



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:45 am GMT

PDB ID : 5AVA
Title : Crystal structure of PHA-E lectin in complex with bisected glycan
Authors : Nagae, M.; Yamaguchi, Y.
Deposited on : 2015-06-12
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

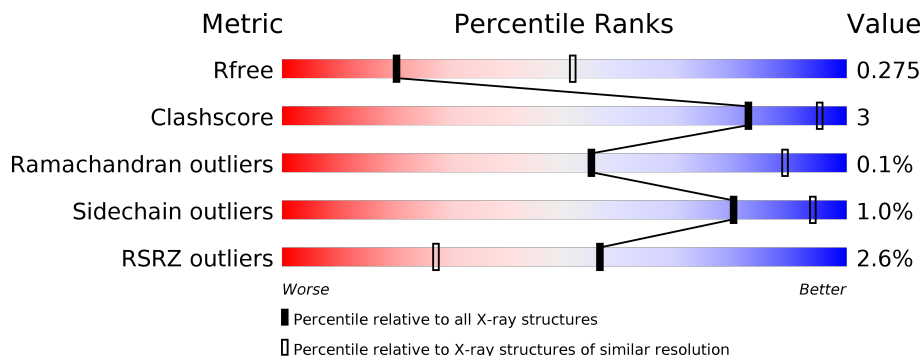
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	275	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>13%</div> </div> </div>
1	B	275	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>13%</div> </div> </div>
1	C	275	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>5%</div> <div>13%</div> </div> </div>
1	D	275	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>6%</div> <div>13%</div> </div> </div>
1	E	275	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>5%</div> <div>13%</div> </div> </div>
1	F	275	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>9%</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	275	
1	H	275	

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
4	NAG	B	2010	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 15504 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 Erythroagglutinin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	0	0	0
			1832	1169	300	363			
1	B	238	Total	C	N	O	0	0	0
			1832	1169	300	363			
1	C	238	Total	C	N	O	0	0	0
			1832	1169	300	363			
1	D	238	Total	C	N	O	0	0	0
			1832	1169	300	363			
1	E	238	Total	C	N	O	0	0	0
			1832	1169	300	363			
1	F	238	Total	C	N	O	0	0	0
			1832	1169	300	363			
1	G	238	Total	C	N	O	0	0	0
			1832	1169	300	363			
1	H	238	Total	C	N	O	0	0	0
			1832	1169	300	363			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	H	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

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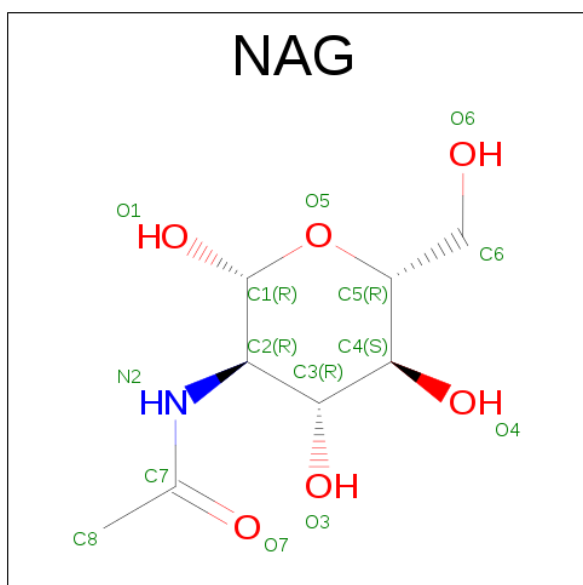
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	F	1	Total 1	Mn 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Ca 1	0	0
3	D	1	Total 1	Ca 1	0	0
3	E	1	Total 1	Ca 1	0	0
3	H	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0
3	F	1	Total 1	Ca 1	0	0

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



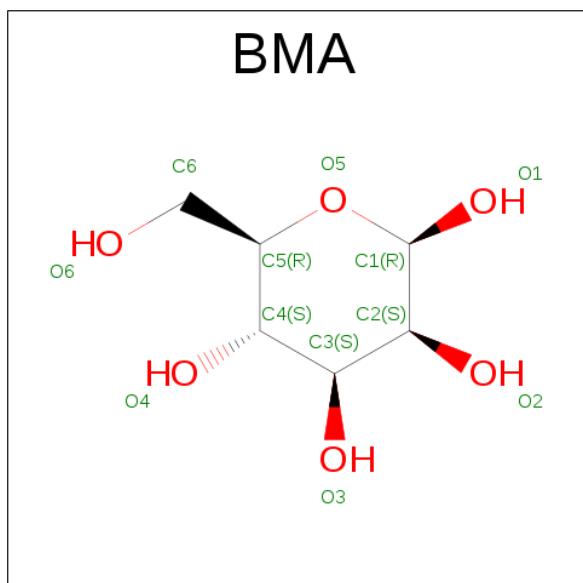
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



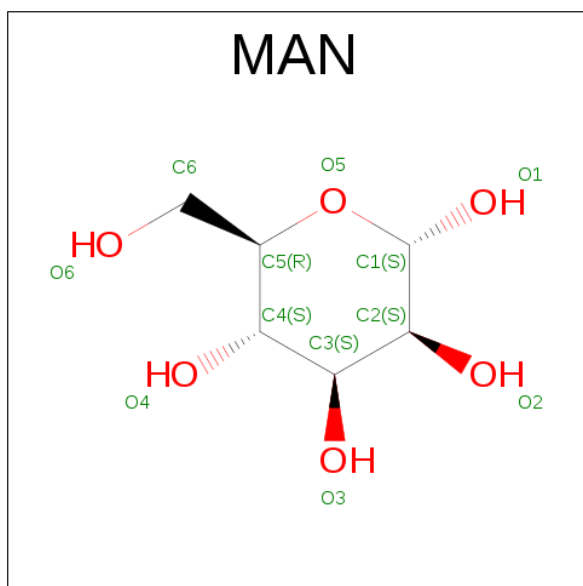
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		
5	E	1	Total	C	O	0	0
			11	6	5		
5	F	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	H	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



