



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2017 – 04:02 PM EDT

PDB ID : 5THB  
Title : Crystal structure of H10 hemagglutinin mutant (T193D-Q226L-G228S) from Jiangxi-Donghu (2013) H10N8 influenza virus  
Authors : Tzarum, N.; Wilson, I.A.  
Deposited on : unknown  
Resolution : 2.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
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) : rb-20029824

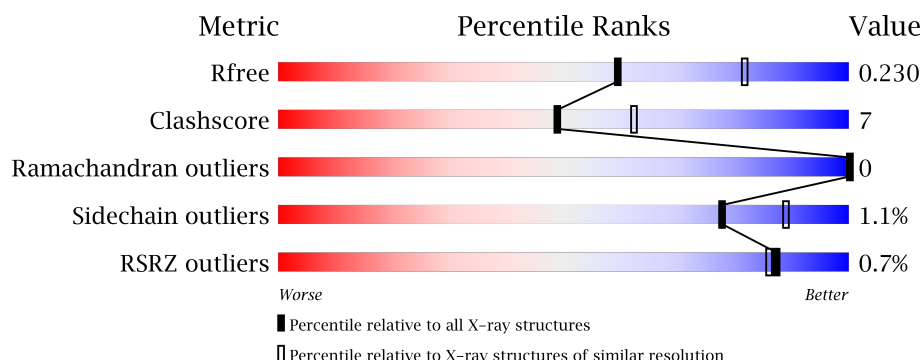
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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	3709 (2.44-2.40)
Clashscore	112137	4241 (2.44-2.40)
Ramachandran outliers	110173	4178 (2.44-2.40)
Sidechain outliers	110143	4179 (2.44-2.40)
RSRZ outliers	101464	3740 (2.44-2.40)

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	323	
1	C	323	
1	E	323	
2	B	180	
2	D	180	

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Mol	Chain	Length	Quality of chain
2	F	180	 73% 19% 6%

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	400	-	-	-	X
3	NAG	B	201	-	-	-	X
3	NAG	C	501	-	-	-	X
3	NAG	E	601	-	-	-	X
3	NAG	F	201	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12224 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2437	1508	448	464	17			
1	C	319	Total	C	N	O	S	0	0	0
			2445	1514	449	465	17			
1	E	318	Total	C	N	O	S	0	0	0
			2437	1508	448	464	17			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	THR	ASP	engineered mutation	UNP A0A0J9X252
A	226	LEU	GLN	engineered mutation	UNP A0A0J9X252
A	228	SER	GLY	engineered mutation	UNP A0A0J9X252
C	193	THR	ASP	engineered mutation	UNP A0A0J9X252
C	226	LEU	GLN	engineered mutation	UNP A0A0J9X252
C	228	SER	GLY	engineered mutation	UNP A0A0J9X252
E	193	THR	ASP	engineered mutation	UNP A0A0J9X252
E	226	LEU	GLN	engineered mutation	UNP A0A0J9X252
E	228	SER	GLY	engineered mutation	UNP A0A0J9X252

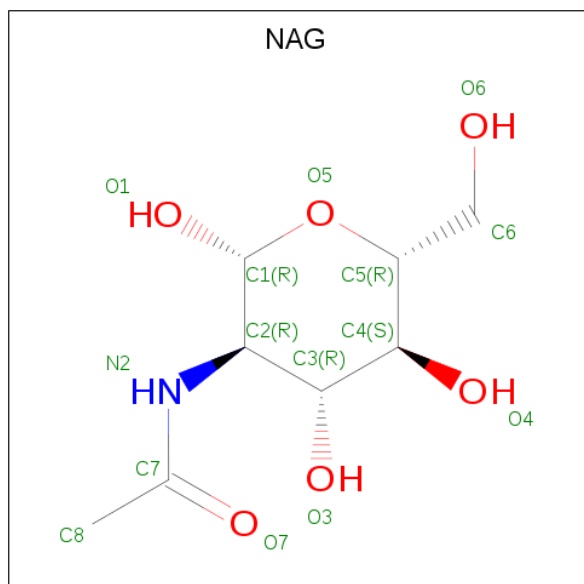
- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1382	854	239	281	8			
2	D	169	Total	C	N	O	S	0	0	0
			1367	846	236	277	8			
2	F	169	Total	C	N	O	S	0	0	0
			1371	848	237	278	8			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A0A0J9X253
B	176	GLY	-	expression tag	UNP A0A0J9X253
B	177	ARG	-	expression tag	UNP A0A0J9X253
B	178	LEU	-	expression tag	UNP A0A0J9X253
B	179	VAL	-	expression tag	UNP A0A0J9X253
B	180	PRO	-	expression tag	UNP A0A0J9X253
B	181	ARG	-	expression tag	UNP A0A0J9X253
D	175	SER	-	expression tag	UNP A0A0J9X253
D	176	GLY	-	expression tag	UNP A0A0J9X253
D	177	ARG	-	expression tag	UNP A0A0J9X253
D	178	LEU	-	expression tag	UNP A0A0J9X253
D	179	VAL	-	expression tag	UNP A0A0J9X253
D	180	PRO	-	expression tag	UNP A0A0J9X253
D	181	ARG	-	expression tag	UNP A0A0J9X253
F	175	SER	-	expression tag	UNP A0A0J9X253
F	176	GLY	-	expression tag	UNP A0A0J9X253
F	177	ARG	-	expression tag	UNP A0A0J9X253
F	178	LEU	-	expression tag	UNP A0A0J9X253
F	179	VAL	-	expression tag	UNP A0A0J9X253
F	180	PRO	-	expression tag	UNP A0A0J9X253
F	181	ARG	-	expression tag	UNP A0A0J9X253

