Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:26 AM GMT

PDB ID	:	2H6O
Title	:	Epstein Barr Virus Major Envelope Glycoprotein
Authors	:	Chen, X.S.
Deposited on	:	2006-05-31
Resolution	:	3.50 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:

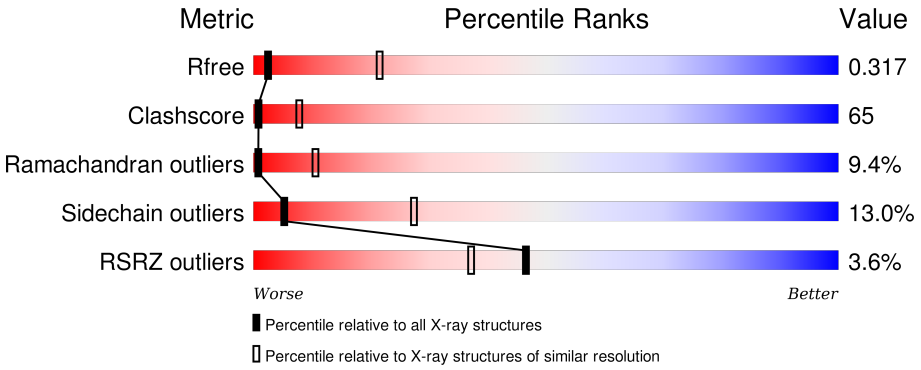
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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 <=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	470	3%, 34%, 47%, 11%, 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
2	NAG	A	1047	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1048	-	-	X	-
2	NAG	A	1166	-	-	X	-
2	NAG	A	1195	-	-	-	X
2	NAG	A	1230	-	-	X	-
2	NAG	A	1328	-	-	X	-
2	NAG	A	1345	-	-	X	-
2	NAG	A	1356	-	-	X	-
2	NAG	A	1386	-	-	X	-
2	NAG	A	1411	-	-	X	-
2	NAG	A	1412	-	-	X	-
3	MAN	A	1049	-	-	X	-
3	MAN	A	1050	-	-	X	-
3	MAN	A	1089	-	-	X	-
3	MAN	A	1117	-	-	X	-
3	MAN	A	1118	-	-	X	-
3	MAN	A	1171	-	-	X	X
3	MAN	A	1231	-	-	X	-
3	MAN	A	1235	-	-	X	-
3	MAN	A	1279	-	-	X	-
3	MAN	A	1283	-	-	X	-
3	MAN	A	1284	-	-	X	-
3	MAN	A	1330	-	-	X	-
3	MAN	A	1347	-	-	X	-
3	MAN	A	1348	-	-	X	-
3	MAN	A	1349	-	-	X	-
3	MAN	A	1359	-	-	X	-
3	MAN	A	1391	-	-	X	-
4	BMA	A	1090	-	-	X	-
4	BMA	A	1168	-	-	X	-
4	BMA	A	1280	-	-	X	-
6	GAL	A	1236	-	-	X	-
7	FUC	A	1364	-	-	-	X

2 Entry composition

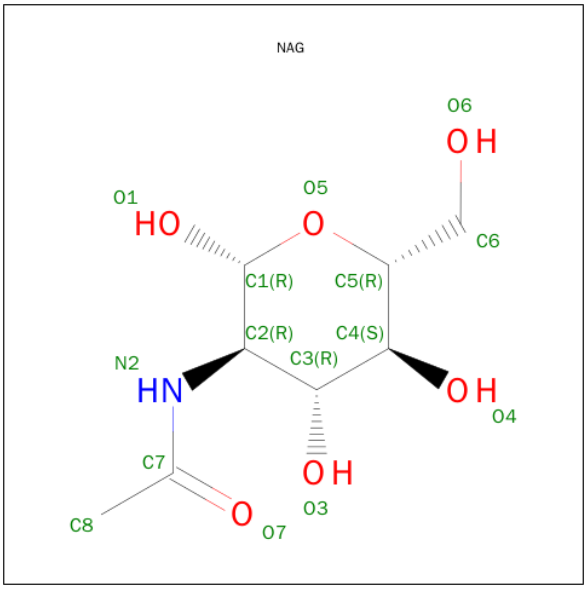
There are 7 unique types of molecules in this entry. The entry contains 4500 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Major outer envelope glycoprotein gp350.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3301	2082	542	660	17			

- Molecule 2 is SUGAR (6-MER) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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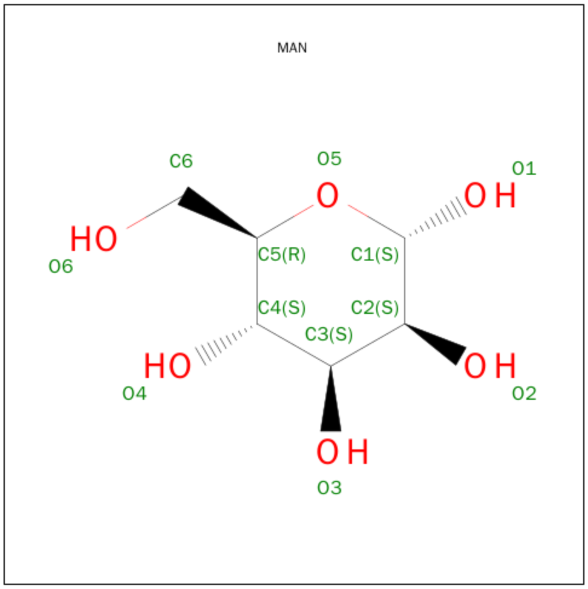
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

- Molecule 3 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

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

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

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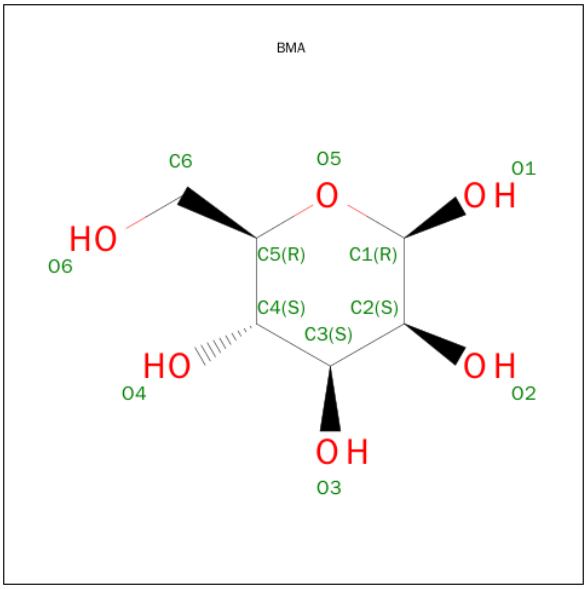
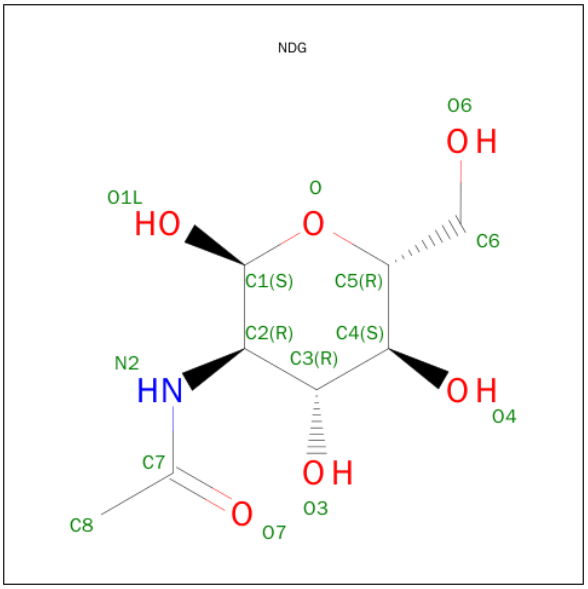
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0

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



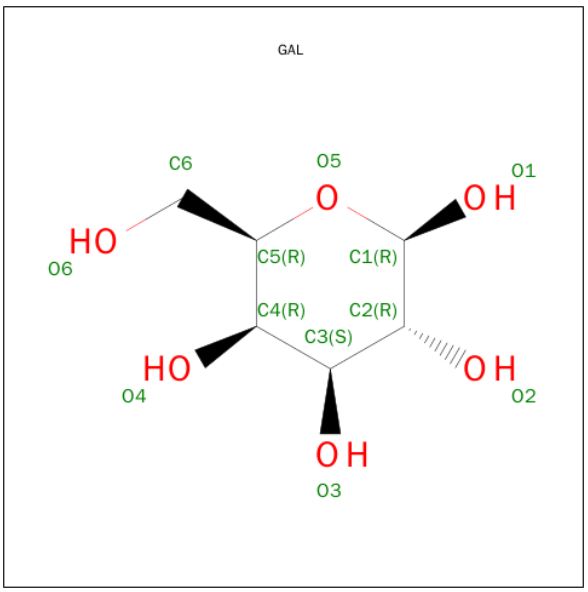
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0

- Molecule 5 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



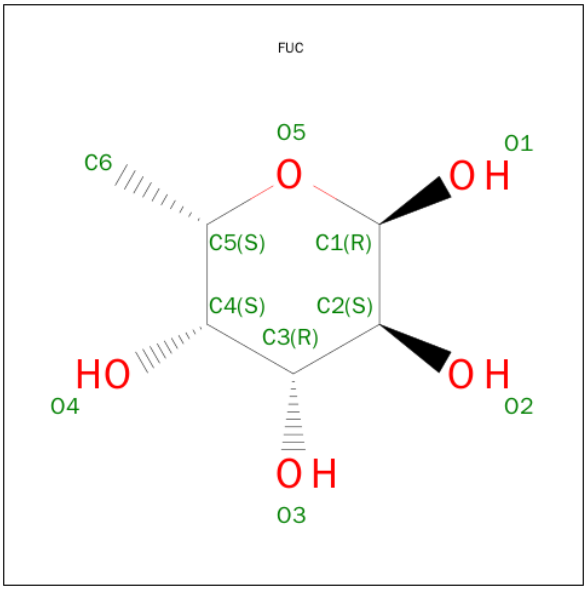
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is SUGAR (D-GALACTOSE) (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



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

- Molecule 7 is SUGAR (ALPHA-L-FUCOSE) (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



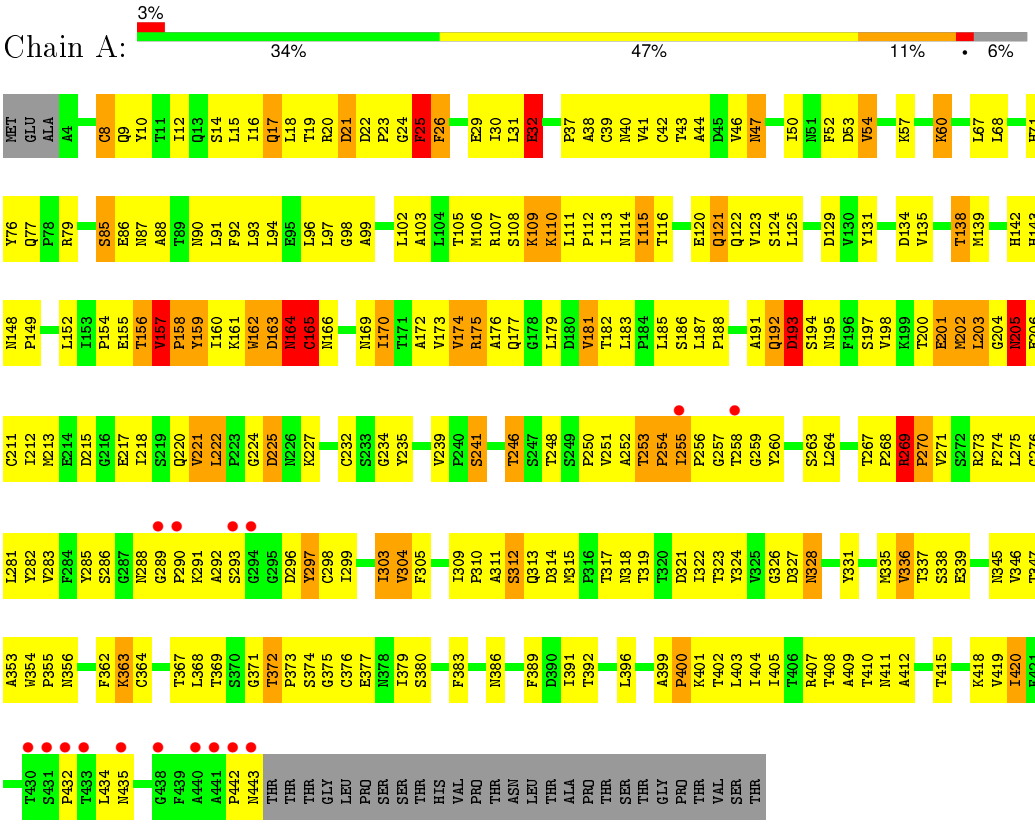
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 10 6 4	0	0
7	A	1	Total C O 10 6 4	0	0

