



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:19 am GMT

PDB ID : 4M40
Title : Crystal structure of hemagglutinin of influenza virus B/Yamanashi/166/1998
Authors : Ni, F.; Kondrashkina, E.; Wang, Q.
Deposited on : 2013-08-06
Resolution : 3.54 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

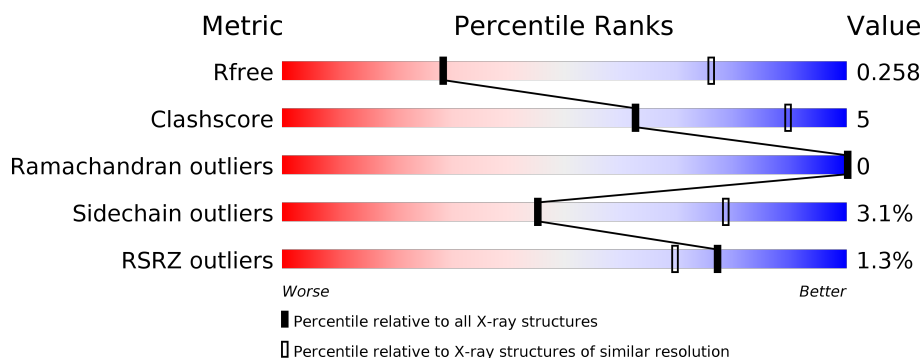
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.54 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	1286 (3.68-3.40)
Clashscore	112137	1070 (3.66-3.42)
Ramachandran outliers	110173	1033 (3.66-3.42)
Sidechain outliers	110143	1033 (3.66-3.42)
RSRZ outliers	101464	1318 (3.68-3.40)

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 ≥ 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	346	<div> <div></div> <div>84% 14% ..</div> </div>
1	C	346	<div> <div></div> <div>86% 11% ..</div> </div>
1	E	346	<div> <div></div> <div>86% 12% ..</div> </div>
2	B	182	<div> <div></div> <div>80% 14% • 6%</div> </div>
2	D	182	<div> <div></div> <div>82% 11% • 7%</div> </div>
2	F	182	<div> <div></div> <div>81% 13% • 6%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12115 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2600	1633	464	487	16			
1	C	343	Total	C	N	O	S	0	0	0
			2600	1633	464	487	16			
1	E	343	Total	C	N	O	S	0	0	0
			2600	1633	464	487	16			

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1301	814	222	259	6			
2	D	170	Total	C	N	O	S	0	0	0
			1293	808	221	258	6			
2	F	171	Total	C	N	O	S	0	0	0
			1301	814	222	259	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	GLY	-	EXPRESSION TAG	UNP A3DQM7
B	178	ALA	-	EXPRESSION TAG	UNP A3DQM7
B	179	LEU	-	EXPRESSION TAG	UNP A3DQM7
B	180	VAL	-	EXPRESSION TAG	UNP A3DQM7
B	181	PRO	-	EXPRESSION TAG	UNP A3DQM7
B	182	ARG	-	EXPRESSION TAG	UNP A3DQM7
D	177	GLY	-	EXPRESSION TAG	UNP A3DQM7
D	178	ALA	-	EXPRESSION TAG	UNP A3DQM7
D	179	LEU	-	EXPRESSION TAG	UNP A3DQM7
D	180	VAL	-	EXPRESSION TAG	UNP A3DQM7
D	181	PRO	-	EXPRESSION TAG	UNP A3DQM7
D	182	ARG	-	EXPRESSION TAG	UNP A3DQM7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	177	GLY	-	EXPRESSION TAG	UNP A3DQM7
F	178	ALA	-	EXPRESSION TAG	UNP A3DQM7
F	179	LEU	-	EXPRESSION TAG	UNP A3DQM7
F	180	VAL	-	EXPRESSION TAG	UNP A3DQM7
F	181	PRO	-	EXPRESSION TAG	UNP A3DQM7
F	182	ARG	-	EXPRESSION TAG	UNP A3DQM7

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).