- 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	C	N	O	0	0
			14	8	1	5		

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

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			11	6	5		

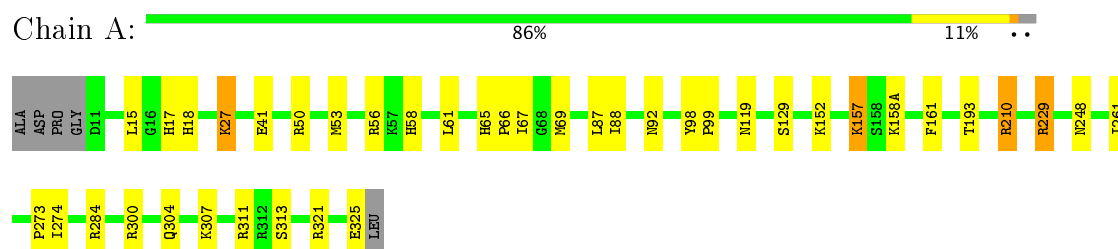
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	138	Total	O	0	0
			138	138		
6	B	64	Total	O	0	0
			64	64		
6	C	150	Total	O	0	0
			150	150		
6	D	72	Total	O	0	0
			72	72		
6	E	135	Total	O	0	0
			135	135		
6	F	78	Total	O	0	0
			78	78		

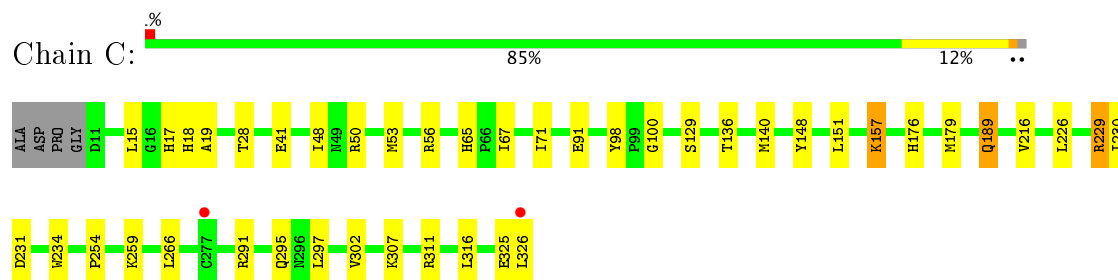
### 3 Residue-property plots [i](#)

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.