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

- Molecule 1: Major outer envelope glycoprotein gp350

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	110.01Å 110.01Å 146.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.50 24.91 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.50) 87.8 (24.91-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.99Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.326 , 0.368 0.287 , 0.317	Depositor DCC
R_{free} test set	947 reflections (7.71%)	DCC
Wilson B-factor (Å^2)	81.4	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.6	EDS
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 20918 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	4500	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, NDG, GAL, FUC, 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	0.58	3/3377 (0.1%)	0.98	11/4621 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	ASN	CA-C	7.14	1.71	1.52
1	A	443	ASN	C-O	7.04	1.36	1.23
1	A	352	TRP	NE1-CE2	-6.49	1.29	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	PHE	CB-CA-C	-7.25	95.90	110.40
1	A	352	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	A	163	ASP	N-CA-C	6.76	129.26	111.00
1	A	443	ASN	CB-CA-C	-6.64	97.12	110.40
1	A	352	TRP	CD2-CE2-CZ2	-6.58	114.40	122.30
1	A	156	THR	N-CA-C	-6.01	94.78	111.00
1	A	25	PHE	CB-CG-CD1	-5.54	116.92	120.80
1	A	218	ILE	N-CA-C	-5.35	96.55	111.00
1	A	432	PRO	N-CA-CB	5.34	109.71	103.30
1	A	442	PRO	N-CA-CB	5.22	109.57	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	PHE	N-CA-CB	5.00	119.61	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	PHE	Sidechain

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	3301	0	3132	356	0
2	A	378	0	326	121	0
3	A	627	0	533	163	0
4	A	66	0	55	28	0
5	A	42	0	38	9	0
6	A	66	0	57	13	0
7	A	20	0	20	5	0
All	All	4500	0	4161	562	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 65.