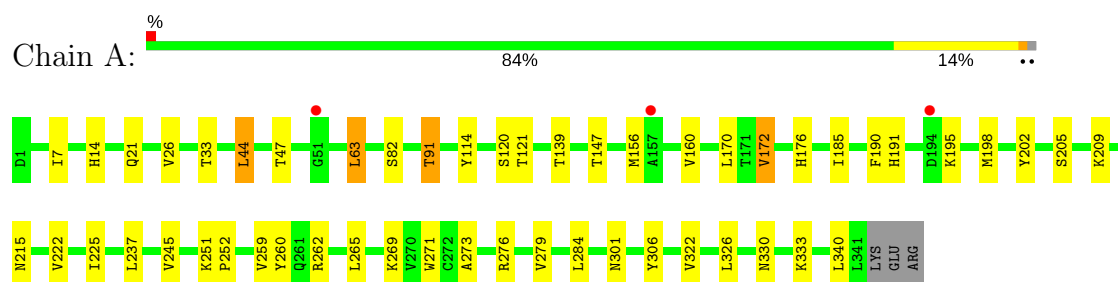


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1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

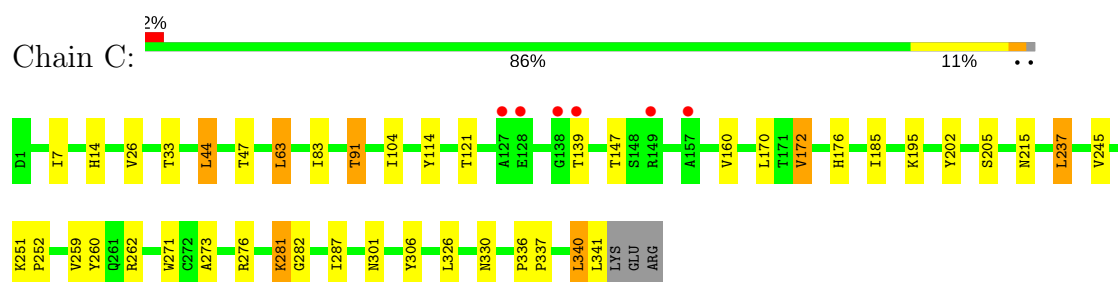
3 Residue-property plots [i](#)

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.