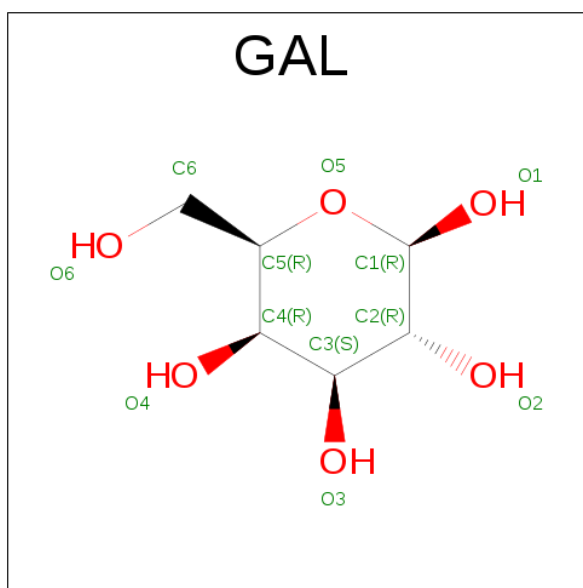
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	F	1	Total	C	O	0	0
			11	6	5		
6	F	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	H	1	Total	C	O	0	0
			11	6	5		
6	H	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 11 6 5	0	0
7	B	1	Total C O 11 6 5	0	0
7	C	1	Total C O 11 6 5	0	0
7	D	1	Total C O 11 6 5	0	0
7	E	1	Total C O 11 6 5	0	0
7	F	1	Total C O 11 6 5	0	0
7	G	1	Total C O 11 6 5	0	0
7	H	1	Total C O 11 6 5	0	0

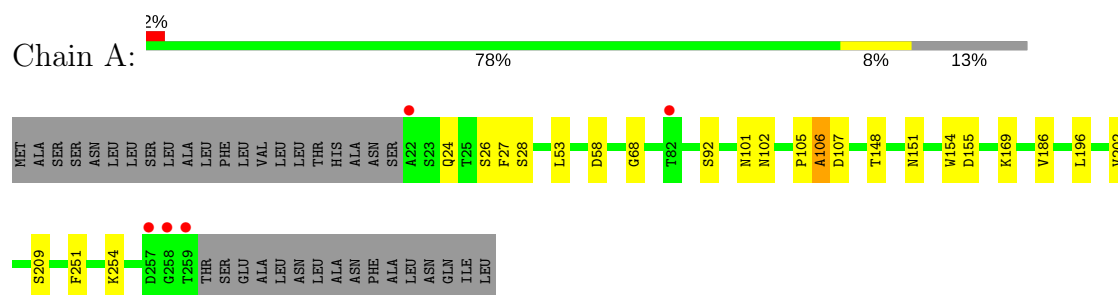
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	4	Total O 4 4	0	0
8	B	4	Total O 4 4	0	0
8	C	4	Total O 4 4	0	0
8	D	4	Total O 4 4	0	0
8	E	4	Total O 4 4	0	0
8	F	4	Total O 4 4	0	0
8	G	4	Total O 4 4	0	0
8	H	4	Total O 4 4	0	0

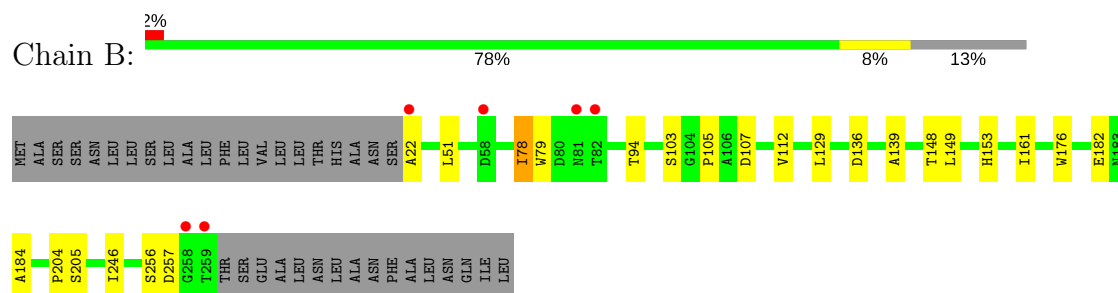
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

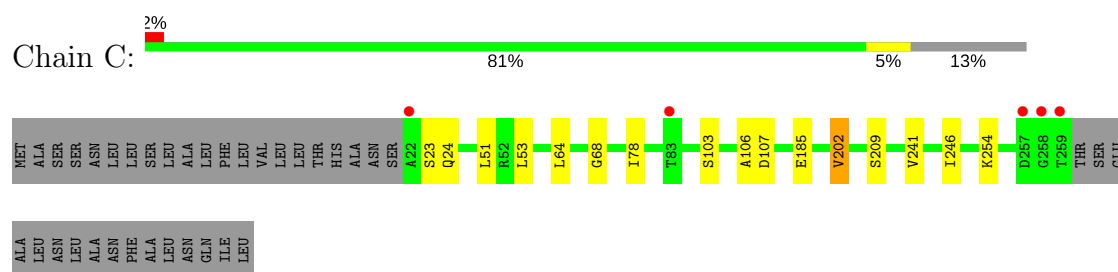
• Molecule 1: Erythroagglutinin



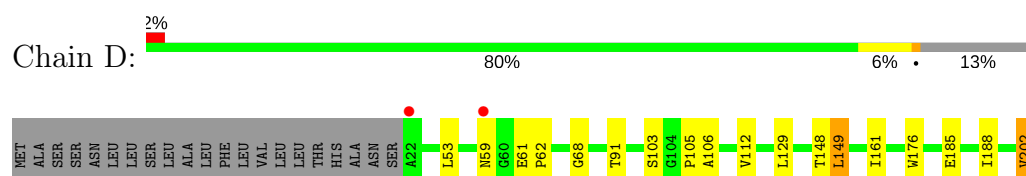
• Molecule 1: Erythroagglutinin



• Molecule 1: Erythroagglutinin

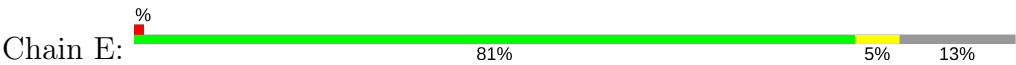


• Molecule 1: Erythroagglutinin



SER
GLU
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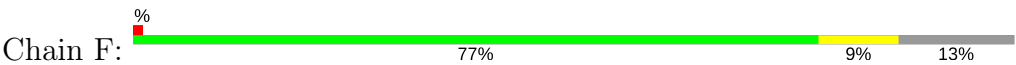
• Molecule 1: Erythroagglutinin



MET
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G68
Y72
S73
A74
I78
N102
A106
A143
L149
D164
S170
T173
E185
L196
V202
D257
G258
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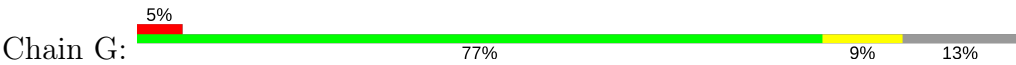
• Molecule 1: Erythroagglutinin