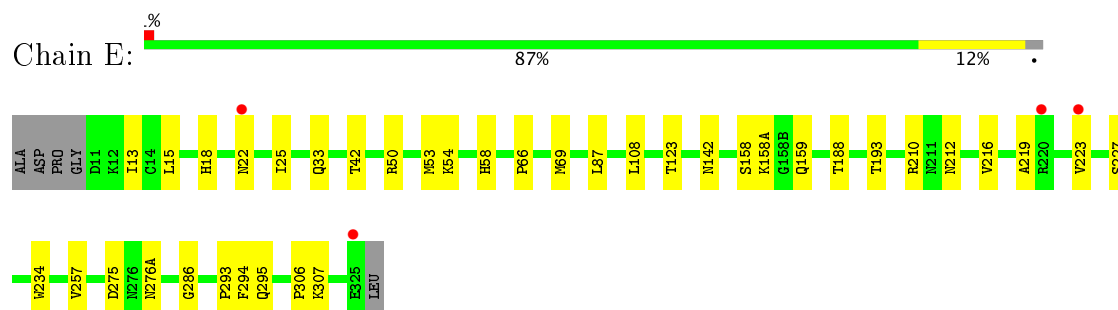
- Molecule 1: Hemagglutinin HA1 chain



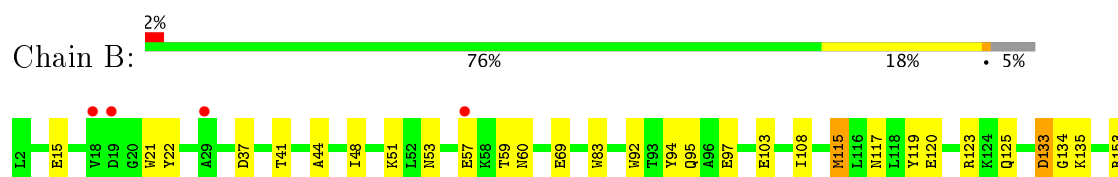
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain



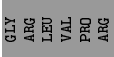
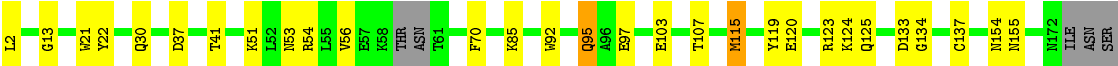
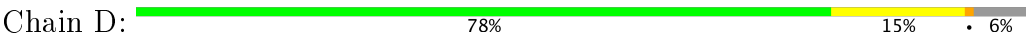
- Molecule 2: Hemagglutinin HA2 chain



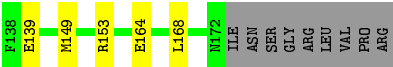
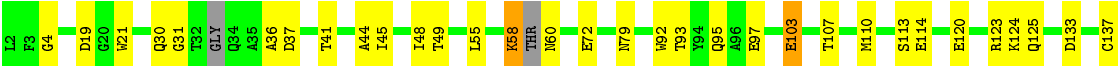




● Molecule 2: Hemagglutinin HA2 chain



● Molecule 2: Hemagglutinin HA2 chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.83 Å   241.29 Å   70.06 Å 90.00°   111.43°   90.00°	Depositor
Resolution (Å)	33.05 – 2.41 47.79 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.8 (33.05-2.41) 95.1 (47.79-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.29 (at 2.39 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.180   ,   0.230 0.179   ,   0.230	Depositor DCC
$R_{free}$ test set	3639 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12224	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.54	0/2486	0.71	3/3369 (0.1%)
1	C	0.54	0/2494	0.68	3/3380 (0.1%)
1	E	0.55	0/2486	0.70	3/3369 (0.1%)
2	B	0.51	0/1407	0.65	1/1899 (0.1%)
2	D	0.53	0/1391	0.64	1/1875 (0.1%)
2	F	0.49	0/1394	0.68	2/1878 (0.1%)
All	All	0.53	0/11658	0.68	13/15770 (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	E	0	1
2	B	0	1
2	F	0	2
All	All	0	4

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	A	210	ARG	NE-CZ-NH1	-8.96	115.82	120.30
1	A	210	ARG	NE-CZ-NH2	8.63	124.62	120.30
1	E	286	GLY	N-CA-C	7.20	131.09	113.10
2	F	31	GLY	N-CA-C	7.00	130.61	113.10
1	A	229	ARG	NE-CZ-NH2	-6.10	117.25	120.30
2	F	168	LEU	CA-CB-CG	5.64	128.28	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	115	MET	CG-SD-CE	-5.62	91.22	100.20
1	C	229	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	B	115	MET	CG-SD-CE	-5.41	91.55	100.20
1	E	15	LEU	CA-CB-CG	-5.36	102.96	115.30
1	E	142	ASN	C-N-CA	-5.12	111.54	122.30
1	C	229	ARG	CG-CD-NE	-5.05	101.20	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	59	THR	Peptide
1	E	219	ALA	Peptide
2	F	30	GLN	Peptide
2	F	4	GLY	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	2437	0	2393	41	0
1	C	2445	0	2405	32	0
1	E	2437	0	2394	25	0
2	B	1382	0	1278	31	0
2	D	1367	0	1264	29	0
2	F	1371	0	1266	29	0
3	A	28	0	26	0	0
3	B	14	0	13	0	0
3	C	28	0	24	0	0
3	D	14	0	13	0	0
3	E	28	0	25	0	0
3	F	14	0	13	1	0
4	C	11	0	9	0	0
5	C	11	0	10	0	0
6	A	138	0	0	4	0
6	B	64	0	0	4	0
6	C	150	0	0	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	72	0	0	6	0
6	E	135	0	0	3	1
6	F	78	0	0	8	0
All	All	12224	0	11133	154	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 7.