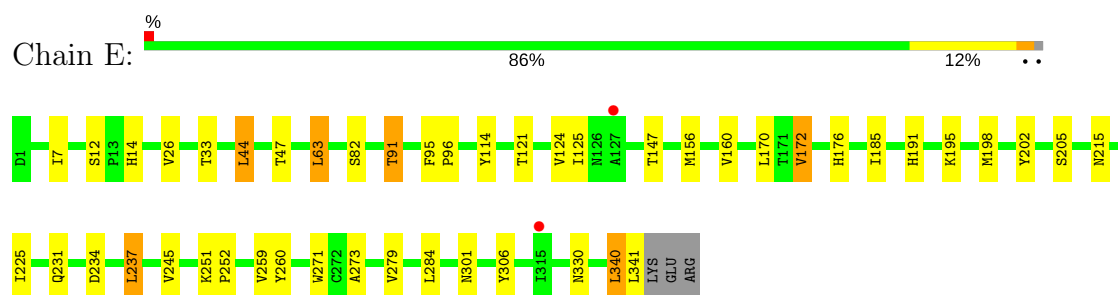
• Molecule 1: Hemagglutinin HA1



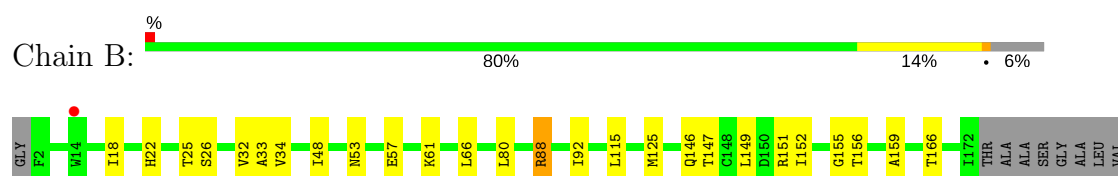
• Molecule 1: Hemagglutinin HA1



• Molecule 1: Hemagglutinin HA1

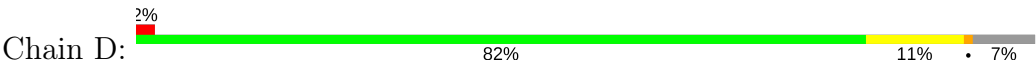


• Molecule 2: Hemagglutinin HA2



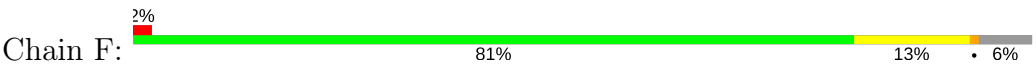
PRO
ARG

• Molecule 2: Hemagglutinin HA2



ARG

• Molecule 2: Hemagglutinin HA2



GLY
ALA
LEU
VAL
PRO
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.91Å 101.29Å 136.81Å 90.00° 115.18° 90.00°	Depositor
Resolution (Å)	42.66 – 3.54 42.66 – 3.54	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.66-3.54) 99.1 (42.66-3.54)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1391)	Depositor
R, R_{free}	0.198 , 0.244 0.217 , 0.258	Depositor DCC
R_{free} test set	1331 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	106.9	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.409 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.409 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12115	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/2659	0.51	0/3613
1	C	0.29	1/2659 (0.0%)	0.52	0/3613
1	E	0.26	0/2659	0.52	0/3613
2	B	0.31	0/1320	0.48	0/1780
2	D	0.28	0/1312	0.48	0/1769
2	F	0.28	0/1320	0.47	0/1780
All	All	0.28	1/11929 (0.0%)	0.50	0/16168