All (562) 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:166:ASN:HD21	2:A:1166:NAG:C1	1.07	1.60
1:A:386:ASN:HD21	2:A:1386:NAG:C1	1.06	1.59
1:A:345:ASN:HD21	2:A:1345:NAG:C1	1.12	1.53
3:A:1330:MAN:O3	3:A:1331:MAN:C1	1.64	1.46
3:A:1169:MAN:O3	3:A:1173:MAN:C1	1.64	1.45
2:A:1345:NAG:O4	2:A:1346:NAG:C1	1.64	1.45
2:A:1356:NAG:O4	5:A:1357:NDG:C1	1.65	1.45
2:A:1115:NAG:O4	3:A:1116:MAN:C1	1.63	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASN:ND2	2:A:1328:NAG:C1	1.76	1.45
2:A:1230:NAG:O4	3:A:1231:MAN:C1	1.66	1.45
3:A:1389:MAN:O2	2:A:1392:NAG:C1	1.63	1.44
2:A:1392:NAG:O3	3:A:1390:MAN:C1	1.65	1.44
2:A:1412:NAG:O4	3:A:1413:MAN:C1	1.65	1.44
3:A:1117:MAN:O3	3:A:1119:MAN:C1	1.64	1.44
3:A:1388:MAN:O6	3:A:1391:MAN:C1	1.65	1.43
2:A:1229:NAG:O4	2:A:1230:NAG:C1	1.67	1.43
3:A:1231:MAN:O6	3:A:1233:MAN:C1	1.64	1.43
3:A:1201:MAN:O3	3:A:1202:MAN:C1	1.66	1.43
6:A:1203:GAL:O3	6:A:1204:GAL:C1	1.65	1.43
3:A:1197:MAN:O6	3:A:1201:MAN:C1	1.65	1.43
3:A:1235:MAN:O3	6:A:1236:GAL:C1	1.66	1.42
1:A:87:ASN:ND2	2:A:1087:NAG:C1	1.80	1.42
3:A:1232:MAN:O2	3:A:1234:MAN:C1	1.67	1.42
3:A:1092:MAN:O2	3:A:1093:MAN:C1	1.66	1.42
2:A:1319:NAG:O3	3:A:1320:MAN:C1	1.64	1.42
4:A:1168:BMA:O3	3:A:1171:MAN:C1	1.66	1.42
3:A:1359:MAN:O2	2:A:1363:NAG:C1	1.65	1.42
3:A:1089:MAN:O3	3:A:1092:MAN:C1	1.67	1.42
6:A:1236:GAL:O3	6:A:1237:GAL:C1	1.65	1.42
2:A:1435:NAG:O4	2:A:1436:NAG:C1	1.68	1.42
3:A:1173:MAN:O2	3:A:1174:MAN:C1	1.68	1.41
3:A:1119:MAN:O2	3:A:1120:MAN:C1	1.69	1.41
1:A:87:ASN:HD22	2:A:1087:NAG:C1	1.31	1.41
3:A:1284:MAN:O2	3:A:1285:MAN:C1	1.67	1.41
2:A:1195:NAG:O3	2:A:1196:NAG:C1	1.66	1.41
2:A:1278:NAG:O4	3:A:1279:MAN:C1	1.67	1.41
3:A:1360:MAN:O6	3:A:1361:MAN:C1	1.65	1.41
3:A:1169:MAN:O6	3:A:1170:MAN:C1	1.67	1.41
5:A:1387:NDG:O3	3:A:1388:MAN:C1	1.67	1.41
3:A:1200:MAN:O3	6:A:1203:GAL:C1	1.65	1.41
2:A:1329:NAG:O3	3:A:1330:MAN:C1	1.69	1.40
2:A:1411:NAG:O3	2:A:1412:NAG:C1	1.69	1.40
2:A:1166:NAG:O4	2:A:1167:NAG:C1	1.69	1.40
2:A:1328:NAG:O4	2:A:1329:NAG:C1	1.65	1.40
3:A:1231:MAN:O3	3:A:1232:MAN:C1	1.67	1.40
2:A:1087:NAG:O4	2:A:1088:NAG:C1	1.68	1.40
2:A:1047:NAG:O4	2:A:1048:NAG:C1	1.65	1.40
5:A:1357:NDG:O3	3:A:1358:MAN:C1	1.68	1.40
4:A:1168:BMA:O6	3:A:1169:MAN:C1	1.70	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ASN:ND2	2:A:1386:NAG:C1	1.79	1.40
4:A:1280:BMA:O3	3:A:1281:MAN:C1	1.67	1.40
2:A:1356:NAG:O6	7:A:1364:FUC:C1	1.69	1.39
3:A:1198:MAN:O2	3:A:1199:MAN:C1	1.71	1.39
3:A:1283:MAN:O2	3:A:1284:MAN:C1	1.70	1.39
3:A:1116:MAN:O6	3:A:1117:MAN:C1	1.70	1.39
3:A:1279:MAN:O6	4:A:1280:BMA:C1	1.69	1.39
1:A:356:ASN:ND2	2:A:1356:NAG:C1	1.85	1.38
1:A:345:ASN:ND2	2:A:1345:NAG:C1	1.80	1.38
3:A:1089:MAN:O6	4:A:1090:BMA:C1	1.71	1.38
3:A:1348:MAN:O2	3:A:1351:MAN:C1	1.71	1.38
2:A:1167:NAG:O4	4:A:1168:BMA:C1	1.70	1.38
2:A:1048:NAG:O4	3:A:1049:MAN:C1	1.66	1.38
3:A:1049:MAN:O3	3:A:1053:MAN:C1	1.70	1.38
6:A:1286:GAL:O3	6:A:1287:GAL:C1	1.68	1.38
2:A:1386:NAG:O6	7:A:1395:FUC:C1	1.69	1.38
3:A:1118:MAN:O2	3:A:1121:MAN:C1	1.70	1.38
5:A:1114:NDG:O4	2:A:1115:NAG:C1	1.71	1.37
3:A:1360:MAN:O3	3:A:1362:MAN:C1	1.70	1.37
3:A:1117:MAN:O6	3:A:1118:MAN:C1	1.70	1.37
3:A:1234:MAN:O2	3:A:1235:MAN:C1	1.71	1.37
3:A:1391:MAN:O3	4:A:1394:BMA:C1	1.70	1.37
2:A:1088:NAG:O4	3:A:1089:MAN:C1	1.73	1.36
4:A:1090:BMA:O6	3:A:1091:MAN:C1	1.69	1.36
3:A:1349:MAN:O6	4:A:1352:BMA:C1	1.73	1.36
3:A:1347:MAN:O6	3:A:1349:MAN:C1	1.72	1.36
3:A:1049:MAN:O6	3:A:1050:MAN:C1	1.71	1.35
1:A:166:ASN:ND2	2:A:1166:NAG:C1	1.83	1.35
3:A:1388:MAN:O3	3:A:1389:MAN:C1	1.73	1.35
3:A:1349:MAN:O3	3:A:1350:MAN:C1	1.74	1.34
3:A:1330:MAN:O6	3:A:1332:MAN:C1	1.73	1.34
3:A:1358:MAN:O3	3:A:1359:MAN:C1	1.73	1.34
3:A:1391:MAN:O6	3:A:1393:MAN:C1	1.75	1.34
3:A:1347:MAN:O3	3:A:1348:MAN:C1	1.75	1.33
3:A:1050:MAN:O6	3:A:1051:MAN:C1	1.75	1.32
1:A:318:ASN:ND2	2:A:1318:NAG:C1	1.92	1.31
1:A:47:ASN:ND2	2:A:1047:NAG:C1	1.92	1.31
3:A:1197:MAN:O3	3:A:1198:MAN:C1	1.79	1.29
3:A:1279:MAN:O3	3:A:1283:MAN:C1	1.80	1.28
1:A:277:ASN:ND2	2:A:1277:NAG:C1	2.01	1.21
1:A:348:VAL:HG11	1:A:389:PHE:CE2	1.80	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:VAL:HG21	1:A:389:PHE:CG	1.81	1.14
1:A:356:ASN:HD21	2:A:1356:NAG:C1	1.47	1.13
2:A:1230:NAG:C4	3:A:1231:MAN:C1	2.27	1.12
1:A:157:VAL:CB	1:A:158:PRO:HD2	1.78	1.12
1:A:318:ASN:HD21	2:A:1318:NAG:C1	1.59	1.12
1:A:435:ASN:ND2	2:A:1435:NAG:C1	2.13	1.11
3:A:1360:MAN:HO3	3:A:1362:MAN:C1	1.52	1.11
6:A:1286:GAL:O3	6:A:1287:GAL:C2	2.02	1.07
5:A:1114:NDG:HC	2:A:1115:NAG:C1	1.60	1.05
1:A:157:VAL:HB	1:A:158:PRO:HD2	1.27	1.05
1:A:348:VAL:HG21	1:A:389:PHE:CD2	1.91	1.04
2:A:1412:NAG:O4	3:A:1413:MAN:C2	2.06	1.03
3:A:1049:MAN:HO6	3:A:1050:MAN:C1	1.58	1.02
3:A:1284:MAN:C2	3:A:1285:MAN:C1	2.36	1.01
2:A:1329:NAG:HO3	3:A:1330:MAN:C1	1.59	1.00
1:A:47:ASN:CG	2:A:1047:NAG:C1	2.30	0.98
2:A:1411:NAG:O3	2:A:1412:NAG:O5	1.78	0.98
2:A:1411:NAG:O3	2:A:1412:NAG:C2	2.11	0.97
3:A:1050:MAN:O4	4:A:1052:BMA:H2	1.63	0.97
1:A:351:PHE:O	1:A:403:LEU:HD12	1.64	0.97
1:A:328:ASN:HD22	2:A:1328:NAG:C1	1.73	0.96
1:A:269:ARG:O	1:A:271:VAL:HG23	1.66	0.96
1:A:435:ASN:HD21	2:A:1435:NAG:C1	1.75	0.96
3:A:1119:MAN:HO2	3:A:1120:MAN:C1	1.65	0.95
1:A:289:GLY:H	1:A:290:PRO:HD3	1.26	0.95
1:A:47:ASN:HD21	2:A:1047:NAG:C1	1.74	0.94
1:A:157:VAL:CG1	1:A:158:PRO:HD2	1.96	0.94
1:A:97:LEU:HD11	1:A:103:ALA:HB2	1.50	0.93
1:A:328:ASN:HD21	2:A:1328:NAG:C1	1.61	0.93
3:A:1118:MAN:HO2	3:A:1121:MAN:C1	1.80	0.92
1:A:157:VAL:HB	1:A:158:PRO:CD	2.01	0.91
2:A:1386:NAG:O6	7:A:1395:FUC:O5	1.89	0.90
3:A:1173:MAN:HO2	3:A:1174:MAN:C1	1.61	0.90
1:A:255:ILE:H	1:A:256:PRO:HD2	1.37	0.90
1:A:345:ASN:CG	2:A:1345:NAG:C1	2.41	0.90
3:A:1348:MAN:HO2	3:A:1351:MAN:C1	1.84	0.90
1:A:200:THR:HG22	1:A:201:GLU:H	1.36	0.90
2:A:1411:NAG:O3	2:A:1412:NAG:H2	1.71	0.89
1:A:324:TYR:CE2	1:A:423:LYS:HA	2.06	0.89
2:A:1278:NAG:C4	3:A:1279:MAN:C1	2.51	0.89
3:A:1049:MAN:C6	3:A:1050:MAN:C1	2.49	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:THR:HG23	1:A:263:SER:HB3	1.54	0.88
2:A:1166:NAG:HO4	2:A:1167:NAG:C1	1.83	0.88
3:A:1391:MAN:HO3	4:A:1394:BMA:C1	1.86	0.87
1:A:291:LYS:HE3	1:A:293:SER:HB3	1.57	0.87
3:A:1283:MAN:HO2	3:A:1284:MAN:C1	1.84	0.86
2:A:1047:NAG:C4	2:A:1048:NAG:C1	2.54	0.86
1:A:352:TRP:HE1	1:A:379:ILE:HD11	1.40	0.86
1:A:356:ASN:CG	2:A:1356:NAG:C1	2.44	0.85
1:A:134:ASP:HB3	1:A:138:THR:H	1.41	0.85
4:A:1168:BMA:C6	3:A:1169:MAN:C1	2.53	0.85
1:A:166:ASN:CG	2:A:1166:NAG:C1	2.45	0.85
3:A:1330:MAN:C3	3:A:1331:MAN:C1	2.54	0.85
2:A:1412:NAG:O4	3:A:1413:MAN:H2	1.75	0.85
3:A:1235:MAN:O3	6:A:1236:GAL:C2	2.26	0.84
1:A:173:VAL:HG12	1:A:304:VAL:HG23	1.60	0.84
1:A:18:LEU:HD12	1:A:19:THR:N	1.93	0.84
1:A:352:TRP:NE1	1:A:379:ILE:HD11	1.93	0.83
1:A:111:LEU:HD21	1:A:123:VAL:HG21	1.58	0.83
2:A:1356:NAG:HO6	7:A:1364:FUC:C1	1.89	0.83
2:A:1345:NAG:C4	2:A:1346:NAG:C1	2.56	0.83
1:A:253:THR:N	1:A:254:PRO:HD3	1.94	0.82
2:A:1411:NAG:H4	2:A:1412:NAG:O7	1.80	0.82
3:A:1089:MAN:O6	4:A:1090:BMA:C2	2.26	0.81
1:A:157:VAL:CB	1:A:158:PRO:CD	2.57	0.81
5:A:1114:NDG:C4	2:A:1115:NAG:C1	2.58	0.81
2:A:1229:NAG:C4	2:A:1230:NAG:C1	2.59	0.81
1:A:60:LYS:NZ	1:A:60:LYS:HB2	1.95	0.81
3:A:1089:MAN:O6	4:A:1090:BMA:O5	1.98	0.80
1:A:25:PHE:O	1:A:107:ARG:HA	1.80	0.80
1:A:166:ASN:ND2	2:A:1166:NAG:O5	2.15	0.79
1:A:318:ASN:HD22	2:A:1318:NAG:C1	1.93	0.79
1:A:277:ASN:CG	2:A:1277:NAG:C1	2.51	0.78
3:A:1173:MAN:C2	3:A:1174:MAN:C1	2.61	0.78
3:A:1330:MAN:O3	3:A:1331:MAN:C2	2.32	0.78
1:A:241:SER:OG	1:A:268:PRO:HA	1.84	0.78
1:A:277:ASN:HD21	2:A:1277:NAG:C1	1.97	0.77
3:A:1231:MAN:C6	3:A:1233:MAN:C1	2.62	0.77
1:A:164:ASN:HD22	1:A:165:CYS:H	1.32	0.76
4:A:1168:BMA:HO6	3:A:1169:MAN:C1	1.98	0.76
2:A:1392:NAG:C3	3:A:1390:MAN:C1	2.63	0.76
1:A:399:ALA:H	1:A:423:LYS:HE3	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1048:NAG:C4	3:A:1049:MAN:C1	2.64	0.76
2:A:1230:NAG:H4	3:A:1231:MAN:C1	2.15	0.76
1:A:255:ILE:H	1:A:256:PRO:CD	1.99	0.76
1:A:122:GLN:HG2	1:A:122:GLN:O	1.86	0.76
3:A:1089:MAN:C3	3:A:1092:MAN:C1	2.64	0.76
1:A:327:ASP:HB3	1:A:396:LEU:HD22	1.68	0.75
1:A:50:ILE:N	1:A:50:ILE:HD12	2.00	0.75
5:A:1357:NDG:C3	3:A:1358:MAN:C1	2.65	0.75
3:A:1234:MAN:HO2	3:A:1235:MAN:C1	1.96	0.75
3:A:1349:MAN:O6	4:A:1352:BMA:O5	1.94	0.75
1:A:348:VAL:CG1	1:A:389:PHE:CE2	2.64	0.75
3:A:1359:MAN:C2	2:A:1363:NAG:C1	2.65	0.74