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Q30
L51
R52
L53
G68
I78
W79
P105
A106
D107
V112
Q119
D122
L126
L129
A143
T148
L149
Y150
N151
D155
P156
K157

D164
L196
V226
T237
T246
S256
D257
G258
T259
THR
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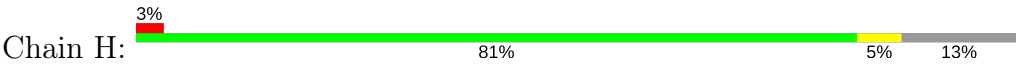
• Molecule 1: Erythroagglutinin



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Q24
L51
R52
L53
N57
D58
N59
G60
T63
G68
Y72
S73
A74
I78
N102
P105
A106
D107
V112
L113
L126
L129
F130
T148
L149

H153
P204
V228
A232
T236
T237
N240
N244
D245
T246
K254
D257
G258
T259
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• Molecule 1: Erythroagglutinin



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A22
L51
G58
Y72
S73
A74
A85
P105
V112
L126
L129
F130
T148
L149
H153
V202
G203
P204
S209
G239
T243
T246
P257

G258
T259
THR
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.21Å 122.84Å 97.66Å 90.00° 90.66° 90.00°	Depositor
Resolution (Å)	100.00 – 3.00 31.73 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (100.00-3.00) 99.9 (31.73-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.24 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.229 , 0.274 0.229 , 0.275	Depositor DCC
R_{free} test set	2267 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 11.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for l,k,-h 0.019 for h,-k,-l 0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15504	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: BMA, NAG, CA, MN, GAL, 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	0.32	0/1874	0.52	0/2559
1	B	0.34	0/1874	0.52	0/2559
1	C	0.32	0/1874	0.52	0/2559
1	D	0.33	0/1874	0.53	0/2559
1	E	0.33	0/1874	0.53	0/2559
1	F	0.33	0/1874	0.50	0/2559
1	G	0.33	0/1874	0.51	0/2559
1	H	0.33	0/1874	0.51	0/2559
All	All	0.33	0/14992	0.52	0/20472

There are no bond length outliers.

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	1832	0	1796	15	0
1	B	1832	0	1796	13	0
1	C	1832	0	1796	9	0
1	D	1832	0	1796	9	0
1	E	1832	0	1796	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1832	0	1796	16	0
1	G	1832	0	1796	14	0
1	H	1832	0	1796	8	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	56	0	50	0	0
4	B	56	0	50	1	0
4	C	56	0	50	0	0
4	D	56	0	50	1	0
4	E	56	0	50	0	0
4	F	56	0	50	0	0
4	G	56	0	50	2	0
4	H	56	0	50	1	0
5	A	11	0	7	0	0
5	B	11	0	7	0	0
5	C	11	0	7	0	0
5	D	11	0	7	0	0
5	E	11	0	7	0	0
5	F	11	0	7	0	0
5	G	11	0	7	0	0
5	H	11	0	7	0	0
6	A	22	0	18	0	0
6	B	22	0	18	0	0
6	C	22	0	18	0	0
6	D	22	0	18	0	0
6	E	22	0	18	0	0
6	F	22	0	18	0	0
6	G	22	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	22	0	18	0	0
7	A	11	0	10	0	0
7	B	11	0	10	0	0
7	C	11	0	10	0	0
7	D	11	0	10	0	0
7	E	11	0	10	0	0
7	F	11	0	10	0	0
7	G	11	0	10	1	0
7	H	11	0	10	0	0
8	A	4	0	0	0	0
8	B	4	0	0	0	0
8	C	4	0	0	0	0
8	D	4	0	0	0	0
8	E	4	0	0	0	0
8	F	4	0	0	0	0
8	G	4	0	0	0	0
8	H	4	0	0	0	0
All	All	15504	0	15048	87	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 3.

The worst 5 of 87 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:202:VAL:HG12	1:A:209:SER:HB3	1.70	0.72
1:A:58:ASP:HB3	1:F:119:GLN:HG3	1.78	0.65
1:F:196:LEU:HD22	1:H:204:PRO:HA	1.83	0.61
1:B:78:ILE:HG22	1:B:79:TRP:HD1	1.67	0.59
1:F:22:ALA:HB3	1:F:256:SER:HA	1.85	0.58

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	236/275 (86%)	227 (96%)	8 (3%)	1 (0%)	38	78
1	B	236/275 (86%)	225 (95%)	11 (5%)	0	100	100
1	C	236/275 (86%)	226 (96%)	10 (4%)	0	100	100
1	D	236/275 (86%)	225 (95%)	11 (5%)	0	100	100
1	E	236/275 (86%)	222 (94%)	14 (6%)	0	100	100
1	F	236/275 (86%)	223 (94%)	13 (6%)	0	100	100
1	G	236/275 (86%)	227 (96%)	9 (4%)	0	100	100
1	H	236/275 (86%)	225 (95%)	11 (5%)	0	100	100
All	All	1888/2200 (86%)	1800 (95%)	87 (5%)	1 (0%)	55	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ALA

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	207/238 (87%)	207 (100%)	0	100	100
1	B	207/238 (87%)	203 (98%)	4 (2%)	62	88
1	C	207/238 (87%)	204 (99%)	3 (1%)	71	91
1	D	207/238 (87%)	203 (98%)	4 (2%)	62	88
1	E	207/238 (87%)	207 (100%)	0	100	100
1	F	207/238 (87%)	204 (99%)	3 (1%)	71	91
1	G	207/238 (87%)	206 (100%)	1 (0%)	91	97
1	H	207/238 (87%)	206 (100%)	1 (0%)	91	97
All	All	1656/1904 (87%)	1640 (99%)	16 (1%)	80	94

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	59	ASN
1	D	103	SER
1	F	78	ILE
1	C	202	VAL
1	F	164	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	59	ASN
1	F	240	ASN
1	H	240	ASN
1	F	138	ASN
1	F	153	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