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	287	ILE	C-N	5.17	1.42	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2600	0	2622	30	0
1	C	2600	0	2622	24	0
1	E	2600	0	2621	26	0
2	B	1301	0	1273	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1293	0	1262	14	0
2	F	1301	0	1273	16	0
3	A	84	0	75	1	0
3	C	84	0	75	1	0
3	E	84	0	75	5	0
4	A	42	0	39	0	0
4	B	14	0	13	0	0
4	C	42	0	39	0	0
4	D	14	0	13	0	0
4	E	42	0	39	1	0
4	F	14	0	13	0	0
All	All	12115	0	12054	120	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (120) 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:340:LEU:HD21	2:B:32:VAL:HG11	1.38	1.03
1:A:209:LYS:HG2	1:A:222:VAL:HG22	1.55	0.88
1:C:83:ILE:HG23	1:C:282:GLY:HA3	1.63	0.79
2:D:61:LYS:O	2:D:88:ARG:NH2	2.19	0.75
2:F:61:LYS:O	2:F:88:ARG:NH2	2.21	0.74
2:B:61:LYS:O	2:B:88:ARG:NH2	2.20	0.73
1:E:7:ILE:HG13	2:F:115:LEU:HD21	1.75	0.67
1:C:63:LEU:HD13	1:C:91:THR:HG23	1.76	0.67
1:C:83:ILE:CG2	1:C:282:GLY:HA3	2.25	0.67
1:C:7:ILE:HG13	2:D:115:LEU:HD21	1.78	0.66
1:A:340:LEU:HD21	2:B:32:VAL:CG1	2.21	0.65
1:C:330:ASN:HA	2:D:48:ILE:HD13	1.80	0.64
2:D:159:ALA:HB3	2:D:166:THR:HG22	1.80	0.63
1:A:340:LEU:CD2	2:B:32:VAL:HG11	2.21	0.63
1:C:340:LEU:HB3	1:C:341:LEU:HD12	1.80	0.62
1:A:7:ILE:HG13	2:B:115:LEU:HD21	1.80	0.62
2:B:159:ALA:HB3	2:B:166:THR:HG22	1.83	0.60
1:E:340:LEU:HB3	1:E:341:LEU:HD12	1.83	0.59
2:D:151:ARG:NH2	2:D:156:THR:O	2.36	0.58
1:C:33:THR:HG22	1:C:306:TYR:HB2	1.84	0.58
1:E:330:ASN:HA	2:F:48:ILE:HD13	1.84	0.58
1:E:63:LEU:HD13	1:E:91:THR:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:LEU:HD12	2:B:152:ILE:HD12	1.86	0.57
1:C:215:ASN:HD21	1:C:251:LYS:H	1.52	0.57
2:B:80:LEU:HD13	2:D:66:LEU:HD11	1.87	0.57
1:A:33:THR:HG22	1:A:306:TYR:HB2	1.87	0.55
3:E:402:NAG:H3	3:E:402:NAG:H83	1.88	0.55
2:F:159:ALA:HB3	2:F:166:THR:HG22	1.89	0.55
2:F:149:LEU:HD12	2:F:152:ILE:HD12	1.89	0.54
1:E:33:THR:HG22	1:E:306:TYR:HB2	1.91	0.53
1:E:172:VAL:HG22	1:E:260:TYR:HE2	1.73	0.52
1:A:156:MET:HE3	1:A:245:VAL:HG13	1.93	0.51
2:B:125:MET:SD	2:B:155:GLY:HA2	2.50	0.51
3:E:407:NAG:H61	3:E:408:NAG:H2	1.92	0.51
1:C:14:HIS:HB2	1:C:26:VAL:HG23	1.93	0.50
1:E:156:MET:HE3	1:E:245:VAL:HG13	1.93	0.50
1:C:172:VAL:HG22	1:C:260:TYR:HE2	1.77	0.50
1:E:82:SER:HB2	1:E:279:VAL:HG22	1.94	0.50
1:E:185:ILE:HB	1:E:271:TRP:HB2	1.93	0.49
2:F:151:ARG:NH2	2:F:156:THR:O	2.45	0.49
1:C:202:TYR:HB3	1:C:262:ARG:HB3	1.95	0.49
1:A:301:ASN:HD22	3:A:404:NAG:H83	1.78	0.49
1:A:330:ASN:HA	2:B:48:ILE:HD13	1.94	0.48
1:E:170:LEU:O	1:E:259:VAL:HA	2.13	0.48
2:B:147:THR:O	2:B:151:ARG:HG3	2.14	0.48
1:A:185:ILE:HB	1:A:271:TRP:HB2	1.96	0.48
1:A:63:LEU:HD13	1:A:91:THR:HG23	1.96	0.47
1:A:170:LEU:O	1:A:259:VAL:HA	2.14	0.47
1:C:326:LEU:HD21	2:D:97:GLU:HG2	1.95	0.47
1:C:301:ASN:HD22	3:C:405:NAG:H83	1.80	0.47
1:A:44:LEU:HB3	1:A:47:THR:HB	1.96	0.47
2:B:66:LEU:HD22	2:F:79:GLU:CG	2.45	0.47
1:A:14:HIS:HB2	1:A:26:VAL:HG23	1.97	0.47
1:A:322:VAL:HG11	1:A:326:LEU:HD11	1.96	0.46