All (154) 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:17:HIS:HB3	2:D:115:MET:HE1	1.49	0.92
2:D:54:ARG:NH1	6:D:301:HOH:O	2.01	0.92
2:B:133:ASP:OD2	2:B:135:LYS:HE3	1.78	0.83
2:B:53:ASN:O	2:B:57:GLU:HG2	1.81	0.80
1:C:53:MET:HE3	1:C:56:ARG:HD2	1.66	0.76
2:F:153:ARG:NH1	6:F:304:HOH:O	2.19	0.74
1:C:28:THR:O	6:C:601:HOH:O	2.04	0.73
1:A:210:ARG:NH1	1:E:227:SER:O	2.22	0.72
2:D:30:GLN:OE1	6:D:302:HOH:O	2.10	0.70
2:F:58:LYS:O	2:F:60:ASN:N	2.25	0.69
2:D:53:ASN:OD1	6:D:303:HOH:O	2.11	0.68
2:B:163:ARG:NH1	6:B:304:HOH:O	2.27	0.68
2:F:120:GLU:OE1	2:F:123:ARG:NH2	2.27	0.67
1:C:266:LEU:HD11	1:C:302:VAL:HG13	1.78	0.66
2:B:95:GLN:NE2	2:F:95:GLN:OE1	2.29	0.66
2:B:165:GLU:OE2	6:B:301:HOH:O	2.13	0.66
2:B:117:ASN:O	6:B:302:HOH:O	2.14	0.65
2:F:103:GLU:OE2	6:F:301:HOH:O	2.14	0.65
2:D:154:ASN:ND2	6:D:304:HOH:O	2.28	0.64
2:D:134:GLY:HA2	2:F:124:LYS:HD3	1.79	0.64
1:C:129:SER:O	1:C:157:LYS:HE3	1.97	0.64
2:D:125:GLN:HE22	2:D:155:ASN:HA	1.64	0.63
1:C:48:ILE:HG22	1:C:50:ARG:H	1.64	0.62
2:F:139:GLU:OE1	6:F:302:HOH:O	2.16	0.62
1:A:17:HIS:HB3	2:B:115:MET:CE	2.31	0.61
2:F:44:ALA:HA	2:F:110:MET:CE	2.30	0.60
1:A:41:GLU:OE2	1:A:313:SER:OG	2.10	0.60
1:C:179:MET:HG2	1:C:234:TRP:HB3	1.82	0.60
1:C:231:ASP:OD2	1:E:210:ARG:NH1	2.35	0.59
1:C:189:GLN:NE2	6:C:603:HOH:O	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:HIS:CB	2:D:115:MET:HE1	2.28	0.59
2:B:37:ASP:O	2:B:41:THR:HG23	2.02	0.59
1:A:284:ARG:NH1	2:B:69:GLU:HG3	2.18	0.58
1:A:69:MET:HE1	1:A:87:LEU:HD21	1.86	0.58
1:E:123:THR:HG22	1:E:257:VAL:HG13	1.85	0.58
2:D:120:GLU:OE1	2:D:123:ARG:NH2	2.22	0.58
2:D:21:TRP:H	2:D:41:THR:CG2	2.17	0.57
1:A:66:PRO:HA	1:A:69:MET:HE3	1.86	0.57
2:B:154:ASN:O	2:B:155:ASN:HB2	2.03	0.57
1:A:88:ILE:HD13	1:A:274:ILE:HD11	1.85	0.57
2:F:79:ASN:OD1	3:F:201:NAG:C8	2.52	0.57
1:C:216:VAL:HG11	1:E:212:ASN:HB2	1.87	0.57
2:F:120:GLU:OE2	6:F:303:HOH:O	2.17	0.55
1:A:92:ASN:ND2	6:A:501:HOH:O	2.19	0.55
1:A:53:MET:CE	1:A:58:HIS:HB3	2.37	0.55
1:C:229:ARG:HD2	6:E:816:HOH:O	2.06	0.55
1:C:15:LEU:HD13	2:D:119:TYR:HA	1.89	0.55
2:D:22:TYR:H	2:D:41:THR:HG22	1.71	0.55
1:C:53:MET:HE3	1:C:56:ARG:CD	2.36	0.55
2:F:164:GLU:HG2	6:F:330:HOH:O	2.07	0.54
1:A:61:LEU:HD11	1:A:69:MET:HE2	1.90	0.54