56 non-standard protein/DNA/RNA residues 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	2003	5	14,14,15	0.53	0	15,19,21	1.00	0
6	MAN	A	2005	5,4	11,11,12	0.68	0	13,15,17	1.04	2 (15%)
4	NAG	A	2006	7,6	14,14,15	0.46	0	15,19,21	1.02	0
7	GAL	A	2007	4	11,11,12	0.60	0	13,15,17	0.72	0
4	NAG	A	2008	5	14,14,15	0.46	0	15,19,21	0.77	0
6	MAN	A	2009	5,4	11,11,12	0.48	0	13,15,17	1.13	1 (7%)
4	NAG	A	2010	6	14,14,15	0.47	0	15,19,21	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	2003	5	14,14,15	0.53	0	15,19,21	0.83	0
6	MAN	B	2005	5,4	11,11,12	0.61	0	13,15,17	0.88	0
4	NAG	B	2006	7,6	14,14,15	0.53	0	15,19,21	1.01	1 (6%)
7	GAL	B	2007	4	11,11,12	0.62	0	13,15,17	0.60	0
4	NAG	B	2008	5	14,14,15	0.49	0	15,19,21	1.34	2 (13%)
6	MAN	B	2009	5,4	11,11,12	0.51	0	13,15,17	1.71	1 (7%)
4	NAG	B	2010	6	14,14,15	0.54	0	15,19,21	0.68	0
4	NAG	C	2003	5	14,14,15	0.49	0	15,19,21	1.05	1 (6%)
6	MAN	C	2005	5,4	11,11,12	0.63	0	13,15,17	0.70	0
4	NAG	C	2006	7,6	14,14,15	0.51	0	15,19,21	0.88	0
7	GAL	C	2007	4	11,11,12	0.60	0	13,15,17	0.63	0
4	NAG	C	2008	5	14,14,15	0.40	0	15,19,21	1.26	1 (6%)
6	MAN	C	2009	5,4	11,11,12	0.52	0	13,15,17	0.97	1 (7%)
4	NAG	C	2010	6	14,14,15	0.51	0	15,19,21	0.74	0
4	NAG	D	2003	5	14,14,15	0.50	0	15,19,21	0.94	0
6	MAN	D	2005	5,4	11,11,12	0.63	0	13,15,17	0.69	0
4	NAG	D	2006	7,6	14,14,15	0.50	0	15,19,21	0.93	0
7	GAL	D	2007	4	11,11,12	0.59	0	13,15,17	0.66	0
4	NAG	D	2008	5	14,14,15	0.46	0	15,19,21	0.95	1 (6%)
6	MAN	D	2009	5,4	11,11,12	0.51	0	13,15,17	1.24	1 (7%)
4	NAG	D	2010	6	14,14,15	0.52	0	15,19,21	0.69	0
4	NAG	E	2003	5	14,14,15	0.52	0	15,19,21	0.79	0
6	MAN	E	2005	5,4	11,11,12	0.60	0	13,15,17	1.09	1 (7%)
4	NAG	E	2006	7,6	14,14,15	0.45	0	15,19,21	0.85	0
7	GAL	E	2007	4	11,11,12	0.65	0	13,15,17	1.02	1 (7%)
4	NAG	E	2008	5	14,14,15	0.39	0	15,19,21	1.41	1 (6%)
6	MAN	E	2009	5,4	11,11,12	0.52	0	13,15,17	1.11	1 (7%)
4	NAG	E	2010	6	14,14,15	0.49	0	15,19,21	0.90	1 (6%)
4	NAG	F	2003	5	14,14,15	0.48	0	15,19,21	0.98	1 (6%)
6	MAN	F	2005	5,4	11,11,12	0.60	0	13,15,17	0.68	0
4	NAG	F	2006	7,6	14,14,15	0.47	0	15,19,21	0.82	0
7	GAL	F	2007	4	11,11,12	0.60	0	13,15,17	0.63	0
4	NAG	F	2008	5	14,14,15	0.39	0	15,19,21	1.11	1 (6%)
6	MAN	F	2009	5,4	11,11,12	0.55	0	13,15,17	0.92	1 (7%)
4	NAG	F	2010	6	14,14,15	0.48	0	15,19,21	1.11	0
4	NAG	G	2003	5	14,14,15	0.53	0	15,19,21	1.07	1 (6%)
6	MAN	G	2005	5,4	11,11,12	0.67	0	13,15,17	0.64	0
4	NAG	G	2006	7,6	14,14,15	0.50	0	15,19,21	1.00	0
7	GAL	G	2007	4	11,11,12	0.59	0	13,15,17	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	2008	5	14,14,15	0.37	0	15,19,21	1.36	1 (6%)
6	MAN	G	2009	5,4	11,11,12	0.53	0	13,15,17	1.20	2 (15%)
4	NAG	G	2010	6	14,14,15	0.45	0	15,19,21	0.95	1 (6%)
4	NAG	H	2003	5	14,14,15	0.54	0	15,19,21	0.91	1 (6%)
6	MAN	H	2005	5,4	11,11,12	0.65	0	13,15,17	0.92	0
4	NAG	H	2006	7,6	14,14,15	0.54	0	15,19,21	1.15	3 (20%)
7	GAL	H	2007	4	11,11,12	0.61	0	13,15,17	0.94	2 (15%)
4	NAG	H	2008	5	14,14,15	0.46	0	15,19,21	1.02	1 (6%)
6	MAN	H	2009	5,4	11,11,12	0.58	0	13,15,17	0.74	0
4	NAG	H	2010	6	14,14,15	0.51	0	15,19,21	0.59	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	2003	5	-	0/6/23/26	0/1/1/1
6	MAN	A	2005	5,4	-	0/2/19/22	0/1/1/1
4	NAG	A	2006	7,6	-	0/6/23/26	0/1/1/1
7	GAL	A	2007	4	-	0/2/19/22	0/1/1/1
4	NAG	A	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	A	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	A	2010	6	-	0/6/23/26	0/1/1/1
4	NAG	B	2003	5	-	0/6/23/26	0/1/1/1
6	MAN	B	2005	5,4	-	0/2/19/22	0/1/1/1
4	NAG	B	2006	7,6	-	0/6/23/26	0/1/1/1
7	GAL	B	2007	4	-	0/2/19/22	0/1/1/1
4	NAG	B	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	B	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	B	2010	6	-	0/6/23/26	0/1/1/1
4	NAG	C	2003	5	-	0/6/23/26	0/1/1/1
6	MAN	C	2005	5,4	-	0/2/19/22	0/1/1/1
4	NAG	C	2006	7,6	-	0/6/23/26	0/1/1/1
7	GAL	C	2007	4	-	0/2/19/22	0/1/1/1
4	NAG	C	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	C	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	C	2010	6	-	0/6/23/26	0/1/1/1
4	NAG	D	2003	5	-	0/6/23/26	0/1/1/1
6	MAN	D	2005	5,4	-	0/2/19/22	0/1/1/1
4	NAG	D	2006	7,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GAL	D	2007	4	-	0/2/19/22	0/1/1/1
4	NAG	D	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	D	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	D	2010	6	-	0/6/23/26	0/1/1/1
4	NAG	E	2003	5	-	0/6/23/26	0/1/1/1
6	MAN	E	2005	5,4	-	0/2/19/22	0/1/1/1
4	NAG	E	2006	7,6	-	0/6/23/26	0/1/1/1