2:B:66:LEU:HD22	2:F:79:GLU:HG2	1.96	0.46
4:E:403:NAG:N2	4:E:403:NAG:O4	2.48	0.46
1:E:301:ASN:HD22	3:E:405:NAG:H83	1.79	0.46
2:D:77:ILE:HD12	2:D:77:ILE:H	1.81	0.46
3:E:408:NAG:N2	3:E:408:NAG:H5	2.31	0.46
1:C:176:HIS:CE1	1:C:252:PRO:HA	2.51	0.46
1:A:176:HIS:CE1	1:A:252:PRO:HA	2.51	0.46
1:C:44:LEU:HB3	1:C:47:THR:HB	1.98	0.46
2:D:147:THR:O	2:D:151:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:SER:OG	2:F:33:ALA:HB3	2.16	0.45
1:A:82:SER:HB2	1:A:279:VAL:HG22	1.97	0.45
1:C:185:ILE:HB	1:C:271:TRP:HB2	1.99	0.45
1:E:44:LEU:HD23	1:E:44:LEU:HA	1.82	0.45
1:C:281:LYS:HB3	1:C:281:LYS:HE2	1.68	0.45
2:D:26:SER:OG	2:D:33:ALA:HB3	2.17	0.45
1:C:104:ILE:HG12	1:C:245:VAL:HG13	1.99	0.45
1:E:176:HIS:CE1	1:E:252:PRO:HA	2.52	0.45
1:C:195:LYS:HG3	1:C:205:SER:HB2	1.99	0.44
2:F:103:SER:O	2:F:107:ILE:HG12	2.16	0.44
1:E:14:HIS:HB2	1:E:26:VAL:HG23	1.98	0.44
2:B:92:ILE:HA	2:B:92:ILE:HD13	1.90	0.44
1:C:170:LEU:O	1:C:259:VAL:HA	2.17	0.44
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.84	0.44
1:E:44:LEU:HB3	1:E:47:THR:HB	1.99	0.43
2:F:33:ALA:HB1	2:F:146:GLN:OE1	2.18	0.43
1:A:195:LYS:HG3	1:A:205:SER:HB2	1.99	0.43
1:E:215:ASN:HD21	1:E:251:LYS:H	1.67	0.43
2:F:147:THR:O	2:F:151:ARG:HG3	2.18	0.43
1:A:202:TYR:HB3	1:A:262:ARG:HB3	2.01	0.43
1:C:114:TYR:CG	1:C:273:ALA:HB1	2.54	0.43
2:B:33:ALA:HB1	2:B:146:GLN:OE1	2.19	0.43
1:A:215:ASN:HD21	1:A:251:LYS:H	1.66	0.42
1:A:190:PHE:HA	1:A:265:LEU:HG	2.00	0.42
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.88	0.42
2:F:92:ILE:HA	2:F:92:ILE:HD13	1.91	0.42
1:A:114:TYR:CG	1:A:273:ALA:HB1	2.54	0.42
2:B:25:THR:HG22	2:B:34:VAL:HG22	2.01	0.42
2:B:151:ARG:NH2	2:B:156:THR:O	2.52	0.42
2:D:125:MET:SD	2:D:155:GLY:HA2	2.59	0.42
2:D:33:ALA:HB1	2:D:146:GLN:OE1	2.20	0.42
1:E:198:MET:HG3	1:E:225:ILE:HD12	2.00	0.42
1:A:21:GLN:OE1	1:A:333:LYS:NZ	2.38	0.42
1:E:124:VAL:HG13	1:E:125:ILE:HG12	2.02	0.42
2:B:92:ILE:HD11	2:F:91:THR:HG23	2.02	0.42
2:D:92:ILE:HA	2:D:92:ILE:HD13	1.92	0.42
1:A:306:TYR:HB3	1:A:322:VAL:HG23	2.02	0.41
1:A:191:HIS:ND1	1:A:202:TYR:OH	2.43	0.41
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.86	0.41
1:E:195:LYS:HG3	1:E:205:SER:HB2	2.01	0.41
2:B:26:SER:OG	2:B:33:ALA:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:SER:O	1:A:269:LYS:HD2	2.20	0.41
1:C:237:LEU:HD12	1:C:237:LEU:HA	1.81	0.41
1:E:95:PHE:CG	1:E:96:PRO:HD2	2.56	0.41
2:F:125:MET:SD	2:F:155:GLY:HA2	2.60	0.41
1:E:284:LEU:HD23	1:E:284:LEU:HA	1.84	0.41
2:B:53:ASN:O	2:B:57:GLU:HG3	2.20	0.41
1:E:114:TYR:CG	1:E:273:ALA:HB1	2.55	0.41
2:D:126:LEU:HA	2:D:126:LEU:HD23	1.86	0.41
1:E:231:GLN:NE2	1:E:234:ASP:OD2	2.48	0.41
2:F:77:ILE:HD12	2:F:77:ILE:H	1.86	0.41
1:E:191:HIS:ND1	1:E:202:TYR:OH	2.44	0.40
1:E:237:LEU:HD12	1:E:237:LEU:HA	1.85	0.40
1:E:12:SER:O	3:E:401:NAG:H83	2.22	0.40
1:C:336:PRO:HA	1:C:337:PRO:HD3	1.95	0.40
1:A:198:MET:HG3	1:A:225:ILE:HD12	2.03	0.40
1:A:172:VAL:HG22	1:A:260:TYR:HE2	1.86	0.40