1:A:348:VAL:HG11	1:A:389:PHE:CD2	2.23	0.74
1:A:289:GLY:N	1:A:290:PRO:HD3	2.01	0.74
1:A:73:LYS:HB3	1:A:76:TYR:CZ	2.22	0.74
2:A:1195:NAG:O3	2:A:1196:NAG:C2	2.36	0.73
3:A:1235:MAN:O4	6:A:1236:GAL:H2	1.88	0.73
1:A:176:ALA:O	1:A:177:GLN:HB2	1.88	0.73
1:A:269:ARG:O	1:A:270:PRO:C	2.25	0.73
1:A:297:TYR:HA	2:A:1166:NAG:O7	1.89	0.73
3:A:1283:MAN:C2	3:A:1284:MAN:C1	2.66	0.73
1:A:25:PHE:HZ	1:A:209:ILE:HD11	1.51	0.73
4:A:1280:BMA:C3	3:A:1281:MAN:C1	2.65	0.73
3:A:1360:MAN:C3	3:A:1362:MAN:C1	2.65	0.72
3:A:1050:MAN:O4	4:A:1052:BMA:C2	2.36	0.72
1:A:402:THR:HG23	1:A:420:ILE:HB	1.71	0.72
3:A:1391:MAN:C6	3:A:1393:MAN:C1	2.67	0.72
1:A:162:TRP:CE3	1:A:162:TRP:HA	2.23	0.72
1:A:195:ASN:OD1	2:A:1195:NAG:O5	2.05	0.72
1:A:277:ASN:O	1:A:278:ASN:HB2	1.87	0.71
5:A:1357:NDG:HB	3:A:1358:MAN:C1	1.99	0.71
2:A:1356:NAG:C4	5:A:1357:NDG:C1	2.68	0.71
2:A:1229:NAG:O4	2:A:1230:NAG:C2	2.38	0.71
1:A:224:GLY:O	1:A:225:ASP:HB2	1.90	0.71
3:A:1089:MAN:C6	4:A:1090:BMA:O5	2.39	0.71
1:A:289:GLY:H	1:A:290:PRO:CD	2.02	0.71
1:A:114:ASN:O	1:A:116:THR:N	2.23	0.71
1:A:25:PHE:CZ	1:A:209:ILE:HD11	2.25	0.70
1:A:39:CYS:HB2	1:A:351:PHE:HZ	1.57	0.70
2:A:1048:NAG:O4	3:A:1049:MAN:C2	2.39	0.70
1:A:201:GLU:HG2	1:A:203:LEU:HD22	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1328:NAG:C4	2:A:1329:NAG:C1	2.68	0.69
1:A:57:LYS:H	1:A:57:LYS:HD3	1.57	0.69
3:A:1089:MAN:O6	4:A:1090:BMA:O2	2.10	0.69
4:A:1168:BMA:C3	3:A:1171:MAN:C1	2.69	0.69
1:A:20:ARG:HG3	1:A:21:ASP:H	1.58	0.69
3:A:1348:MAN:O2	3:A:1351:MAN:C2	2.41	0.69
1:A:250:PRO:HB2	1:A:253:THR:HB	1.74	0.68
3:A:1231:MAN:O3	3:A:1232:MAN:O5	2.10	0.68
1:A:38:ALA:HB3	1:A:404:ILE:HD11	1.75	0.68
1:A:114:ASN:C	1:A:116:THR:H	1.95	0.68
1:A:337:THR:HG22	1:A:338:SER:N	2.08	0.68
3:A:1234:MAN:O2	3:A:1235:MAN:C2	2.42	0.67
1:A:87:ASN:HD21	2:A:1087:NAG:C1	2.03	0.67
1:A:348:VAL:HG11	1:A:389:PHE:HE2	1.50	0.67
1:A:60:LYS:HZ3	1:A:60:LYS:HB2	1.59	0.67
1:A:53:ASP:HB3	1:A:124:SER:HB2	1.75	0.67
1:A:116:THR:HG23	1:A:120:GLU:O	1.95	0.67
6:A:1286:GAL:O3	6:A:1287:GAL:O2	2.11	0.67
1:A:250:PRO:HG2	1:A:254:PRO:HG3	1.77	0.67
1:A:159:TYR:H	1:A:159:TYR:HD2	1.41	0.67
1:A:12:ILE:HG13	1:A:32:GLU:HG2	1.77	0.66
1:A:157:VAL:HG12	1:A:158:PRO:HD2	1.73	0.66
1:A:356:ASN:ND2	2:A:1356:NAG:C2	2.58	0.66
3:A:1388:MAN:O3	3:A:1389:MAN:O5	2.14	0.66
3:A:1049:MAN:HO3	3:A:1053:MAN:C1	2.07	0.66
3:A:1279:MAN:HO3	3:A:1283:MAN:C1	2.05	0.65
1:A:289:GLY:N	1:A:290:PRO:CD	2.57	0.65
3:A:1349:MAN:HO3	3:A:1350:MAN:C1	2.04	0.65
1:A:323:THR:HA	1:A:422:SER:OG	1.97	0.65
1:A:380:SER:HB3	1:A:392:THR:HB	1.78	0.65
1:A:25:PHE:O	1:A:106:MET:O	2.14	0.65
1:A:288:ASN:HB3	1:A:290:PRO:HD2	1.78	0.65
3:A:1284:MAN:H2	3:A:1285:MAN:O5	1.97	0.65
1:A:157:VAL:HG12	1:A:158:PRO:CD	2.27	0.65
1:A:204:GLY:HA3	1:A:279:SER:HB3	1.77	0.64
1:A:345:ASN:HB2	1:A:410:THR:HB	1.79	0.64
3:A:1284:MAN:H2	3:A:1285:MAN:C1	2.28	0.64
3:A:1279:MAN:O6	4:A:1280:BMA:O5	2.16	0.64
1:A:92:PHE:CE1	1:A:106:MET:HG3	2.33	0.64
1:A:12:ILE:HG13	1:A:32:GLU:CG	2.27	0.63
3:A:1089:MAN:O2	3:A:1092:MAN:H2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ASN:ND2	1:A:165:CYS:H	1.97	0.63
1:A:345:ASN:OD1	2:A:1345:NAG:C1	2.47	0.62
1:A:317:THR:HG21	1:A:418:LYS:HD3	1.81	0.62
1:A:280:ILE:HD12	1:A:282:TYR:OH	1.99	0.62
3:A:1347:MAN:HO6	3:A:1349:MAN:C1	2.07	0.62
1:A:391:ILE:HD12	1:A:405:ILE:HD13	1.81	0.62
1:A:373:PRO:HG2	1:A:376:CYS:CB	2.29	0.62
1:A:9:GLN:CB	2:A:1345:NAG:H83	2.28	0.62
2:A:1115:NAG:O4	3:A:1116:MAN:C2	2.45	0.62
1:A:252:ALA:C	1:A:254:PRO:HD3	2.19	0.62
3:A:1116:MAN:C6	3:A:1117:MAN:C1	2.75	0.62
1:A:164:ASN:HD22	1:A:165:CYS:N	1.97	0.62
1:A:352:TRP:CZ3	1:A:401:LYS:HB3	2.33	0.62
1:A:166:ASN:OD1	2:A:1166:NAG:C1	2.48	0.61
1:A:435:ASN:CG	2:A:1435:NAG:C1	2.69	0.61
1:A:8:CYS:HA	1:A:139:MET:HB3	1.81	0.61
1:A:9:GLN:H	1:A:9:GLN:CD	2.02	0.61
1:A:18:LEU:HD12	1:A:19:THR:H	1.64	0.61
3:A:1089:MAN:H61	4:A:1090:BMA:O5	1.99	0.61
1:A:39:CYS:HB2	1:A:351:PHE:CZ	2.36	0.60
1:A:200:THR:HG21	1:A:281:LEU:HD11	1.81	0.60
6:A:1236:GAL:O3	6:A:1237:GAL:O5	2.19	0.60
1:A:29:GLU:HA	1:A:103:ALA:HA	1.82	0.60
1:A:273:ARG:HA	1:A:305:PHE:CD2	2.37	0.60
1:A:251:VAL:HG23	1:A:252:ALA:H	1.65	0.60
6:A:1203:GAL:O3	6:A:1204:GAL:O5	2.19	0.60
1:A:348:VAL:CG2	1:A:389:PHE:CD2	2.77	0.60
1:A:411:ASN:O	1:A:412:ALA:HB3	2.01	0.60
1:A:253:THR:O	1:A:253:THR:HG22	2.01	0.59
1:A:57:LYS:N	1:A:57:LYS:HD3	2.17	0.59
1:A:351:PHE:HB3	1:A:404:ILE:HB	1.84	0.59
1:A:31:LEU:O	1:A:32:GLU:HB2	2.03	0.59
3:A:1284:MAN:C2	3:A:1285:MAN:O5	2.50	0.59
1:A:200:THR:HG22	1:A:201:GLU:N	2.15	0.59
1:A:202:MET:HG2	1:A:209:ILE:HB	1.84	0.59
1:A:411:ASN:OD1	2:A:1411:NAG:O5	2.21	0.58
1:A:25:PHE:HZ	1:A:209:ILE:CD1	2.17	0.58
1:A:12:ILE:HD11	1:A:412:ALA:CB	2.34	0.58
1:A:46:VAL:HG21	1:A:68:LEU:HD11	1.85	0.58
1:A:348:VAL:HG21	1:A:389:PHE:CD1	2.37	0.58
1:A:205:ASN:C	1:A:207:ILE:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ALA:O	1:A:303:ILE:HA	2.04	0.57
1:A:211:CYS:HA	1:A:232:CYS:HA	1.85	0.57
1:A:194:SER:HB3	1:A:221:VAL:HG21	1.86	0.57
3:A:1117:MAN:O5	3:A:1118:MAN:H5	2.04	0.57
1:A:269:ARG:O	1:A:271:VAL:N	2.37	0.57
1:A:273:ARG:HA	1:A:305:PHE:CE2	2.40	0.57
3:A:1235:MAN:C3	6:A:1236:GAL:C1	2.76	0.57
1:A:175:ARG:HH11	1:A:175:ARG:HG3	1.68	0.57
1:A:116:THR:HG23	1:A:120:GLU:HG3	1.85	0.57
1:A:356:ASN:HD21	2:A:1356:NAG:C2	2.15	0.56
1:A:420:ILE:O	1:A:420:ILE:HG23	2.04	0.56
1:A:44:ALA:HB3	1:A:68:LEU:HB2	1.87	0.56
1:A:192:GLN:O	1:A:194:SER:N	2.37	0.56
1:A:347:THR:O	1:A:347:THR:HG22	2.03	0.56
1:A:336:VAL:CB	1:A:407:ARG:HH21	2.19	0.56
1:A:77:GLN:NE2	1:A:90:ASN:HB2	2.20	0.56
3:A:1197:MAN:O3	3:A:1198:MAN:O5	2.23	0.56
4:A:1168:BMA:O3	3:A:1171:MAN:O5	2.24	0.56
1:A:166:ASN:HD21	2:A:1166:NAG:C2	2.02	0.56
1:A:12:ILE:HD11	1:A:412:ALA:HB3	1.87	0.56
1:A:221:VAL:O	1:A:222:LEU:O	2.22	0.56
3:A:1049:MAN:H62	3:A:1050:MAN:C1	2.34	0.55
1:A:96:LEU:HD23	1:A:102:LEU:CD2	2.37	0.55
1:A:267:THR:HG22	1:A:267:THR:O	2.06	0.55
1:A:9:GLN:HB2	2:A:1345:NAG:H83	1.87	0.55
1:A:47:ASN:OD1	2:A:1047:NAG:C1	2.54	0.55
1:A:26:PHE:HA	1:A:235:TYR:CE1	2.41	0.55
1:A:111:LEU:CD2	1:A:123:VAL:HG21	2.32	0.55
1:A:248:THR:HG22	1:A:248:THR:O	2.07	0.55
3:A:1391:MAN:O6	3:A:1393:MAN:O5	2.25	0.55
2:A:1392:NAG:H3	3:A:1390:MAN:H2	1.89	0.55
1:A:92:PHE:CZ	1:A:106:MET:HG3	2.41	0.55
1:A:52:PHE:CG	1:A:113:ILE:HD11	2.42	0.55
2:A:1115:NAG:C4	3:A:1116:MAN:C1	2.78	0.54
1:A:201:GLU:CG	1:A:203:LEU:HD22	2.35	0.54
1:A:107:ARG:HH22	1:A:206:GLU:CB	2.20	0.54
1:A:191:ALA:HB2	1:A:260:TYR:CZ	2.42	0.54
3:A:1050:MAN:C6	3:A:1051:MAN:C1	2.80	0.54
1:A:37:PRO:HA	1:A:314:ASP:HB3	1.88	0.54
1:A:377:GLU:O	1:A:379:ILE:HD12	2.08	0.54
1:A:37:PRO:HD3	1:A:315:MET:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASN:ND2	2:A:1345:NAG:O5	2.14	0.54
3:A:1359:MAN:O2	2:A:1363:NAG:O5	2.24	0.54
1:A:269:ARG:CB	1:A:270:PRO:HD2	2.37	0.54
1:A:336:VAL:CG2	1:A:409:ALA:HB2	2.37	0.54
1:A:52:PHE:HE2	1:A:152:LEU:HD11	1.72	0.54
2:A:1088:NAG:C4	3:A:1089:MAN:C1	2.82	0.54
1:A:352:TRP:HZ3	1:A:401:LYS:HB3	1.71	0.54
1:A:96:LEU:HD23	1:A:102:LEU:HD21	1.90	0.54
1:A:336:VAL:HB	1:A:407:ARG:HH21	1.72	0.54
1:A:336:VAL:O	1:A:337:THR:HB	2.08	0.54
1:A:367:THR:HG22	1:A:368:LEU:N	2.22	0.54
1:A:255:ILE:N	1:A:256:PRO:CD	2.69	0.53
2:A:1318:NAG:H4	2:A:1319:NAG:C7	2.39	0.53
2:A:1386:NAG:C6	7:A:1395:FUC:C1	2.79	0.53
1:A:204:GLY:HA3	1:A:279:SER:CB	2.39	0.53
1:A:191:ALA:O	1:A:192:GLN:HB2	2.09	0.53
1:A:386:ASN:ND2	2:A:1386:NAG:C2	2.66	0.53
1:A:291:LYS:HE3	1:A:293:SER:CB	2.34	0.53
1:A:185:LEU:HD23	1:A:185:LEU:N	2.24	0.53
1:A:54:VAL:HG12	1:A:120:GLU:HB2	1.89	0.53
1:A:116:THR:CG2	1:A:120:GLU:O	2.58	0.52
1:A:43:THR:O	1:A:135:VAL:HG22	2.09	0.52
3:A:1089:MAN:O2	3:A:1092:MAN:C2	2.58	0.52
1:A:346:VAL:H	1:A:368:LEU:HD23	1.75	0.52
2:A:1328:NAG:O4	2:A:1329:NAG:C2	2.53	0.52
1:A:373:PRO:HG2	1:A:376:CYS:HB3	1.91	0.52
1:A:20:ARG:HG3	1:A:21:ASP:N	2.24	0.52
1:A:185:LEU:HD12	1:A:285:TYR:CD1	2.45	0.52
1:A:109:LYS:N	1:A:109:LYS:HD2	2.24	0.52
1:A:399:ALA:H	1:A:423:LYS:CE	2.22	0.52
1:A:114:ASN:C	1:A:116:THR:N	2.62	0.52
1:A:79:ARG:O	1:A:79:ARG:HG3	2.09	0.52
1:A:269:ARG:CB	1:A:270:PRO:CD	2.87	0.51
1:A:420:ILE:O	1:A:420:ILE:HD13	2.10	0.51
1:A:336:VAL:HG22	1:A:409:ALA:HB2	1.91	0.51
1:A:337:THR:HG22	1:A:338:SER:H	1.74	0.51
1:A:336:VAL:H	1:A:407:ARG:NH2	2.09	0.51
1:A:225:ASP:OD1	1:A:246:THR:HB	2.11	0.51