7	GAL	E	2007	4	-	0/2/19/22	0/1/1/1
4	NAG	E	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	E	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	E	2010	6	-	0/6/23/26	0/1/1/1
4	NAG	F	2003	5	-	0/6/23/26	0/1/1/1
6	MAN	F	2005	5,4	-	0/2/19/22	0/1/1/1
4	NAG	F	2006	7,6	-	0/6/23/26	0/1/1/1
7	GAL	F	2007	4	-	0/2/19/22	0/1/1/1
4	NAG	F	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	F	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	F	2010	6	-	0/6/23/26	0/1/1/1
4	NAG	G	2003	5	-	0/6/23/26	0/1/1/1
6	MAN	G	2005	5,4	-	0/2/19/22	0/1/1/1
4	NAG	G	2006	7,6	-	0/6/23/26	0/1/1/1
7	GAL	G	2007	4	-	0/2/19/22	0/1/1/1
4	NAG	G	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	G	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	G	2010	6	-	0/6/23/26	0/1/1/1
4	NAG	H	2003	5	-	0/6/23/26	0/1/1/1
6	MAN	H	2005	5,4	-	0/2/19/22	0/1/1/1
4	NAG	H	2006	7,6	-	0/6/23/26	0/1/1/1
7	GAL	H	2007	4	-	0/2/19/22	0/1/1/1
4	NAG	H	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	H	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	H	2010	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	2007	GAL	O5-C1-C2	-2.54	106.81	110.79
4	C	2003	NAG	O5-C1-C2	-2.31	108.26	111.47
4	B	2008	NAG	C6-C5-C4	-2.29	107.65	113.00
7	H	2007	GAL	O5-C1-C2	-2.25	107.26	110.79
6	G	2009	MAN	O5-C1-C2	-2.25	107.27	110.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2006	NAG	1	0
4	D	2006	NAG	1	0
4	G	2006	NAG	1	0
7	G	2007	GAL	1	0
4	G	2008	NAG	1	0
6	G	2009	MAN	1	0
4	H	2006	NAG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 80 ligands modelled in this entry, 16 are monoatomic - leaving 64 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	$\# Z > 2$
4	NAG	A	2003	5	14,14,15	0.53	0	15,19,21	1.00	0
5	BMA	A	2004	4,6	11,11,12	0.65	0	13,15,17	0.79	0
6	MAN	A	2005	5,4	11,11,12	0.68	0	13,15,17	1.04	2 (15%)
4	NAG	A	2006	7,6	14,14,15	0.46	0	15,19,21	1.02	0
7	GAL	A	2007	4	11,11,12	0.60	0	13,15,17	0.72	0
4	NAG	A	2008	5	14,14,15	0.46	0	15,19,21	0.77	0
6	MAN	A	2009	5,4	11,11,12	0.48	0	13,15,17	1.13	1 (7%)
4	NAG	A	2010	6	14,14,15	0.47	0	15,19,21	0.89	0
4	NAG	B	2003	5	14,14,15	0.53	0	15,19,21	0.83	0
5	BMA	B	2004	4,6	11,11,12	0.59	0	13,15,17	0.87	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	B	2005	5,4	11,11,12	0.61	0	13,15,17	0.88	0
4	NAG	B	2006	7,6	14,14,15	0.53	0	15,19,21	1.01	1 (6%)
7	GAL	B	2007	4	11,11,12	0.62	0	13,15,17	0.60	0
4	NAG	B	2008	5	14,14,15	0.49	0	15,19,21	1.34	2 (13%)
6	MAN	B	2009	5,4	11,11,12	0.51	0	13,15,17	1.71	1 (7%)
4	NAG	B	2010	6	14,14,15	0.54	0	15,19,21	0.68	0
4	NAG	C	2003	5	14,14,15	0.49	0	15,19,21	1.05	1 (6%)
5	BMA	C	2004	4,6	11,11,12	0.61	0	13,15,17	0.79	0
6	MAN	C	2005	5,4	11,11,12	0.63	0	13,15,17	0.70	0
4	NAG	C	2006	7,6	14,14,15	0.51	0	15,19,21	0.88	0
7	GAL	C	2007	4	11,11,12	0.60	0	13,15,17	0.63	0
4	NAG	C	2008	5	14,14,15	0.40	0	15,19,21	1.26	1 (6%)
6	MAN	C	2009	5,4	11,11,12	0.52	0	13,15,17	0.97	1 (7%)
4	NAG	C	2010	6	14,14,15	0.51	0	15,19,21	0.74	0
4	NAG	D	2003	5	14,14,15	0.50	0	15,19,21	0.94	0
5	BMA	D	2004	4,6	11,11,12	0.55	0	13,15,17	0.68	0
6	MAN	D	2005	5,4	11,11,12	0.63	0	13,15,17	0.69	0
4	NAG	D	2006	7,6	14,14,15	0.50	0	15,19,21	0.93	0
7	GAL	D	2007	4	11,11,12	0.59	0	13,15,17	0.66	0
4	NAG	D	2008	5	14,14,15	0.46	0	15,19,21	0.95	1 (6%)
6	MAN	D	2009	5,4	11,11,12	0.51	0	13,15,17	1.24	1 (7%)
4	NAG	D	2010	6	14,14,15	0.52	0	15,19,21	0.69	0
4	NAG	E	2003	5	14,14,15	0.52	0	15,19,21	0.79	0
5	BMA	E	2004	4,6	11,11,12	0.56	0	13,15,17	0.86	1 (7%)
6	MAN	E	2005	5,4	11,11,12	0.60	0	13,15,17	1.09	1 (7%)
4	NAG	E	2006	7,6	14,14,15	0.45	0	15,19,21	0.85	0
7	GAL	E	2007	4	11,11,12	0.65	0	13,15,17	1.02	1 (7%)
4	NAG	E	2008	5	14,14,15	0.39	0	15,19,21	1.41	1 (6%)
6	MAN	E	2009	5,4	11,11,12	0.52	0	13,15,17	1.11	1 (7%)
4	NAG	E	2010	6	14,14,15	0.49	0	15,19,21	0.90	1 (6%)
4	NAG	F	2003	5	14,14,15	0.48	0	15,19,21	0.98	1 (6%)
5	BMA	F	2004	4,6	11,11,12	0.57	0	13,15,17	0.79	0
6	MAN	F	2005	5,4	11,11,12	0.60	0	13,15,17	0.68	0
4	NAG	F	2006	7,6	14,14,15	0.47	0	15,19,21	0.82	0
7	GAL	F	2007	4	11,11,12	0.60	0	13,15,17	0.63	0
4	NAG	F	2008	5	14,14,15	0.39	0	15,19,21	1.11	1 (6%)
6	MAN	F	2009	5,4	11,11,12	0.55	0	13,15,17	0.92	1 (7%)
4	NAG	F	2010	6	14,14,15	0.48	0	15,19,21	1.11	0
4	NAG	G	2003	5	14,14,15	0.53	0	15,19,21	1.07	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	G	2004	4,6	11,11,12	0.58	0	13,15,17	0.79	0
6	MAN	G	2005	5,4	11,11,12	0.67	0	13,15,17	0.64	0
4	NAG	G	2006	7,6	14,14,15	0.50	0	15,19,21	1.00	0
7	GAL	G	2007	4	11,11,12	0.59	0	13,15,17	0.75	0