There are no symmetry-related clashes.

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	341/346 (99%)	327 (96%)	14 (4%)	0	100	100
1	C	341/346 (99%)	327 (96%)	14 (4%)	0	100	100
1	E	341/346 (99%)	328 (96%)	13 (4%)	0	100	100
2	B	169/182 (93%)	163 (96%)	6 (4%)	0	100	100
2	D	168/182 (92%)	163 (97%)	5 (3%)	0	100	100
2	F	169/182 (93%)	164 (97%)	5 (3%)	0	100	100
All	All	1529/1584 (96%)	1472 (96%)	57 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	291/294 (99%)	281 (97%)	10 (3%)	42	76
1	C	291/294 (99%)	279 (96%)	12 (4%)	35	72
1	E	291/294 (99%)	282 (97%)	9 (3%)	45	78
2	B	139/145 (96%)	136 (98%)	3 (2%)	57	84
2	D	138/145 (95%)	135 (98%)	3 (2%)	57	84
2	F	139/145 (96%)	136 (98%)	3 (2%)	57	84
All	All	1289/1317 (98%)	1249 (97%)	40 (3%)	45	78

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	63	LEU
1	A	91	THR
1	A	121	THR
1	A	139	THR
1	A	147	THR
1	A	160	VAL
1	A	172	VAL
1	A	237	LEU
1	A	276	ARG
2	B	18	ILE
2	B	22	HIS
2	B	88	ARG
1	C	44	LEU
1	C	63	LEU
1	C	91	THR
1	C	121	THR
1	C	139	THR
1	C	147	THR

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Mol	Chain	Res	Type
1	C	160	VAL
1	C	172	VAL
1	C	237	LEU
1	C	276	ARG
1	C	281	LYS
1	C	340	LEU
2	D	18	ILE
2	D	22	HIS
2	D	88	ARG
1	E	44	LEU
1	E	63	LEU
1	E	91	THR
1	E	121	THR
1	E	147	THR
1	E	160	VAL
1	E	172	VAL
1	E	237	LEU
1	E	340	LEU
2	F	22	HIS
2	F	51	ASN
2	F	88	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	42	GLN
1	C	215	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

18 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	401	1,3	14,14,15	0.29	0	15,19,21	0.86	1 (6%)
3	NAG	A	402	3	14,14,15	0.38	0	15,19,21	0.63	0
3	NAG	A	404	1,3	14,14,15	0.40	0	15,19,21	0.74	0
3	NAG	A	405	3	14,14,15	1.10	1 (7%)	15,19,21	1.30	1 (6%)
3	NAG	A	407	1,3	14,14,15	0.30	0	15,19,21	0.74	0
3	NAG	A	408	3	14,14,15	0.88	1 (7%)	15,19,21	1.12	1 (6%)
3	NAG	C	401	1,3	14,14,15	0.63	0	15,19,21	1.20	2 (13%)
3	NAG	C	402	3	14,14,15	0.82	1 (7%)	15,19,21	1.05	1 (6%)
3	NAG	C	405	1,3	14,14,15	0.49	0	15,19,21	0.84	1 (6%)
3	NAG	C	406	3	14,14,15	1.02	1 (7%)	15,19,21	1.32	1 (6%)
3	NAG	C	407	1,3	14,14,15	0.28	0	15,19,21	1.29	2 (13%)
3	NAG	C	408	3	14,14,15	0.68	0	15,19,21	0.97	1 (6%)
3	NAG	E	401	1,3	14,14,15	0.55	0	15,19,21	0.62	0
3	NAG	E	402	3	14,14,15	0.40	0	15,19,21	1.39	2 (13%)
3	NAG	E	405	1,3	14,14,15	0.35	0	15,19,21	0.82	1 (6%)
3	NAG	E	406	3	14,14,15	1.05	1 (7%)	15,19,21	1.25	1 (6%)
3	NAG	E	407	1,3	14,14,15	0.25	0	15,19,21	0.65	0
3	NAG	E	408	3	14,14,15	1.02	2 (14%)	15,19,21	0.91	1 (6%)