1:A:53:MET:HE1	1:A:56:ARG:HD3	1.90	0.54
2:D:133:ASP:OD2	2:D:137:CYS:HB2	2.08	0.54
2:F:60:ASN:ND2	6:F:305:HOH:O	2.20	0.53
1:A:321:ARG:HG3	2:B:108:ILE:HG23	1.92	0.52
2:B:21:TRP:H	2:B:41:THR:CG2	2.22	0.52
1:A:17:HIS:HB3	2:B:115:MET:HE1	1.89	0.52
2:F:19:ASP:HB3	2:F:36:ALA:HB2	1.91	0.52
2:F:93:THR:O	2:F:97:GLU:HG3	2.09	0.52
1:A:284:ARG:HG3	2:B:69:GLU:HG2	1.92	0.52
1:A:304:GLN:HB3	2:B:60:ASN:CB	2.41	0.51
1:A:50:ARG:NH2	1:A:273:PRO:HG2	2.26	0.51
2:D:37:ASP:O	2:D:41:THR:HG23	2.10	0.51
1:A:300:ARG:NE	6:A:510:HOH:O	2.44	0.50
1:A:53:MET:HE2	1:A:58:HIS:CB	2.41	0.50
1:C:151:LEU:HD23	1:C:254:PRO:HA	1.93	0.50
1:A:152:LYS:NZ	6:A:511:HOH:O	2.44	0.50
1:C:307:LYS:HG3	2:D:92:TRP:CE2	2.47	0.50
2:B:22:TYR:H	2:B:41:THR:HG22	1.75	0.50
2:B:125:GLN:OE1	2:B:155:ASN:HA	2.12	0.50
2:F:21:TRP:H	2:F:41:THR:CG2	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:HD2	6:A:595:HOH:O	2.11	0.50
1:A:158(A):LYS:O	1:A:193:THR:O	2.28	0.50
2:F:44:ALA:HA	2:F:110:MET:HE3	1.93	0.49
1:A:15:LEU:HD13	2:B:119:TYR:HA	1.94	0.49
2:B:21:TRP:H	2:B:41:THR:HG21	1.78	0.48
1:C:176:HIS:CD2	1:C:259:LYS:HG3	2.48	0.48
1:C:91:GLU:HB2	2:D:70:PHE:CE1	2.47	0.48
2:F:45:ILE:O	2:F:49:THR:HG23	2.13	0.48
1:A:65:HIS:CE1	1:A:67:ILE:HG12	2.48	0.48
2:F:110:MET:O	2:F:113:SER:HB3	2.13	0.48
1:E:42:THR:HG22	2:F:55:LEU:HD21	1.96	0.48
1:C:98:TYR:HD2	1:C:136:THR:HG21	1.79	0.48
1:A:304:GLN:HB3	2:B:60:ASN:HB2	1.96	0.47
1:E:22:ASN:N	1:E:22:ASN:OD1	2.41	0.47
2:F:44:ALA:HA	2:F:110:MET:HE1	1.95	0.47
1:E:295:GLN:HG2	1:E:306:PRO:HG2	1.96	0.47
2:D:2:LEU:HB3	6:F:320:HOH:O	2.14	0.47
1:E:53:MET:HB3	1:E:53:MET:HE3	1.79	0.47
1:A:311:ARG:NE	2:B:97:GLU:OE1	2.36	0.47
1:A:53:MET:HE1	1:A:56:ARG:CD	2.45	0.47
1:A:119:ASN:ND2	1:A:261:ILE:HD11	2.30	0.47
1:A:66:PRO:HA	1:A:69:MET:CE	2.44	0.47
2:B:94:TYR:HE1	2:D:95:GLN:NE2	2.13	0.47
1:E:69:MET:HE1	1:E:87:LEU:HD21	1.97	0.47
2:F:125:GLN:HG2	6:F:317:HOH:O	2.15	0.47
1:E:188:THR:HG22	6:E:812:HOH:O	2.15	0.46
2:B:44:ALA:O	2:B:48:ILE:HG12	2.15	0.46
1:A:210:ARG:NH2	1:E:216:VAL:O	2.47	0.46
2:D:54:ARG:NE	6:D:305:HOH:O	2.33	0.45
1:A:53:MET:HE2	1:A:58:HIS:HB3	1.97	0.45
1:E:22:ASN:ND2	6:E:713:HOH:O	2.49	0.45
1:A:53:MET:HE3	1:A:58:HIS:HB3	1.98	0.45
1:E:13:ILE:HB	2:F:149:MET:HE1	1.98	0.45
2:B:134:GLY:HA2	2:D:124:LYS:HD3	1.97	0.45
