NAG	B	601	14/15	0.90	0.15	-	86,88,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.