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	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	402	3	-	0/6/23/26	0/1/1/1
3	NAG	A	404	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	405	3	-	0/6/23/26	0/1/1/1
3	NAG	A	407	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	408	3	-	0/6/23/26	0/1/1/1
3	NAG	C	401	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	402	3	-	0/6/23/26	0/1/1/1
3	NAG	C	405	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	406	3	-	0/6/23/26	0/1/1/1
3	NAG	C	407	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	408	3	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	402	3	-	0/6/23/26	0/1/1/1
3	NAG	E	405	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	406	3	-	0/6/23/26	0/1/1/1
3	NAG	E	407	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	408	3	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	408	NAG	C1-C2	2.36	1.55	1.52
3	E	408	NAG	O5-C1	2.75	1.48	1.43
3	C	402	NAG	O5-C1	2.80	1.48	1.43
3	A	408	NAG	O5-C1	3.18	1.48	1.43
3	C	406	NAG	O5-C1	3.68	1.49	1.43
3	E	406	NAG	O5-C1	3.82	1.50	1.43
3	A	405	NAG	O5-C1	4.01	1.50	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAG	O4-C4-C3	-2.75	104.37	110.36
3	C	401	NAG	O5-C1-C2	-2.39	108.14	111.47
3	C	407	NAG	O5-C1-C2	-2.02	108.67	111.47
3	C	405	NAG	C1-O5-C5	2.01	114.93	112.17
3	E	408	NAG	C2-N2-C7	2.02	125.89	122.94
3	E	405	NAG	C1-O5-C5	2.23	115.23	112.17
3	E	402	NAG	C1-C2-N2	2.27	114.36	110.49
3	C	401	NAG	C1-O5-C5	2.65	115.83	112.17
3	C	408	NAG	C1-O5-C5	3.43	116.89	112.17
3	C	402	NAG	C1-O5-C5	3.74	117.32	112.17
3	A	408	NAG	C1-O5-C5	4.00	117.67	112.17
3	E	402	NAG	C2-N2-C7	4.18	129.04	122.94
3	C	407	NAG	C1-O5-C5	4.27	118.06	112.17
3	E	406	NAG	C1-O5-C5	4.54	118.42	112.17
3	A	405	NAG	C1-O5-C5	4.76	118.73	112.17
3	C	406	NAG	C1-O5-C5	4.88	118.90	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	NAG	1	0
3	C	405	NAG	1	0
3	E	401	NAG	1	0
3	E	402	NAG	1	0
3	E	405	NAG	1	0
3	E	407	NAG	1	0
3	E	408	NAG	2	0

5.6 Ligand geometry

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	A	403	1	14,14,15	0.39	0	15,19,21	0.70	0
4	NAG	A	406	1	14,14,15	0.26	0	15,19,21	0.53	0
4	NAG	A	409	1	14,14,15	0.51	0	15,19,21	0.58	0
4	NAG	B	201	2	14,14,15	0.25	0	15,19,21	0.70	0
4	NAG	C	403	1	14,14,15	0.60	1 (7%)	15,19,21	0.65	0
4	NAG	C	404	1	14,14,15	0.27	0	15,19,21	1.13	1 (6%)
4	NAG	C	409	1	14,14,15	0.25	0	15,19,21	0.55	0
4	NAG	D	201	2	14,14,15	0.18	0	15,19,21	0.53	0
4	NAG	E	403	1	14,14,15	1.31	1 (7%)	15,19,21	2.10	1 (6%)
4	NAG	E	404	1	14,14,15	0.69	1 (7%)	15,19,21	1.10	1 (6%)
4	NAG	E	409	1	14,14,15	0.25	0	15,19,21	0.91	1 (6%)
4	NAG	F	201	2	14,14,15	0.16	0	15,19,21	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	403	1	-	0/6/23/26	0/1/1/1
4	NAG	A	406	1	-	0/6/23/26	0/1/1/1
4	NAG	A	409	1	-	0/6/23/26	0/1/1/1
4	NAG	B	201	2	-	0/6/23/26	0/1/1/1
4	NAG	C	403	1	-	0/6/23/26	0/1/1/1
4	NAG	C	404	1	-	0/6/23/26	0/1/1/1
4	NAG	C	409	1	-	0/6/23/26	0/1/1/1
4	NAG	D	201	2	-	0/6/23/26	0/1/1/1
4	NAG	E	403	1	-	0/6/23/26	0/1/1/1
4	NAG	E	404	1	-	0/6/23/26	0/1/1/1
4	NAG	E	409	1	-	0/6/23/26	0/1/1/1
4	NAG	F	201	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	403	NAG	O5-C1	2.07	1.47	1.43
4	E	404	NAG	O5-C1	2.15	1.47	1.43
4	E	403	NAG	O5-C1	4.76	1.51	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	409	NAG	C1-O5-C5	2.79	116.02	112.17
4	C	404	NAG	C1-O5-C5	3.48	116.96	112.17
4	E	404	NAG	C1-O5-C5	3.74	117.32	112.17
4	E	403	NAG	C1-O5-C5	7.77	122.87	112.17