3:A:1347:MAN:C3	3:A:1348:MAN:C1	2.82	0.51
1:A:373:PRO:HG2	1:A:376:CYS:HB2	1.92	0.51
1:A:8:CYS:HB3	1:A:139:MET:CG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:VAL:HG12	1:A:347:THR:N	2.26	0.51
1:A:331:TYR:CG	1:A:419:VAL:HG11	2.46	0.51
3:A:1349:MAN:HO6	4:A:1352:BMA:C1	1.87	0.51
1:A:9:GLN:HB3	2:A:1345:NAG:H83	1.92	0.51
1:A:93:LEU:HD22	1:A:274:PHE:CE2	2.46	0.51
1:A:19:THR:HG22	1:A:234:GLY:O	2.11	0.50
1:A:362:PHE:N	1:A:362:PHE:CD1	2.79	0.50
1:A:351:PHE:H	1:A:403:LEU:HD11	1.75	0.50
3:A:1118:MAN:O2	3:A:1121:MAN:C2	2.52	0.50
1:A:401:LYS:HG2	1:A:423:LYS:HZ3	1.77	0.50
1:A:399:ALA:N	1:A:423:LYS:HE3	2.23	0.50
1:A:337:THR:CG2	1:A:338:SER:H	2.24	0.50
2:A:1166:NAG:C4	2:A:1167:NAG:C1	2.82	0.50
3:A:1283:MAN:O2	3:A:1284:MAN:O5	2.28	0.50
2:A:1048:NAG:C4	3:A:1049:MAN:H2	2.41	0.50
1:A:386:ASN:HD22	2:A:1386:NAG:C1	2.08	0.50
1:A:286:SER:HB3	1:A:288:ASN:ND2	2.26	0.50
1:A:99:ALA:HA	1:A:312:SER:O	2.12	0.50
1:A:162:TRP:HE3	1:A:162:TRP:HA	1.72	0.50
6:A:1286:GAL:C3	6:A:1287:GAL:C1	2.81	0.49
1:A:73:LYS:HB3	1:A:76:TYR:OH	2.11	0.49
3:A:1330:MAN:O3	3:A:1331:MAN:H2	2.09	0.49
1:A:86:GLU:O	1:A:87:ASN:HB2	2.12	0.49
1:A:346:VAL:HB	1:A:368:LEU:CD2	2.43	0.49
3:A:1173:MAN:C1	3:A:1174:MAN:C1	2.90	0.49
1:A:376:CYS:SG	1:A:379:ILE:HB	2.52	0.49
1:A:107:ARG:HH22	1:A:206:GLU:HB2	1.77	0.49
1:A:283:VAL:HB	1:A:299:ILE:HG22	1.94	0.49
1:A:50:ILE:N	1:A:50:ILE:CD1	2.70	0.49
1:A:94:LEU:HD11	1:A:102:LEU:HD13	1.95	0.49
3:A:1347:MAN:C6	3:A:1349:MAN:C1	2.85	0.49
1:A:324:TYR:CE2	1:A:423:LYS:CA	2.88	0.49
1:A:197:SER:OG	1:A:292:ALA:HB1	2.12	0.49
1:A:86:GLU:C	1:A:88:ALA:N	2.64	0.49
1:A:176:ALA:O	1:A:177:GLN:CB	2.57	0.49
1:A:336:VAL:HG12	1:A:407:ARG:HH21	1.78	0.49
2:A:1345:NAG:O4	2:A:1346:NAG:O5	2.26	0.49
1:A:156:THR:HA	1:A:206:GLU:OE2	2.13	0.49
3:A:1349:MAN:O3	3:A:1350:MAN:O5	2.28	0.48
1:A:146:MET:HE1	1:A:235:TYR:CE2	2.48	0.48
1:A:155:GLU:HB3	1:A:157:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:HD12	1:A:285:TYR:CE1	2.48	0.48
1:A:32:GLU:OE1	1:A:32:GLU:HA	2.12	0.48
1:A:336:VAL:CG1	1:A:407:ARG:HH21	2.26	0.48
1:A:250:PRO:CB	1:A:253:THR:HB	2.43	0.48
1:A:188:PRO:HA	3:A:1171:MAN:O6	2.14	0.48
2:A:1048:NAG:H4	3:A:1049:MAN:H2	1.95	0.48
1:A:8:CYS:HB3	1:A:139:MET:HG3	1.95	0.48
2:A:1167:NAG:O4	4:A:1168:BMA:O5	2.30	0.47
2:A:1319:NAG:O3	3:A:1320:MAN:O5	2.28	0.47
1:A:269:ARG:HB3	1:A:270:PRO:CD	2.44	0.47
1:A:18:LEU:HD12	1:A:18:LEU:C	2.35	0.47
1:A:207:ILE:HB	1:A:275:LEU:HD12	1.96	0.47
1:A:309:ILE:HG22	1:A:310:PRO:O	2.13	0.47
2:A:1048:NAG:C4	3:A:1049:MAN:C2	2.92	0.47
1:A:239:VAL:HB	1:A:269:ARG:HD2	1.96	0.47
1:A:74:ALA:HB2	1:A:309:ILE:HG13	1.96	0.47
1:A:111:LEU:HD21	1:A:123:VAL:CG2	2.38	0.47
1:A:328:ASN:O	1:A:328:ASN:OD1	2.33	0.47
1:A:120:GLU:HA	1:A:122:GLN:OE1	2.14	0.47
1:A:191:ALA:HB2	1:A:260:TYR:OH	2.15	0.47
1:A:22:ASP:HB2	1:A:23:PRO:CD	2.45	0.47
1:A:212:ILE:HG12	1:A:213:MET:O	2.15	0.46
1:A:47:ASN:ND2	2:A:1047:NAG:C2	2.73	0.46
1:A:351:PHE:H	1:A:403:LEU:CD1	2.29	0.46
1:A:241:SER:HB2	1:A:269:ARG:N	2.30	0.46
1:A:23:PRO:HB3	1:A:209:ILE:HA	1.98	0.46
1:A:38:ALA:HB3	1:A:404:ILE:CD1	2.41	0.46
3:A:1050:MAN:H4	3:A:1051:MAN:H3	1.97	0.46
1:A:174:VAL:HG13	1:A:179:LEU:HB2	1.96	0.46
1:A:188:PRO:CA	3:A:1171:MAN:O6	2.63	0.46
1:A:399:ALA:HA	1:A:400:PRO:HD2	1.57	0.46
1:A:364:CYS:SG	1:A:379:ILE:HD13	2.56	0.46
1:A:159:TYR:CD2	1:A:159:TYR:N	2.84	0.46
1:A:317:THR:HG21	1:A:418:LYS:CD	2.46	0.46
1:A:94:LEU:HD21	1:A:102:LEU:CD2	2.46	0.46
1:A:269:ARG:HB2	1:A:270:PRO:HD2	1.97	0.46
1:A:91:LEU:HD21	1:A:110:LYS:HB3	1.98	0.46
3:A:1358:MAN:HO3	3:A:1359:MAN:C1	2.16	0.46
1:A:348:VAL:CB	1:A:389:PHE:CE2	2.99	0.46
3:A:1232:MAN:C2	3:A:1234:MAN:C1	2.83	0.45
1:A:23:PRO:HB3	1:A:208:ASP:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:THR:HG22	1:A:368:LEU:H	1.81	0.45
1:A:220:GLN:O	1:A:220:GLN:HG3	2.16	0.45
2:A:1230:NAG:C4	3:A:1231:MAN:O5	2.64	0.45
1:A:371:GLY:O	1:A:372:THR:HB	2.16	0.45
1:A:200:THR:O	1:A:201:GLU:HB2	2.17	0.45
1:A:25:PHE:HB3	1:A:105:THR:CG2	2.46	0.45
1:A:183:LEU:CD1	1:A:283:VAL:HG21	2.46	0.45
1:A:169:ASN:O	1:A:170:ILE:HG13	2.16	0.45
1:A:188:PRO:CB	3:A:1171:MAN:O6	2.64	0.45
1:A:23:PRO:CD	1:A:24:GLY:H	2.25	0.45
1:A:319:THR:HG22	1:A:418:LYS:CG	2.46	0.45
1:A:115:ILE:O	1:A:115:ILE:HG22	2.16	0.45
1:A:154:PRO:O	1:A:155:GLU:HG3	2.16	0.45
1:A:309:ILE:HD12	1:A:309:ILE:H	1.82	0.45
1:A:9:GLN:O	1:A:10:TYR:HB2	2.17	0.45
1:A:399:ALA:C	1:A:423:LYS:HE2	2.37	0.45
1:A:94:LEU:HD21	1:A:102:LEU:HD22	1.98	0.45
1:A:12:ILE:HG13	1:A:32:GLU:HG3	1.99	0.45
1:A:111:LEU:HA	1:A:112:PRO:HD3	1.85	0.45
1:A:23:PRO:CD	1:A:24:GLY:N	2.75	0.45
1:A:363:LYS:HG2	1:A:375:GLY:HA3	1.98	0.45
1:A:21:ASP:N	1:A:21:ASP:OD1	2.50	0.45
1:A:165:CYS:SG	1:A:298:CYS:C	2.95	0.44
3:A:1117:MAN:O6	3:A:1118:MAN:O5	2.31	0.44
1:A:52:PHE:CD1	1:A:113:ILE:HD11	2.52	0.44
1:A:122:GLN:O	1:A:122:GLN:CG	2.63	0.44
1:A:143:HIS:CE1	1:A:145:GLU:HB2	2.52	0.44
3:A:1283:MAN:C2	3:A:1284:MAN:O5	2.65	0.44
3:A:1360:MAN:O3	3:A:1362:MAN:O5	2.20	0.44
2:A:1230:NAG:H4	3:A:1231:MAN:O5	2.17	0.44
1:A:411:ASN:O	1:A:412:ALA:CB	2.65	0.44
1:A:25:PHE:O	1:A:26:PHE:HB3	2.18	0.44
1:A:172:ALA:HA	1:A:181:VAL:HG13	1.99	0.44
1:A:41:VAL:O	1:A:41:VAL:HG12	2.18	0.44
1:A:16:ILE:HG22	1:A:17:GLN:N	2.32	0.44
1:A:253:THR:N	1:A:254:PRO:CD	2.74	0.44
1:A:336:VAL:CG2	1:A:409:ALA:CB	2.95	0.44
1:A:23:PRO:HD2	1:A:24:GLY:N	2.33	0.44
1:A:383:PHE:CD1	1:A:389:PHE:HD1	2.36	0.43
1:A:73:LYS:HD3	1:A:76:TYR:CE2	2.53	0.43
1:A:311:ALA:O	1:A:313:GLN:N	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ALA:HA	1:A:425:PRO:HD2	1.81	0.43
3:A:1391:MAN:H4	3:A:1393:MAN:C1	2.48	0.43
1:A:75:VAL:C	1:A:76:TYR:CD1	2.91	0.43
1:A:336:VAL:HB	1:A:407:ARG:HE	1.83	0.43
1:A:186:SER:HA	1:A:260:TYR:O	2.18	0.43
2:A:1392:NAG:C3	3:A:1390:MAN:C2	2.96	0.43
1:A:256:PRO:O	1:A:258:THR:N	2.52	0.43
1:A:336:VAL:N	1:A:407:ARG:NH2	2.67	0.43
1:A:157:VAL:HB	1:A:158:PRO:CG	2.49	0.43
1:A:17:GLN:HG2	1:A:18:LEU:N	2.34	0.43
1:A:322:ILE:HG22	1:A:323:THR:N	2.34	0.43
1:A:121:GLN:O	1:A:121:GLN:HG2	2.18	0.43
1:A:203:LEU:HD12	1:A:203:LEU:O	2.19	0.43
1:A:116:THR:HG23	1:A:120:GLU:CG	2.48	0.43
1:A:336:VAL:CG2	1:A:409:ALA:HA	2.49	0.43
3:A:1050:MAN:O6	3:A:1051:MAN:C2	2.61	0.42
1:A:25:PHE:HB3	1:A:105:THR:HG23	2.01	0.42
1:A:30:ILE:HG23	1:A:142:HIS:CD2	2.54	0.42
1:A:254:PRO:O	1:A:254:PRO:HD2	2.19	0.42
1:A:160:ILE:HG13	1:A:161:LYS:O	2.19	0.42
1:A:92:PHE:CD2	1:A:106:MET:HB2	2.54	0.42
1:A:148:ASN:O	1:A:149:PRO:C	2.56	0.42
1:A:40:ASN:ND2	1:A:71:HIS:CD2	2.86	0.42
3:A:1359:MAN:O3	2:A:1363:NAG:H5	2.19	0.42
3:A:1050:MAN:C4	3:A:1051:MAN:H3	2.50	0.42
1:A:331:TYR:CD2	1:A:419:VAL:HG11	2.55	0.42
1:A:206:GLU:O	1:A:207:ILE:HD13	2.20	0.42
1:A:75:VAL:HG12	1:A:76:TYR:N	2.34	0.42
3:A:1279:MAN:O6	4:A:1280:BMA:C2	2.60	0.42
1:A:241:SER:CB	1:A:268:PRO:HA	2.49	0.42
1:A:396:LEU:O	1:A:396:LEU:HD12	2.19	0.42
1:A:46:VAL:HG23	1:A:68:LEU:HG	2.02	0.42
2:A:1328:NAG:C3	2:A:1329:NAG:C1	2.97	0.42
1:A:203:LEU:HA	1:A:203:LEU:HD13	1.75	0.42
1:A:23:PRO:HB3	1:A:209:ILE:CA	2.50	0.41
1:A:193:ASP:OD2	2:A:1196:NAG:C6	2.68	0.41
1:A:288:ASN:HB3	1:A:290:PRO:CD	2.48	0.41
1:A:173:VAL:HG12	1:A:304:VAL:CG2	2.41	0.41
1:A:185:LEU:HD23	1:A:185:LEU:H	1.84	0.41
1:A:317:THR:CG2	1:A:418:LYS:CB	2.98	0.41
1:A:351:PHE:HB2	1:A:404:ILE:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:THR:HA	1:A:264:LEU:O	2.21	0.41
4:A:1280:BMA:O4	3:A:1281:MAN:H2	2.21	0.41
1:A:107:ARG:HH22	1:A:206:GLU:HB3	1.84	0.41
2:A:1392:NAG:C3	3:A:1390:MAN:H2	2.50	0.41
2:A:1411:NAG:C4	2:A:1412:NAG:H2	2.51	0.41
1:A:290:PRO:HD3	2:A:1195:NAG:O7	2.19	0.41
1:A:46:VAL:HG21	1:A:68:LEU:CD1	2.51	0.41
1:A:221:VAL:O	1:A:222:LEU:C	2.59	0.41
1:A:187:LEU:HD21	1:A:285:TYR:HD1	1.85	0.41
1:A:129:ASP:HB3	1:A:131:TYR:CE1	2.55	0.41
1:A:157:VAL:O	1:A:158:PRO:C	2.59	0.41
1:A:200:THR:CG2	1:A:281:LEU:HD11	2.48	0.41
1:A:52:PHE:CE2	1:A:152:LEU:HD11	2.54	0.41
1:A:108:SER:OG	1:A:109:LYS:HD2	2.21	0.41
1:A:12:ILE:HB	1:A:142:HIS:CD2	2.56	0.40
1:A:217:GLU:OE2	1:A:289:GLY:HA2	2.20	0.40
1:A:235:TYR:N	1:A:235:TYR:CD1	2.89	0.40
1:A:50:ILE:HD12	1:A:50:ILE:H	1.81	0.40
1:A:354:TRP:N	1:A:355:PRO:HD3	2.36	0.40
3:A:1347:MAN:O3	3:A:1348:MAN:O5	2.33	0.40
1:A:205:ASN:C	1:A:207:ILE:N	2.74	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	438/470 (93%)	327 (75%)	70 (16%)	41 (9%)	1 10