2:B:153:ARG:NH2	6:B:307:HOH:O	2.50	0.45
2:F:21:TRP:H	2:F:41:THR:HG22	1.82	0.44
1:E:307:LYS:HG3	2:F:92:TRP:CE2	2.53	0.44
2:F:110:MET:HE1	2:F:114:GLU:HG3	1.99	0.44
1:C:226:LEU:O	1:C:229:ARG:NH2	2.51	0.44
1:E:158:SER:HB2	1:E:159:GLN:HG3	2.00	0.44
1:A:129:SER:O	1:A:157:LYS:HE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:TYR:H	2:D:41:THR:CG2	2.31	0.44
2:F:48:ILE:HD11	2:F:107:THR:HG23	1.99	0.44
1:A:284:ARG:HH11	2:B:69:GLU:HG3	1.82	0.44
1:A:50:ARG:CZ	1:A:273:PRO:HG2	2.47	0.44
2:F:149:MET:HE3	2:F:149:MET:HB3	1.85	0.44
2:D:54:ARG:NH2	6:D:305:HOH:O	2.40	0.44
1:E:50:ARG:NE	1:E:275:ASP:OD2	2.39	0.43
1:C:316:LEU:HD11	2:D:103:GLU:HG2	1.99	0.43
1:E:54:LYS:HD2	1:E:276(A):ASN:O	2.17	0.43
1:C:100:GLY:HA3	1:C:230:ILE:O	2.18	0.43
1:C:176:HIS:HD2	1:C:259:LYS:HG3	1.84	0.43
1:A:27:LYS:HE3	1:A:27:LYS:HB2	1.75	0.43
1:C:53:MET:HB3	1:C:53:MET:HE2	1.80	0.43
2:D:21:TRP:H	2:D:41:THR:HG21	1.84	0.43
2:F:133:ASP:CG	2:F:137:CYS:HB2	2.39	0.43
1:C:71:ILE:O	1:C:148:TYR:HB3	2.19	0.43
1:E:223:VAL:HG23	1:E:223:VAL:O	2.19	0.43
2:B:51:LYS:HD3	2:B:103:GLU:HG3	2.00	0.43
1:E:53:MET:HE2	1:E:58:HIS:CB	2.49	0.43
1:E:66:PRO:HA	1:E:69:MET:CE	2.49	0.43
1:A:161:PHE:HB3	1:A:248:ASN:O	2.19	0.42
2:D:51:LYS:NZ	2:D:107:THR:OG1	2.31	0.42
1:E:293:PRO:HG2	1:E:294:PHE:CD2	2.55	0.42
1:E:158(A):LYS:HG2	1:E:193:THR:HG23	2.02	0.42
1:C:295:GLN:OE1	1:C:297:LEU:N	2.53	0.42
1:E:66:PRO:HA	1:E:69:MET:HE3	2.01	0.42
1:C:291:ARG:HG3	2:D:56:VAL:HB	2.02	0.42
1:A:325:GLU:HG3	2:B:15:GLU:HG3	2.01	0.42
1:E:25:ILE:HG23	1:E:33:GLN:HA	2.02	0.42
1:A:53:MET:HE2	1:A:58:HIS:HB2	2.03	0.41
1:C:311:ARG:HE	2:D:97:GLU:CD	2.23	0.41
1:C:65:HIS:CE1	1:C:67:ILE:HG12	2.55	0.41
1:C:19:ALA:HB2	2:D:13:GLY:HA3	2.02	0.41
1:C:325:GLU:OE2	1:C:326:LEU:N	2.52	0.41
1:E:108:LEU:HB2	1:E:234:TRP:CE2	2.56	0.41
1:A:50:ARG:HD3	1:A:50:ARG:HA	1.93	0.41
2:F:37:ASP:O	2:F:41:THR:HG23	2.20	0.41
2:B:83:TRP:CH2	2:D:85:LYS:HG2	2.55	0.41
2:B:120:GLU:OE1	2:B:123:ARG:NH1	2.54	0.40
1:A:307:LYS:HG3	2:B:92:TRP:CE2	2.57	0.40
1:A:98:TYR:CD1	1:A:99:PRO:HD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LYS:NZ	6:C:609:HOH:O	2.49	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)
6:C:740:HOH:O	6:E:721:HOH:O[1_454]	2.17	0.03