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
4	E	403	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, 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	343/346 (99%)	0.13	3 (0%) 84 77	90, 117, 143, 177	0
1	C	343/346 (99%)	0.16	6 (1%) 70 62	90, 118, 142, 176	0
1	E	343/346 (99%)	0.15	2 (0%) 89 84	92, 118, 144, 174	0
2	B	171/182 (93%)	0.18	1 (0%) 89 84	88, 117, 151, 168	0
2	D	170/182 (93%)	0.21	4 (2%) 59 50	86, 117, 153, 168	0
2	F	171/182 (93%)	0.14	4 (2%) 61 52	86, 117, 151, 171	0
All	All	1541/1584 (97%)	0.16	20 (1%) 77 69	86, 118, 149, 177	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	138	GLY	3.8
1	A	51	GLY	3.6
2	D	34	VAL	3.6
2	D	12	GLY	3.5
2	D	14	TRP	3.4
1	C	128	GLU	2.9
1	E	127	ALA	2.7
1	C	149	ARG	2.7
2	F	12	GLY	2.5
2	F	24	TYR	2.4
1	C	127	ALA	2.4
2	D	133	ILE	2.3
2	F	122	LEU	2.3
2	B	14	TRP	2.3
1	A	157	ALA	2.3
1	E	315	ILE	2.2
1	A	194	ASP	2.2
1	C	139	THR	2.0
1	C	157	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	14	TRP	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](#)

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
3	NAG	C	401	14/15	0.90	0.24	0.20	48,62,68,72	0
3	NAG	E	401	14/15	0.93	0.19	-0.54	48,56,62,67	0
3	NAG	A	401	14/15	0.89	0.23	-0.56	53,59,70,73	0
3	NAG	A	404	14/15	0.92	0.16	-0.75	55,63,73,75	0
3	NAG	C	407	14/15	0.84	0.23	-0.89	47,61,69,71	0
3	NAG	E	405	14/15	0.92	0.17	-0.99	57,65,74,75	0
3	NAG	C	405	14/15	0.92	0.14	-1.18	57,65,72,78	0
3	NAG	E	408	14/15	0.86	0.20	-	79,94,100,101	0
3	NAG	A	402	14/15	0.83	0.21	-	72,89,99,109	0
3	NAG	E	407	14/15	0.84	0.18	-	51,60,71,74	0
3	NAG	E	406	14/15	0.72	0.27	-	69,85,89,94	0
3	NAG	A	405	14/15	0.76	0.23	-	68,78,86,87	0
3	NAG	C	408	14/15	0.91	0.16	-	71,89,93,94	0
3	NAG	C	406	14/15	0.73	0.22	-	69,82,88,89	0
3	NAG	C	402	14/15	0.86	0.22	-	72,75,80,80	0
3	NAG	E	402	14/15	0.90	0.15	-	70,79,84,87	0
3	NAG	A	407	14/15	0.87	0.20	-	48,59,70,71	0
3	NAG	A	408	14/15	0.94	0.13	-	64,86,92,94	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
4	NAG	E	403	14/15	0.83	0.23	-0.65	80,90,97,103	0
4	NAG	C	403	14/15	0.87	0.19	-	63,71,78,80	0
4	NAG	A	406	14/15	0.65	0.31	-	109,126,133,134	0
4	NAG	F	201	14/15	0.81	0.23	-	79,94,102,104	0
4	NAG	D	201	14/15	0.80	0.21	-	81,93,100,105	0
4	NAG	E	404	14/15	0.83	0.35	-	106,115,122,124	0
4	NAG	E	409	14/15	0.78	0.19	-	105,124,129,129	0
4	NAG	C	404	14/15	0.73	0.35	-	106,124,128,134	0
4	NAG	C	409	14/15	0.82	0.21	-	110,124,129,131	0
4	NAG	B	201	14/15	0.72	0.30	-	79,92,105,107	0
4	NAG	A	409	14/15	0.53	0.34	-	105,122,126,127	0
4	NAG	A	403	14/15	0.78	0.26	-	68,73,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.