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	CYS
1	A	32	GLU
1	A	85	SER
1	A	115	ILE
1	A	158	PRO
1	A	165	CYS
1	A	201	GLU
1	A	205	ASN
1	A	254	PRO
1	A	255	ILE
1	A	257	GLY
1	A	269	ARG
1	A	270	PRO
1	A	312	SER
1	A	374	SER
1	A	42	CYS
1	A	98	GLY
1	A	110	LYS
1	A	164	ASN
1	A	193	ASP
1	A	221	VAL
1	A	259	GLY
1	A	296	ASP
1	A	326	GLY
1	A	400	PRO
1	A	434	LEU
1	A	222	LEU
1	A	225	ASP
1	A	253	THR
1	A	353	ALA
1	A	423	LYS
1	A	26	PHE
1	A	192	GLN
1	A	335	MET
1	A	339	GLU
1	A	157	VAL
1	A	328	ASN
1	A	372	THR
1	A	276	GLY
1	A	170	ILE
1	A	424	ALA

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	362/404 (90%)	315 (87%)	47 (13%)	5 27

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	15	LEU
1	A	17	GLN
1	A	21	ASP
1	A	25	PHE
1	A	32	GLU
1	A	47	ASN
1	A	54	VAL
1	A	60	LYS
1	A	67	LEU
1	A	85	SER
1	A	109	LYS
1	A	121	GLN
1	A	125	LEU
1	A	138	THR
1	A	157	VAL
1	A	159	TYR
1	A	162	TRP
1	A	163	ASP
1	A	164	ASN
1	A	165	CYS
1	A	174	VAL
1	A	175	ARG
1	A	181	VAL
1	A	193	ASP
1	A	198	VAL
1	A	202	MET
1	A	203	LEU
1	A	205	ASN
1	A	215	ASP

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Mol	Chain	Res	Type
1	A	227	LYS
1	A	241	SER
1	A	246	THR
1	A	269	ARG
1	A	277	ASN
1	A	280	ILE
1	A	297	TYR
1	A	303	ILE
1	A	304	VAL
1	A	321	ASP
1	A	336	VAL
1	A	351	PHE
1	A	363	LYS
1	A	369	THR
1	A	408	THR
1	A	415	THR
1	A	420	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	47	ASN
1	A	77	GLN
1	A	87	ASN
1	A	143	HIS
1	A	164	ASN
1	A	166	ASN
1	A	177	GLN
1	A	277	ASN
1	A	278	ASN
1	A	318	ASN
1	A	328	ASN
1	A	345	ASN
1	A	356	ASN
1	A	378	ASN
1	A	386	ASN
1	A	435	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