## 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	316/323 (98%)	309 (98%)	7 (2%)	0	100	100
1	C	317/323 (98%)	308 (97%)	9 (3%)	0	100	100
1	E	316/323 (98%)	310 (98%)	6 (2%)	0	100	100
2	B	169/180 (94%)	162 (96%)	7 (4%)	0	100	100
2	D	165/180 (92%)	162 (98%)	3 (2%)	0	100	100
2	F	163/180 (91%)	157 (96%)	6 (4%)	0	100	100
All	All	1446/1509 (96%)	1408 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	270/273 (99%)	267 (99%)	3 (1%)	78	89
1	C	271/273 (99%)	266 (98%)	5 (2%)	64	80
1	E	270/273 (99%)	269 (100%)	1 (0%)	93	97
2	B	146/154 (95%)	145 (99%)	1 (1%)	87	94
2	D	144/154 (94%)	143 (99%)	1 (1%)	87	94
2	F	145/154 (94%)	142 (98%)	3 (2%)	59	76
All	All	1246/1281 (97%)	1232 (99%)	14 (1%)	78	89

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	27	LYS
1	A	157	LYS
2	B	133	ASP
1	C	18	HIS
1	C	41	GLU
1	C	140	MET
1	C	157	LYS
1	C	189	GLN
2	D	95	GLN
1	E	18	HIS
2	F	58	LYS
2	F	72	GLU
2	F	103	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
2	B	95	GLN
2	D	95	GLN
2	D	125	GLN
2	F	26	HIS
2	F	47	GLN