4	NAG	G	2008	5	14,14,15	0.37	0	15,19,21	1.36	1 (6%)
6	MAN	G	2009	5,4	11,11,12	0.53	0	13,15,17	1.20	2 (15%)
4	NAG	G	2010	6	14,14,15	0.45	0	15,19,21	0.95	1 (6%)
4	NAG	H	2003	5	14,14,15	0.54	0	15,19,21	0.91	1 (6%)
5	BMA	H	2004	4,6	11,11,12	0.54	0	13,15,17	0.58	0
6	MAN	H	2005	5,4	11,11,12	0.65	0	13,15,17	0.92	0
4	NAG	H	2006	7,6	14,14,15	0.54	0	15,19,21	1.15	3 (20%)
7	GAL	H	2007	4	11,11,12	0.61	0	13,15,17	0.94	2 (15%)
4	NAG	H	2008	5	14,14,15	0.46	0	15,19,21	1.02	1 (6%)
6	MAN	H	2009	5,4	11,11,12	0.58	0	13,15,17	0.74	0
4	NAG	H	2010	6	14,14,15	0.51	0	15,19,21	0.59	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	2003	5	-	0/6/23/26	0/1/1/1
5	BMA	A	2004	4,6	-	0/2/19/22	0/1/1/1
6	MAN	A	2005	5,4	-	0/2/19/22	0/1/1/1
4	NAG	A	2006	7,6	-	0/6/23/26	0/1/1/1
7	GAL	A	2007	4	-	0/2/19/22	0/1/1/1
4	NAG	A	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	A	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	A	2010	6	-	0/6/23/26	0/1/1/1
4	NAG	B	2003	5	-	0/6/23/26	0/1/1/1
5	BMA	B	2004	4,6	-	0/2/19/22	0/1/1/1
6	MAN	B	2005	5,4	-	0/2/19/22	0/1/1/1
4	NAG	B	2006	7,6	-	0/6/23/26	0/1/1/1
7	GAL	B	2007	4	-	0/2/19/22	0/1/1/1
4	NAG	B	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	B	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	B	2010	6	-	0/6/23/26	0/1/1/1
4	NAG	C	2003	5	-	0/6/23/26	0/1/1/1
5	BMA	C	2004	4,6	-	0/2/19/22	0/1/1/1
6	MAN	C	2005	5,4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	2006	7,6	-	0/6/23/26	0/1/1/1
7	GAL	C	2007	4	-	0/2/19/22	0/1/1/1
4	NAG	C	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	C	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	C	2010	6	-	0/6/23/26	0/1/1/1
4	NAG	D	2003	5	-	0/6/23/26	0/1/1/1
5	BMA	D	2004	4,6	-	0/2/19/22	0/1/1/1
6	MAN	D	2005	5,4	-	0/2/19/22	0/1/1/1
4	NAG	D	2006	7,6	-	0/6/23/26	0/1/1/1
7	GAL	D	2007	4	-	0/2/19/22	0/1/1/1
4	NAG	D	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	D	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	D	2010	6	-	0/6/23/26	0/1/1/1
4	NAG	E	2003	5	-	0/6/23/26	0/1/1/1
5	BMA	E	2004	4,6	-	0/2/19/22	0/1/1/1
6	MAN	E	2005	5,4	-	0/2/19/22	0/1/1/1
4	NAG	E	2006	7,6	-	0/6/23/26	0/1/1/1
7	GAL	E	2007	4	-	0/2/19/22	0/1/1/1
4	NAG	E	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	E	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	E	2010	6	-	0/6/23/26	0/1/1/1
4	NAG	F	2003	5	-	0/6/23/26	0/1/1/1
5	BMA	F	2004	4,6	-	0/2/19/22	0/1/1/1
6	MAN	F	2005	5,4	-	0/2/19/22	0/1/1/1
4	NAG	F	2006	7,6	-	0/6/23/26	0/1/1/1
7	GAL	F	2007	4	-	0/2/19/22	0/1/1/1
4	NAG	F	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	F	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	F	2010	6	-	0/6/23/26	0/1/1/1
4	NAG	G	2003	5	-	0/6/23/26	0/1/1/1
5	BMA	G	2004	4,6	-	0/2/19/22	0/1/1/1
6	MAN	G	2005	5,4	-	0/2/19/22	0/1/1/1
4	NAG	G	2006	7,6	-	0/6/23/26	0/1/1/1
7	GAL	G	2007	4	-	0/2/19/22	0/1/1/1
4	NAG	G	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	G	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	G	2010	6	-	0/6/23/26	0/1/1/1
4	NAG	H	2003	5	-	0/6/23/26	0/1/1/1
5	BMA	H	2004	4,6	-	0/2/19/22	0/1/1/1
6	MAN	H	2005	5,4	-	0/2/19/22	0/1/1/1
4	NAG	H	2006	7,6	-	0/6/23/26	0/1/1/1
7	GAL	H	2007	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	H	2008	5	-	0/6/23/26	0/1/1/1
6	MAN	H	2009	5,4	-	0/2/19/22	0/1/1/1
4	NAG	H	2010	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	2007	GAL	O5-C1-C2	-2.54	106.81	110.79
4	C	2003	NAG	O5-C1-C2	-2.31	108.26	111.47
4	B	2008	NAG	C6-C5-C4	-2.29	107.65	113.00
7	H	2007	GAL	O5-C1-C2	-2.25	107.26	110.79
6	G	2009	MAN	O5-C1-C2	-2.25	107.27	110.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2006	NAG	1	0
4	D	2006	NAG	1	0
4	G	2006	NAG	1	0
7	G	2007	GAL	1	0
4	G	2008	NAG	1	0
6	G	2009	MAN	1	0
4	H	2006	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	238/275 (86%)	-0.40	5 (2%) 64 34	20, 32, 50, 139	0
1	B	238/275 (86%)	-0.38	6 (2%) 58 29	22, 33, 51, 97	0
1	C	238/275 (86%)	-0.32	5 (2%) 64 34	23, 38, 68, 115	0
1	D	238/275 (86%)	-0.27	5 (2%) 64 34	24, 36, 61, 116	0
1	E	238/275 (86%)	-0.46	4 (1%) 70 42	19, 32, 51, 116	0
1	F	238/275 (86%)	-0.34	4 (1%) 70 42	20, 35, 62, 119	0
1	G	238/275 (86%)	0.06	13 (5%) 26 10	25, 50, 82, 131	0
1	H	238/275 (86%)	0.15	8 (3%) 46 20	30, 54, 83, 120	0
All	All	1904/2200 (86%)	-0.25	50 (2%) 56 27	19, 37, 73, 139	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	THR	10.8
1	D	259	THR	9.8
1	H	259	THR	9.5
1	E	259	THR	8.7
1	F	259	THR	8.3