101 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	$\#\|Z\| > 2$
2	NAG	A	1047	-	14,14,15	1.56	4 (28%)	15,19,21	1.39	2 (13%)
2	NAG	A	1048	-	14,14,15	1.14	2 (14%)	15,19,21	1.95	5 (33%)
3	MAN	A	1049	-	11,11,12	1.35	1 (9%)	14,15,17	1.10	1 (7%)
3	MAN	A	1050	-	11,11,12	1.53	2 (18%)	14,15,17	1.48	5 (35%)
3	MAN	A	1051	-	11,11,12	1.16	0	14,15,17	1.53	3 (21%)
4	BMA	A	1052	-	11,11,12	1.18	2 (18%)	14,15,17	1.65	3 (21%)
3	MAN	A	1053	-	11,11,12	1.31	1 (9%)	14,15,17	1.52	2 (14%)
2	NAG	A	1087	-	14,14,15	1.02	1 (7%)	15,19,21	0.80	1 (6%)
2	NAG	A	1088	-	14,14,15	0.94	1 (7%)	15,19,21	0.81	1 (6%)
3	MAN	A	1089	-	11,11,12	1.26	2 (18%)	14,15,17	1.16	1 (7%)
4	BMA	A	1090	-	11,11,12	1.66	3 (27%)	14,15,17	1.66	4 (28%)
3	MAN	A	1091	-	11,11,12	0.91	1 (9%)	14,15,17	1.34	2 (14%)
3	MAN	A	1092	-	11,11,12	1.38	2 (18%)	14,15,17	1.53	1 (7%)
3	MAN	A	1093	-	11,11,12	1.24	1 (9%)	14,15,17	1.70	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NDG	A	1114	-	14,14,15	1.52	1 (7%)	15,19,21	1.38	3 (20%)
2	NAG	A	1115	-	14,14,15	0.90	0	15,19,21	1.28	1 (6%)
3	MAN	A	1116	-	11,11,12	1.52	2 (18%)	14,15,17	1.28	2 (14%)
3	MAN	A	1117	-	11,11,12	1.24	2 (18%)	14,15,17	1.76	5 (35%)
3	MAN	A	1118	-	11,11,12	1.25	2 (18%)	14,15,17	0.96	1 (7%)
3	MAN	A	1119	-	11,11,12	1.28	2 (18%)	14,15,17	1.56	1 (7%)
3	MAN	A	1120	-	11,11,12	1.32	1 (9%)	14,15,17	1.54	2 (14%)
3	MAN	A	1121	-	11,11,12	0.97	0	14,15,17	1.23	1 (7%)
2	NAG	A	1166	-	14,14,15	1.01	2 (14%)	15,19,21	0.85	1 (6%)
2	NAG	A	1167	-	14,14,15	1.05	1 (7%)	15,19,21	0.83	1 (6%)
4	BMA	A	1168	-	11,11,12	1.73	3 (27%)	14,15,17	2.45	6 (42%)
3	MAN	A	1169	-	11,11,12	1.94	4 (36%)	14,15,17	2.36	6 (42%)
3	MAN	A	1170	-	11,11,12	1.04	1 (9%)	14,15,17	1.28	2 (14%)
3	MAN	A	1171	-	11,11,12	1.57	3 (27%)	14,15,17	1.07	1 (7%)
3	MAN	A	1172	-	11,11,12	0.90	0	14,15,17	1.87	5 (35%)
3	MAN	A	1173	-	11,11,12	1.14	1 (9%)	14,15,17	1.25	2 (14%)
3	MAN	A	1174	-	11,11,12	1.17	1 (9%)	14,15,17	1.51	1 (7%)
2	NAG	A	1195	1	14,14,15	2.57	4 (28%)	15,19,21	2.17	3 (20%)
2	NAG	A	1196	-	14,14,15	1.03	0	15,19,21	1.45	4 (26%)
3	MAN	A	1197	-	11,11,12	2.91	5 (45%)	14,15,17	2.40	6 (42%)
3	MAN	A	1198	-	11,11,12	1.78	4 (36%)	14,15,17	1.02	0
3	MAN	A	1199	-	11,11,12	1.79	3 (27%)	14,15,17	2.37	5 (35%)
3	MAN	A	1200	-	11,11,12	1.31	3 (27%)	14,15,17	0.96	1 (7%)
3	MAN	A	1201	-	11,11,12	1.26	2 (18%)	14,15,17	1.37	2 (14%)
3	MAN	A	1202	-	11,11,12	0.96	1 (9%)	14,15,17	1.44	1 (7%)
6	GAL	A	1203	-	11,11,12	1.17	2 (18%)	14,15,17	1.03	1 (7%)
6	GAL	A	1204	-	11,11,12	0.31	0	14,15,17	0.92	2 (14%)
2	NAG	A	1229	-	14,14,15	1.01	1 (7%)	15,19,21	1.08	1 (6%)
2	NAG	A	1230	-	14,14,15	1.11	1 (7%)	15,19,21	1.87	4 (26%)
3	MAN	A	1231	-	11,11,12	1.38	1 (9%)	14,15,17	3.02	7 (50%)
3	MAN	A	1232	-	11,11,12	1.22	1 (9%)	14,15,17	1.10	0
3	MAN	A	1233	-	11,11,12	0.83	0	14,15,17	1.62	2 (14%)
3	MAN	A	1234	-	11,11,12	1.43	3 (27%)	14,15,17	1.10	1 (7%)
3	MAN	A	1235	-	11,11,12	1.07	1 (9%)	14,15,17	1.44	2 (14%)
6	GAL	A	1236	-	11,11,12	1.14	1 (9%)	14,15,17	1.15	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GAL	A	1237	-	11,11,12	0.36	0	14,15,17	0.92	2 (14%)
2	NAG	A	1277	-	14,14,15	0.95	1 (7%)	15,19,21	1.42	2 (13%)
2	NAG	A	1278	-	14,14,15	0.95	1 (7%)	15,19,21	1.54	1 (6%)
3	MAN	A	1279	-	11,11,12	1.33	2 (18%)	14,15,17	1.00	1 (7%)
4	BMA	A	1280	-	11,11,12	1.48	1 (9%)	14,15,17	1.94	4 (28%)
3	MAN	A	1281	-	11,11,12	1.00	1 (9%)	14,15,17	1.55	2 (14%)
3	MAN	A	1282	-	11,11,12	1.12	2 (18%)	14,15,17	1.52	3 (21%)
3	MAN	A	1283	-	11,11,12	1.39	1 (9%)	14,15,17	1.40	3 (21%)
3	MAN	A	1284	-	11,11,12	1.21	2 (18%)	14,15,17	1.42	2 (14%)
3	MAN	A	1285	-	11,11,12	1.35	3 (27%)	14,15,17	1.79	2 (14%)
6	GAL	A	1286	-	11,11,12	1.10	1 (9%)	14,15,17	1.34	3 (21%)
6	GAL	A	1287	-	11,11,12	1.13	2 (18%)	14,15,17	0.87	0
2	NAG	A	1318	-	14,14,15	2.46	4 (28%)	15,19,21	1.64	2 (13%)
2	NAG	A	1319	-	14,14,15	1.62	3 (21%)	15,19,21	1.97	5 (33%)
3	MAN	A	1320	-	11,11,12	1.55	3 (27%)	14,15,17	2.07	2 (14%)
2	NAG	A	1328	-	14,14,15	1.24	3 (21%)	15,19,21	1.61	3 (20%)
2	NAG	A	1329	-	14,14,15	1.44	2 (14%)	15,19,21	1.32	4 (26%)
3	MAN	A	1330	-	11,11,12	1.78	3 (27%)	14,15,17	2.12	1 (7%)
3	MAN	A	1331	-	11,11,12	0.99	1 (9%)	14,15,17	1.61	1 (7%)
3	MAN	A	1332	-	11,11,12	0.95	0	14,15,17	0.85	1 (7%)
2	NAG	A	1345	-	14,14,15	1.49	3 (21%)	15,19,21	1.37	3 (20%)
2	NAG	A	1346	-	14,14,15	2.01	1 (7%)	15,19,21	2.13	5 (33%)
3	MAN	A	1347	-	11,11,12	1.58	2 (18%)	14,15,17	2.78	8 (57%)
3	MAN	A	1348	-	11,11,12	1.02	1 (9%)	14,15,17	1.10	2 (14%)
3	MAN	A	1349	-	11,11,12	1.47	2 (18%)	14,15,17	1.26	2 (14%)
3	MAN	A	1350	-	11,11,12	2.23	3 (27%)	14,15,17	1.97	2 (14%)
3	MAN	A	1351	-	11,11,12	1.01	0	14,15,17	1.23	1 (7%)
4	BMA	A	1352	-	11,11,12	2.35	3 (27%)	14,15,17	1.97	2 (14%)
2	NAG	A	1356	-	14,14,15	1.19	2 (14%)	15,19,21	1.39	2 (13%)
5	NDG	A	1357	-	14,14,15	1.53	4 (28%)	15,19,21	1.12	2 (13%)
3	MAN	A	1358	-	11,11,12	1.02	1 (9%)	14,15,17	2.52	3 (21%)
3	MAN	A	1359	-	11,11,12	0.93	1 (9%)	14,15,17	1.73	2 (14%)
3	MAN	A	1360	-	11,11,12	0.99	0	14,15,17	1.87	1 (7%)
3	MAN	A	1361	-	11,11,12	0.59	0	14,15,17	1.77	3 (21%)
3	MAN	A	1362	-	11,11,12	1.03	1 (9%)	14,15,17	1.73	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	1363	-	14,14,15	1.67	3 (21%)	15,19,21	1.25	1 (6%)
7	FUC	A	1364	-	10,10,11	0.56	0	14,14,16	0.79	0
2	NAG	A	1386	-	14,14,15	1.22	1 (7%)	15,19,21	1.93	4 (26%)
5	NDG	A	1387	-	14,14,15	0.97	1 (7%)	15,19,21	1.70	4 (26%)
3	MAN	A	1388	-	11,11,12	1.35	1 (9%)	14,15,17	1.22	3 (21%)
3	MAN	A	1389	-	11,11,12	1.75	3 (27%)	14,15,17	1.74	3 (21%)
3	MAN	A	1390	-	11,11,12	1.15	2 (18%)	14,15,17	1.05	1 (7%)
3	MAN	A	1391	-	11,11,12	1.31	2 (18%)	14,15,17	1.87	3 (21%)
2	NAG	A	1392	-	14,14,15	1.47	1 (7%)	15,19,21	2.06	5 (33%)
3	MAN	A	1393	-	11,11,12	1.65	3 (27%)	14,15,17	2.55	7 (50%)
4	BMA	A	1394	-	11,11,12	1.19	2 (18%)	14,15,17	1.33	3 (21%)
7	FUC	A	1395	-	10,10,11	1.22	2 (20%)	14,14,16	0.33	0
2	NAG	A	1411	1	14,14,15	2.04	2 (14%)	15,19,21	1.42	2 (13%)
2	NAG	A	1412	-	14,14,15	1.38	2 (14%)	15,19,21	1.90	4 (26%)
3	MAN	A	1413	-	11,11,12	1.40	1 (9%)	14,15,17	0.95	0
2	NAG	A	1435	-	14,14,15	1.30	2 (14%)	15,19,21	1.55	5 (33%)
2	NAG	A	1436	-	14,14,15	0.97	0	15,19,21	1.71	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
2	NAG	A	1047	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1048	-	-	0/6/23/26	0/1/1/1
3	MAN	A	1049	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1050	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1051	-	-	0/2/19/22	0/1/1/1
4	BMA	A	1052	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1053	-	-	0/2/19/22	0/1/1/1
2	NAG	A	1087	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1088	-	-	0/6/23/26	0/1/1/1
3	MAN	A	1089	-	-	0/2/19/22	0/1/1/1
4	BMA	A	1090	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1091	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1092	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1093	-	-	0/2/19/22	0/1/1/1
5	NDG	A	1114	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1115	-	-	0/6/23/26	0/1/1/1
3	MAN	A	1116	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1117	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1118	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1119	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1120	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1121	-	-	0/2/19/22	0/1/1/1
2	NAG	A	1166	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1167	-	-	0/6/23/26	0/1/1/1
4	BMA	A	1168	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1169	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1170	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1171	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1172	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1173	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1174	-	-	0/2/19/22	0/1/1/1
2	NAG	A	1195	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1196	-	-	0/6/23/26	0/1/1/1
3	MAN	A	1197	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1198	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1199	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1200	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1201	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1202	-	-	0/2/19/22	0/1/1/1
6	GAL	A	1203	-	-	0/2/19/22	0/1/1/1
6	GAL	A	1204	-	-	0/2/19/22	0/1/1/1
2	NAG	A	1229	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1230	-	-	0/6/23/26	0/1/1/1
3	MAN	A	1231	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1232	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1233	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1234	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1235	-	-	0/2/19/22	0/1/1/1
6	GAL	A	1236	-	-	0/2/19/22	0/1/1/1
6	GAL	A	1237	-	-	0/2/19/22	0/1/1/1
2	NAG	A	1277	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1278	-	-	0/6/23/26	0/1/1/1
3	MAN	A	1279	-	-	0/2/19/22	0/1/1/1
4	BMA	A	1280	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1281	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1282	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1283	-	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	A	1284	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1285	-	-	0/2/19/22	0/1/1/1
6	GAL	A	1286	-	-	0/2/19/22	0/1/1/1
6	GAL	A	1287	-	-	0/2/19/22	0/1/1/1
2	NAG	A	1318	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1319	-	-	0/6/23/26	0/1/1/1
3	MAN	A	1320	-	-	0/2/19/22	0/1/1/1
2	NAG	A	1328	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1329	-	-	0/6/23/26	0/1/1/1
3	MAN	A	1330	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1331	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1332	-	-	0/2/19/22	0/1/1/1
2	NAG	A	1345	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1346	-	-	0/6/23/26	0/1/1/1
3	MAN	A	1347	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1348	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1349	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1350	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1351	-	-	0/2/19/22	0/1/1/1
4	BMA	A	1352	-	-	0/2/19/22	0/1/1/1
2	NAG	A	1356	-	-	0/6/23/26	0/1/1/1
5	NDG	A	1357	-	-	0/6/23/26	0/1/1/1
3	MAN	A	1358	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1359	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1360	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1361	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1362	-	-	0/2/19/22	0/1/1/1
2	NAG	A	1363	-	-	0/6/23/26	0/1/1/1
7	FUC	A	1364	-	-	0/0/17/20	0/1/1/1
2	NAG	A	1386	-	-	0/6/23/26	0/1/1/1
5	NDG	A	1387	-	-	0/6/23/26	0/1/1/1
3	MAN	A	1388	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1389	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1390	-	-	0/2/19/22	0/1/1/1
3	MAN	A	1391	-	-	0/2/19/22	0/1/1/1
2	NAG	A	1392	-	-	0/6/23/26	0/1/1/1
3	MAN	A	1393	-	-	0/2/19/22	0/1/1/1
4	BMA	A	1394	-	-	0/2/19/22	0/1/1/1
7	FUC	A	1395	-	-	0/0/17/20	0/1/1/1
2	NAG	A	1411	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1412	-	-	0/6/23/26	0/1/1/1
3	MAN	A	1413	-	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1435	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1436	-	-	0/6/23/26	0/1/1/1