### 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 ⓘ

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	NAG	A	400	1	14,14,15	0.66	1 (7%)	15,19,21	1.41	2 (13%)
3	NAG	A	401	1	14,14,15	0.75	1 (7%)	15,19,21	0.94	0
3	NAG	B	201	2	14,14,15	0.66	1 (7%)	15,19,21	1.42	2 (13%)
3	NAG	C	501	1,3	14,14,15	1.04	2 (14%)	15,19,21	1.52	3 (20%)
3	NAG	C	502	3,4	14,14,15	0.22	0	15,19,21	0.60	0
4	BMA	C	503	3,5	11,11,12	1.43	2 (18%)	13,15,17	0.90	1 (7%)
5	MAN	C	504	4	11,11,12	1.56	3 (27%)	13,15,17	1.25	2 (15%)
3	NAG	D	201	2	14,14,15	0.81	1 (7%)	15,19,21	3.05	4 (26%)
3	NAG	E	601	1,3	14,14,15	1.14	2 (14%)	15,19,21	1.17	0
3	NAG	E	602	3	14,14,15	0.33	0	15,19,21	0.84	0
3	NAG	F	201	2	14,14,15	0.81	1 (7%)	15,19,21	3.06	4 (26%)

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	400	1	-	0/6/23/26	0/1/1/1
3	NAG	A	401	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	201	2	-	0/6/23/26	0/1/1/1
3	NAG	C	501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	502	3,4	-	0/6/23/26	0/1/1/1
4	BMA	C	503	3,5	-	0/2/19/22	0/1/1/1
5	MAN	C	504	4	-	0/2/19/22	0/1/1/1
3	NAG	D	201	2	-	0/6/23/26	0/1/1/1
3	NAG	E	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	602	3	-	0/6/23/26	0/1/1/1
3	NAG	F	201	2	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	NAG	O5-C1	-2.40	1.39	1.43
3	A	401	NAG	O5-C1	-2.36	1.39	1.43
3	E	601	NAG	O5-C1	-2.35	1.39	1.43
3	B	201	NAG	O5-C1	-2.21	1.40	1.43
3	A	400	NAG	O5-C1	-2.19	1.40	1.43
3	D	201	NAG	O5-C1	-2.19	1.40	1.43
3	F	201	NAG	O5-C1	-2.18	1.40	1.43
3	E	601	NAG	C2-N2	-2.12	1.42	1.46
3	C	501	NAG	O7-C7	-2.06	1.18	1.23
5	C	504	MAN	O5-C5	2.30	1.48	1.43
5	C	504	MAN	O3-C3	2.30	1.48	1.43
4	C	503	BMA	O5-C5	2.56	1.48	1.43
4	C	503	BMA	O5-C1	2.93	1.48	1.43
5	C	504	MAN	O5-C1	3.16	1.48	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	201	NAG	O3-C3-C2	-7.92	92.42	109.39
3	D	201	NAG	O3-C3-C2	-7.91	92.44	109.39
3	F	201	NAG	C1-C2-N2	-6.25	99.81	110.49
3	D	201	NAG	C1-C2-N2	-6.24	99.83	110.49
3	A	400	NAG	O4-C4-C3	-3.45	102.85	110.36
3	B	201	NAG	O4-C4-C3	-3.44	102.86	110.36
3	C	501	NAG	C1-C2-N2	-3.35	104.77	110.49
3	C	501	NAG	C6-C5-C4	-3.03	105.91	113.00
3	A	400	NAG	O3-C3-C4	2.10	114.92	110.36
4	C	503	BMA	C1-O5-C5	2.11	115.07	112.17
3	B	201	NAG	O3-C3-C4	2.11	114.94	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	201	NAG	C6-C5-C4	2.26	118.29	113.00
3	D	201	NAG	C6-C5-C4	2.26	118.30	113.00
3	C	501	NAG	O3-C3-C2	2.43	114.59	109.39
5	C	504	MAN	C1-C2-C3	2.52	112.85	109.65
5	C	504	MAN	C1-O5-C5	2.69	115.87	112.17
3	F	201	NAG	O4-C4-C5	4.45	120.50	109.28
3	D	201	NAG	O4-C4-C5	4.46	120.52	109.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	201	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	318/323 (98%)	-0.57	0 100 100	11, 21, 36, 58	0
1	C	319/323 (98%)	-0.50	2 (0%) 89 87	12, 21, 36, 59	0
1	E	318/323 (98%)	-0.46	4 (1%) 77 75	12, 22, 41, 58	0
2	B	171/180 (95%)	-0.16	4 (2%) 61 57	14, 30, 49, 55	0
2	D	169/180 (93%)	-0.36	0 100 100	15, 27, 41, 56	0
2	F	169/180 (93%)	-0.25	0 100 100	14, 29, 47, 59	0
All	All	1464/1509 (97%)	-0.42	10 (0%) 87 86	11, 24, 44, 59	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	220	ARG	5.4
1	E	22	ASN	3.1
1	C	326	LEU	3.1
2	B	29	ALA	2.9
1	E	325	GLU	2.8
2	B	57	GLU	2.7
1	E	223	VAL	2.7
2	B	18	VAL	2.5
2	B	19	ASP	2.2
1	C	277	CYS	2.1

### 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 [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, 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
3	NAG	A	400	14/15	0.69	0.34	11.99	51,60,68,72	0
3	NAG	B	201	14/15	0.69	0.34	6.73	47,58,68,81	0
3	NAG	F	201	14/15	0.68	0.30	6.08	47,57,63,70	0
3	NAG	C	501	14/15	0.93	0.17	3.32	28,34,41,43	0
3	NAG	E	601	14/15	0.84	0.18	3.29	26,44,59,67	0
3	NAG	A	401	14/15	0.76	0.27	1.05	41,50,61,67	0
3	NAG	D	201	14/15	0.72	0.21	1.05	47,54,60,63	0
4	BMA	C	503	11/12	0.84	0.25	-	56,63,71,77	0
3	NAG	E	602	14/15	0.61	0.43	-	63,75,91,91	0
5	MAN	C	504	11/12	0.59	0.40	-	70,83,87,88	0
3	NAG	C	502	14/15	0.85	0.22	-	34,43,57,60	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.