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
4	NAG	B	2010	14/15	0.87	0.36	7.36	59,61,63,64	0
6	MAN	E	2005	11/12	0.90	0.22	0.45	47,49,50,50	0
6	MAN	B	2005	11/12	0.94	0.19	0.14	35,37,38,38	0
6	MAN	A	2005	11/12	0.93	0.21	0.03	37,38,38,39	0
4	NAG	B	2006	14/15	0.97	0.20	-0.07	33,34,35,38	0
4	NAG	A	2006	14/15	0.96	0.21	-0.11	34,36,40,41	0
6	MAN	C	2005	11/12	0.91	0.18	-0.12	49,52,53,54	0
4	NAG	C	2006	14/15	0.92	0.20	-0.34	45,47,48,49	0
6	MAN	F	2005	11/12	0.89	0.18	-0.52	53,55,57,58	0
4	NAG	H	2006	14/15	0.80	0.30	-0.61	67,71,79,82	0
4	NAG	E	2006	14/15	0.95	0.17	-0.62	42,44,45,46	0
6	MAN	G	2005	11/12	0.85	0.21	-0.66	65,68,69,72	0
4	NAG	F	2006	14/15	0.92	0.18	-0.85	55,58,62,63	0
4	NAG	D	2006	14/15	0.93	0.18	-0.85	45,47,51,51	0
4	NAG	G	2006	14/15	0.92	0.24	-0.95	58,61,62,64	0
6	MAN	D	2005	11/12	0.94	0.14	-2.41	48,50,52,53	0
6	MAN	H	2005	11/12	0.82	0.17	-2.53	78,83,84,85	0
4	NAG	C	2003	14/15	0.84	0.25	-	57,59,61,61	0
7	GAL	A	2007	11/12	0.94	0.17	-	31,32,33,34	0
6	MAN	B	2009	11/12	0.90	0.30	-	50,51,52,56	0
4	NAG	A	2003	14/15	0.90	0.23	-	40,42,43,43	0
7	GAL	E	2007	11/12	0.93	0.20	-	40,41,41,41	0
4	NAG	H	2003	14/15	0.71	0.35	-	84,89,96,97	0
4	NAG	H	2008	14/15	0.82	0.28	-	69,73,80,81	0
4	NAG	E	2008	14/15	0.92	0.24	-	43,44,45,46	0
4	NAG	C	2008	14/15	0.90	0.20	-	48,49,51,53	0
4	NAG	B	2003	14/15	0.85	0.21	-	45,48,49,51	0
7	GAL	F	2007	11/12	0.89	0.20	-	54,57,58,59	0
6	MAN	A	2009	11/12	0.90	0.25	-	55,56,57,62	0
4	NAG	G	2008	14/15	0.90	0.29	-	57,58,60,60	0
6	MAN	D	2009	11/12	0.85	0.30	-	66,68,70,71	0
4	NAG	G	2003	14/15	0.84	0.23	-	55,60,66,66	0
4	NAG	D	2010	14/15	0.83	0.36	-	69,72,74,76	0
4	NAG	F	2008	14/15	0.87	0.34	-	55,59,61,62	0
7	GAL	H	2007	11/12	0.88	0.21	-	64,66,69,69	0
4	NAG	A	2008	14/15	0.93	0.23	-	39,40,43,45	0
6	MAN	F	2009	11/12	0.85	0.37	-	74,76,77,82	0
4	NAG	A	2010	14/15	0.83	0.30	-	66,68,72,73	0
7	GAL	B	2007	11/12	0.93	0.23	-	40,42,43,44	0
6	MAN	C	2009	11/12	0.77	0.30	-	67,69,72,73	0
6	MAN	E	2009	11/12	0.84	0.28	-	66,70,74,76	0
4	NAG	H	2010	14/15	0.89	0.40	-	82,84,84,84	0
6	MAN	G	2009	11/12	0.75	0.33	-	79,82,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	GAL	D	2007	11/12	0.96	0.21	-	40,41,43,43	0
4	NAG	E	2003	14/15	0.85	0.19	-	48,54,57,58	0
7	GAL	G	2007	11/12	0.86	0.24	-	64,65,66,66	0
4	NAG	F	2003	14/15	0.82	0.29	-	63,66,70,71	0
4	NAG	D	2008	14/15	0.92	0.25	-	51,53,61,63	0
7	GAL	C	2007	11/12	0.90	0.21	-	47,49,50,50	0
4	NAG	F	2010	14/15	0.79	0.42	-	83,86,87,90	0
4	NAG	E	2010	14/15	0.88	0.27	-	71,71,72,74	0
4	NAG	B	2008	14/15	0.92	0.29	-	35,38,40,40	0
4	NAG	D	2003	14/15	0.88	0.29	-	53,58,59,60	0
4	NAG	C	2010	14/15	0.82	0.25	-	62,67,71,72	0
6	MAN	H	2009	11/12	0.82	0.36	-	77,80,82,82	0
4	NAG	G	2010	14/15	0.77	0.37	-	75,80,81,81	0

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(\AA^2)	Q<0.9
4	NAG	B	2010	14/15	0.87	0.36	7.36	59,61,63,64	0
6	MAN	E	2005	11/12	0.90	0.22	0.45	47,49,50,50	0
6	MAN	B	2005	11/12	0.94	0.19	0.14	35,37,38,38	0
6	MAN	A	2005	11/12	0.93	0.21	0.03	37,38,38,39	0
4	NAG	B	2006	14/15	0.97	0.20	-0.07	33,34,35,38	0
4	NAG	A	2006	14/15	0.96	0.21	-0.11	34,36,40,41	0
6	MAN	C	2005	11/12	0.91	0.18	-0.12	49,52,53,54	0
4	NAG	C	2006	14/15	0.92	0.20	-0.34	45,47,48,49	0
6	MAN	F	2005	11/12	0.89	0.18	-0.52	53,55,57,58	0
4	NAG	H	2006	14/15	0.80	0.30	-0.61	67,71,79,82	0
4	NAG	E	2006	14/15	0.95	0.17	-0.62	42,44,45,46	0
6	MAN	G	2005	11/12	0.85	0.21	-0.66	65,68,69,72	0
4	NAG	D	2006	14/15	0.93	0.18	-0.85	45,47,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	F	2006	14/15	0.92	0.18	-0.85	55,58,62,63	0
3	CA	E	2002	1/1	0.95	0.12	-0.89	40,40,40,40	0
4	NAG	G	2006	14/15	0.92	0.24	-0.95	58,61,62,64	0
3	CA	G	2002	1/1	0.88	0.09	-1.56	61,61,61,61	0
3	CA	C	2002	1/1	0.95	0.07	-1.71	42,42,42,42	0
3	CA	D	2002	1/1	0.89	0.09	-1.85	44,44,44,44	0
2	MN	G	2001	1/1	0.96	0.07	-1.94	54,54,54,54	0
3	CA	A	2002	1/1	0.95	0.06	-2.10	34,34,34,34	0
3	CA	H	2002	1/1	0.86	0.08	-2.29	72,72,72,72	0
2	MN	A	2001	1/1	0.97	0.05	-2.37	33,33,33,33	0
6	MAN	D	2005	11/12	0.94	0.14	-2.41	48,50,52,53	0
3	CA	F	2002	1/1	0.97	0.05	-2.49	44,44,44,44	0
6	MAN	H	2005	11/12	0.82	0.17	-2.53	78,83,84,85	0
3	CA	B	2002	1/1	0.96	0.07	-2.64	35,35,35,35	0
2	MN	C	2001	1/1	0.94	0.06	-2.97	41,41,41,41	0
2	MN	H	2001	1/1	0.95	0.04	-3.03	63,63,63,63	0
2	MN	F	2001	1/1	0.99	0.04	-3.09	43,43,43,43	0
2	MN	D	2001	1/1	0.96	0.04	-3.20	40,40,40,40	0
2	MN	E	2001	1/1	0.97	0.06	-3.44	40,40,40,40	0
2	MN	B	2001	1/1	0.97	0.04	-5.50	34,34,34,34	0
5	BMA	A	2004	11/12	0.94	0.18	-	39,42,45,50	0
4	NAG	C	2008	14/15	0.90	0.20	-	48,49,51,53	0
5	BMA	D	2004	11/12	0.88	0.20	-	52,57,59,63	0
4	NAG	B	2003	14/15	0.85	0.21	-	45,48,49,51	0
4	NAG	G	2010	14/15	0.77	0.37	-	75,80,81,81	0
6	MAN	D	2009	11/12	0.85	0.30	-	66,68,70,71	0
4	NAG	E	2008	14/15	0.92	0.24	-	43,44,45,46	0
6	MAN	G	2009	11/12	0.75	0.33	-	79,82,86,86	0
5	BMA	G	2004	11/12	0.90	0.19	-	62,64,69,73	0
5	BMA	F	2004	11/12	0.90	0.21	-	58,63,66,69	0
4	NAG	G	2003	14/15	0.84	0.23	-	55,60,66,66	0
5	BMA	C	2004	11/12	0.93	0.14	-	53,55,58,63	0
4	NAG	H	2008	14/15	0.82	0.28	-	69,73,80,81	0
5	BMA	E	2004	11/12	0.92	0.18	-	50,53,55,60	0
4	NAG	D	2010	14/15	0.83	0.36	-	69,72,74,76	0
4	NAG	F	2008	14/15	0.87	0.34	-	55,59,61,62	0
6	MAN	H	2009	11/12	0.82	0.36	-	77,80,82,82	0
4	NAG	A	2008	14/15	0.93	0.23	-	39,40,43,45	0
6	MAN	A	2009	11/12	0.90	0.25	-	55,56,57,62	0
4	NAG	A	2010	14/15	0.83	0.30	-	66,68,72,73	0
7	GAL	B	2007	11/12	0.93	0.23	-	40,42,43,44	0
6	MAN	C	2009	11/12	0.77	0.30	-	67,69,72,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	GAL	F	2007	11/12	0.89	0.20	-	54,57,58,59	0
4	NAG	C	2003	14/15	0.84	0.25	-	57,59,61,61	0
4	NAG	G	2008	14/15	0.90	0.29	-	57,58,60,60	0
4	NAG	C	2010	14/15	0.82	0.25	-	62,67,71,72	0
7	GAL	D	2007	11/12	0.96	0.21	-	40,41,43,43	0
6	MAN	F	2009	11/12	0.85	0.37	-	74,76,77,82	0
6	MAN	E	2009	11/12	0.84	0.28	-	66,70,74,76	0
5	BMA	B	2004	11/12	0.91	0.18	-	39,43,44,47	0
7	GAL	H	2007	11/12	0.88	0.21	-	64,66,69,69	0
7	GAL	A	2007	11/12	0.94	0.17	-	31,32,33,34	0
4	NAG	D	2008	14/15	0.92	0.25	-	51,53,61,63	0
6	MAN	B	2009	11/12	0.90	0.30	-	50,51,52,56	0
4	NAG	F	2003	14/15	0.82	0.29	-	63,66,70,71	0
7	GAL	C	2007	11/12	0.90	0.21	-	47,49,50,50	0
4	NAG	A	2003	14/15	0.90	0.23	-	40,42,43,43	0
4	NAG	F	2010	14/15	0.79	0.42	-	83,86,87,90	0
7	GAL	E	2007	11/12	0.93	0.20	-	40,41,41,41	0
4	NAG	E	2003	14/15	0.85	0.19	-	48,54,57,58	0
4	NAG	H	2010	14/15	0.89	0.40	-	82,84,84,84	0
4	NAG	E	2010	14/15	0.88	0.27	-	71,71,72,74	0
4	NAG	B	2008	14/15	0.92	0.29	-	35,38,40,40	0
4	NAG	D	2003	14/15	0.88	0.29	-	53,58,59,60	0
5	BMA	H	2004	11/12	0.84	0.17	-	76,79,83,84	0
4	NAG	H	2003	14/15	0.71	0.35	-	84,89,96,97	0
7	GAL	G	2007	11/12	0.86	0.24	-	64,65,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.