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1195	NAG	C1-C2	-7.76	1.41	1.52
2	A	1318	NAG	O3-C3	-6.45	1.27	1.43
2	A	1411	NAG	C1-C2	-6.22	1.43	1.52
3	A	1197	MAN	O3-C3	-5.77	1.29	1.43
5	A	1114	NDG	C1-C2	-4.83	1.45	1.52
3	A	1197	MAN	C4-C3	-4.68	1.40	1.52
2	A	1363	NAG	C1-C2	-4.35	1.46	1.52
2	A	1318	NAG	C4-C5	-4.31	1.44	1.53
3	A	1199	MAN	O2-C2	-4.20	1.33	1.43
2	A	1392	NAG	C1-C2	-3.91	1.47	1.52
2	A	1411	NAG	O3-C3	-3.81	1.33	1.43
4	A	1168	BMA	C6-C5	-3.77	1.38	1.51
3	A	1049	MAN	O5-C1	-3.59	1.37	1.43
3	A	1413	MAN	O5-C1	-3.46	1.37	1.43
4	A	1280	BMA	C2-C3	-3.44	1.47	1.52
3	A	1169	MAN	C6-C5	-3.40	1.39	1.51
3	A	1347	MAN	O2-C2	-3.36	1.35	1.43
3	A	1197	MAN	C4-C5	-3.35	1.46	1.53
2	A	1412	NAG	O4-C4	-3.35	1.34	1.43
3	A	1116	MAN	O5-C1	-3.20	1.38	1.43
2	A	1345	NAG	C1-C2	-3.20	1.48	1.52
3	A	1169	MAN	O3-C3	-3.15	1.35	1.43
6	A	1236	GAL	O3-C3	-3.15	1.35	1.43
6	A	1286	GAL	O3-C3	-3.10	1.35	1.43
3	A	1393	MAN	O2-C2	-3.06	1.36	1.43
3	A	1198	MAN	O2-C2	-3.03	1.36	1.43
3	A	1232	MAN	C1-C2	-2.99	1.45	1.52
6	A	1203	GAL	O3-C3	-2.97	1.35	1.43
3	A	1389	MAN	O2-C2	-2.97	1.36	1.43
2	A	1318	NAG	C1-C2	-2.95	1.48	1.52
3	A	1234	MAN	O2-C2	-2.88	1.36	1.43
3	A	1350	MAN	O2-C2	-2.88	1.36	1.43
3	A	1171	MAN	O2-C2	-2.88	1.36	1.43
2	A	1319	NAG	C1-C2	-2.84	1.48	1.52
3	A	1388	MAN	O3-C3	-2.84	1.36	1.43
3	A	1092	MAN	O2-C2	-2.83	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1195	NAG	O3-C3	-2.80	1.36	1.43
2	A	1167	NAG	O4-C4	-2.80	1.36	1.43
3	A	1118	MAN	O2-C2	-2.75	1.37	1.43
4	A	1352	BMA	O2-C2	-2.75	1.37	1.43
3	A	1198	MAN	C1-C2	-2.74	1.45	1.52
4	A	1090	BMA	C2-C3	-2.71	1.48	1.52
3	A	1285	MAN	O3-C3	-2.70	1.36	1.43
4	A	1052	BMA	O5-C1	-2.69	1.39	1.43
2	A	1048	NAG	O5-C1	-2.68	1.39	1.43
2	A	1087	NAG	O4-C4	-2.62	1.36	1.43
2	A	1047	NAG	C1-C2	-2.61	1.48	1.52
3	A	1050	MAN	C1-C2	-2.54	1.46	1.52
2	A	1166	NAG	C1-C2	-2.54	1.48	1.52
3	A	1348	MAN	O2-C2	-2.53	1.37	1.43
2	A	1386	NAG	O4-C4	-2.52	1.36	1.43
3	A	1330	MAN	O6-C6	-2.50	1.31	1.42
3	A	1234	MAN	O5-C1	-2.49	1.39	1.43
6	A	1287	GAL	O5-C1	-2.44	1.39	1.43
3	A	1285	MAN	C1-C2	-2.44	1.46	1.52
3	A	1119	MAN	O2-C2	-2.42	1.37	1.43
7	A	1395	FUC	C1-C2	-2.41	1.46	1.52
3	A	1201	MAN	O3-C3	-2.39	1.37	1.43
2	A	1345	NAG	O6-C6	-2.37	1.32	1.42
2	A	1319	NAG	O3-C3	-2.37	1.37	1.43
3	A	1117	MAN	C2-C3	-2.35	1.49	1.52
4	A	1168	BMA	O3-C3	-2.35	1.37	1.43
3	A	1359	MAN	O2-C2	-2.35	1.38	1.43
2	A	1278	NAG	O5-C1	-2.31	1.39	1.43
2	A	1048	NAG	C1-C2	-2.31	1.49	1.52
3	A	1171	MAN	C1-C2	-2.29	1.46	1.52
3	A	1169	MAN	C1-C2	-2.28	1.46	1.52
2	A	1230	NAG	O5-C1	-2.28	1.39	1.43
2	A	1088	NAG	C1-C2	-2.27	1.49	1.52
3	A	1279	MAN	O6-C6	-2.25	1.32	1.42
3	A	1282	MAN	O5-C1	-2.24	1.40	1.43
5	A	1357	NDG	C1-C2	-2.23	1.49	1.52
3	A	1200	MAN	O3-C3	-2.21	1.37	1.43
3	A	1284	MAN	C1-C2	-2.20	1.46	1.52
6	A	1203	GAL	O5-C1	-2.20	1.40	1.43
2	A	1329	NAG	O3-C3	-2.20	1.37	1.43
3	A	1200	MAN	C1-C2	-2.19	1.46	1.52
3	A	1117	MAN	O3-C3	-2.15	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1390	MAN	O5-C1	-2.13	1.40	1.43
5	A	1357	NDG	C4-C5	-2.07	1.48	1.53
6	A	1287	GAL	C2-C3	-2.07	1.49	1.52
2	A	1166	NAG	O4-C4	-2.06	1.38	1.43
2	A	1328	NAG	C1-C2	-2.04	1.49	1.52
3	A	1391	MAN	O3-C3	-2.02	1.38	1.43
3	A	1089	MAN	O6-C6	-2.00	1.33	1.42
2	A	1328	NAG	C4-C3	2.00	1.57	1.52
2	A	1229	NAG	C1-C2	2.01	1.55	1.52
3	A	1284	MAN	O5-C1	2.02	1.47	1.43
2	A	1318	NAG	C8-C7	2.02	1.54	1.50
3	A	1200	MAN	O5-C1	2.06	1.47	1.43
3	A	1320	MAN	O5-C5	2.07	1.48	1.43
3	A	1285	MAN	O5-C5	2.08	1.48	1.43
3	A	1198	MAN	O5-C5	2.08	1.48	1.43
2	A	1328	NAG	C8-C7	2.09	1.54	1.50
3	A	1358	MAN	O5-C5	2.09	1.48	1.43
3	A	1331	MAN	O5-C5	2.15	1.48	1.43
3	A	1118	MAN	C4-C5	2.15	1.57	1.53
3	A	1390	MAN	C2-C3	2.17	1.55	1.52
3	A	1091	MAN	C4-C5	2.18	1.57	1.53
5	A	1387	NDG	O-C5	2.22	1.48	1.43
3	A	1234	MAN	C4-C5	2.24	1.57	1.53
3	A	1173	MAN	C4-C5	2.24	1.57	1.53
3	A	1201	MAN	C4-C5	2.25	1.57	1.53
2	A	1047	NAG	O7-C7	2.29	1.28	1.23
4	A	1052	BMA	C4-C5	2.30	1.58	1.53
3	A	1362	MAN	O5-C1	2.31	1.47	1.43
3	A	1197	MAN	O2-C2	2.31	1.48	1.43
2	A	1277	NAG	O5-C5	2.32	1.48	1.43
4	A	1394	BMA	C4-C5	2.32	1.58	1.53
3	A	1170	MAN	C4-C5	2.33	1.58	1.53
3	A	1282	MAN	C4-C5	2.34	1.58	1.53
2	A	1363	NAG	C4-C3	2.37	1.58	1.52
3	A	1349	MAN	C4-C5	2.37	1.58	1.53
2	A	1047	NAG	O5-C5	2.40	1.48	1.43
2	A	1195	NAG	C8-C7	2.45	1.55	1.50
4	A	1394	BMA	O5-C5	2.47	1.48	1.43
2	A	1435	NAG	C3-C2	2.47	1.58	1.52
2	A	1363	NAG	O5-C5	2.47	1.48	1.43
2	A	1356	NAG	C4-C3	2.47	1.58	1.52
2	A	1356	NAG	O5-C5	2.48	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1330	MAN	O5-C5	2.50	1.48	1.43
3	A	1347	MAN	C2-C3	2.52	1.56	1.52
3	A	1092	MAN	O5-C5	2.54	1.49	1.43
3	A	1279	MAN	C4-C3	2.56	1.59	1.52
3	A	1174	MAN	O5-C5	2.58	1.49	1.43
3	A	1281	MAN	O5-C5	2.59	1.49	1.43
5	A	1357	NDG	C4-C3	2.60	1.59	1.52
4	A	1168	BMA	C4-C5	2.60	1.58	1.53
3	A	1393	MAN	C2-C3	2.65	1.56	1.52
2	A	1412	NAG	O5-C1	2.66	1.48	1.43
7	A	1395	FUC	O5-C1	2.67	1.48	1.43
3	A	1199	MAN	O5-C5	2.69	1.49	1.43
3	A	1089	MAN	C4-C3	2.72	1.59	1.52
3	A	1198	MAN	C4-C3	2.73	1.59	1.52
3	A	1119	MAN	O5-C5	2.73	1.49	1.43
3	A	1202	MAN	O5-C5	2.75	1.49	1.43
3	A	1389	MAN	O5-C5	2.75	1.49	1.43
3	A	1320	MAN	O5-C1	2.76	1.48	1.43
2	A	1435	NAG	C4-C3	2.80	1.59	1.52
4	A	1090	BMA	O5-C1	2.81	1.48	1.43
3	A	1235	MAN	O5-C5	2.82	1.49	1.43
3	A	1199	MAN	O5-C1	2.86	1.48	1.43
3	A	1393	MAN	O5-C1	2.86	1.48	1.43
3	A	1389	MAN	O5-C1	2.88	1.48	1.43
3	A	1349	MAN	O5-C5	2.88	1.49	1.43
2	A	1329	NAG	C1-C2	2.88	1.56	1.52
3	A	1169	MAN	C4-C5	2.89	1.59	1.53
3	A	1171	MAN	C4-C3	2.93	1.60	1.52
3	A	1391	MAN	O5-C5	2.93	1.49	1.43
3	A	1116	MAN	C4-C3	2.94	1.60	1.52
2	A	1047	NAG	C8-C7	2.96	1.56	1.50
5	A	1357	NDG	C3-C2	2.96	1.59	1.52
2	A	1345	NAG	C8-C7	2.97	1.56	1.50
3	A	1231	MAN	O5-C5	3.18	1.50	1.43
3	A	1050	MAN	C4-C3	3.18	1.60	1.52
2	A	1195	NAG	O5-C1	3.19	1.49	1.43
3	A	1330	MAN	C2-C3	3.25	1.57	1.52
3	A	1093	MAN	C2-C3	3.31	1.57	1.52
4	A	1090	BMA	C1-C2	3.39	1.60	1.52
3	A	1320	MAN	C2-C3	3.40	1.57	1.52
3	A	1283	MAN	C2-C3	3.43	1.57	1.52
3	A	1120	MAN	C2-C3	3.47	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1053	MAN	C2-C3	3.57	1.57	1.52
3	A	1197	MAN	C2-C3	3.60	1.57	1.52
3	A	1350	MAN	O5-C1	3.63	1.49	1.43
2	A	1319	NAG	C3-C2	4.37	1.62	1.52
4	A	1352	BMA	C2-C3	4.98	1.59	1.52
4	A	1352	BMA	O5-C1	5.03	1.52	1.43
3	A	1350	MAN	C2-C3	5.36	1.59	1.52
2	A	1346	NAG	O5-C1	6.47	1.54	1.43

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1195	NAG	C1-O5-C5	-6.92	103.47	112.25
2	A	1346	NAG	C1-O5-C5	-5.02	105.88	112.25
3	A	1169	MAN	C3-C4-C5	-4.60	102.19	110.20
4	A	1168	BMA	C3-C4-C5	-4.46	102.42	110.20
2	A	1278	NAG	C1-O5-C5	-4.32	106.77	112.25
4	A	1052	BMA	C1-C2-C3	-4.25	104.51	109.54
3	A	1231	MAN	C1-C2-C3	-4.21	104.56	109.54
2	A	1392	NAG	C2-N2-C7	-4.01	117.89	123.04
4	A	1168	BMA	O3-C3-C4	-3.98	101.38	110.34
2	A	1048	NAG	C1-O5-C5	-3.96	107.22	112.25
3	A	1169	MAN	O4-C4-C5	-3.91	98.87	109.24
4	A	1280	BMA	C1-C2-C3	-3.88	104.95	109.54
2	A	1386	NAG	C2-N2-C7	-3.88	118.06	123.04
4	A	1168	BMA	O4-C4-C5	-3.80	99.18	109.24
2	A	1328	NAG	C2-N2-C7	-3.75	118.22	123.04
3	A	1347	MAN	O3-C3-C2	-3.72	103.28	110.00
4	A	1280	BMA	C1-O5-C5	-3.70	107.55	112.25
3	A	1282	MAN	C1-C2-C3	-3.68	105.19	109.54
2	A	1412	NAG	C2-N2-C7	-3.58	118.44	123.04
3	A	1201	MAN	C1-C2-C3	-3.50	105.40	109.54
2	A	1328	NAG	C4-C3-C2	-3.48	105.82	111.23
3	A	1172	MAN	C1-O5-C5	-3.43	107.89	112.25
2	A	1230	NAG	C1-O5-C5	-3.39	107.95	112.25
6	A	1286	GAL	C1-C2-C3	-3.37	105.55	109.54
2	A	1363	NAG	C2-N2-C7	-3.30	118.80	123.04
3	A	1117	MAN	C3-C4-C5	-3.29	104.46	110.20
2	A	1048	NAG	O4-C4-C3	-3.27	102.97	110.34
2	A	1115	NAG	C1-O5-C5	-3.25	108.13	112.25
3	A	1347	MAN	O5-C5-C6	-3.24	100.33	107.35
3	A	1091	MAN	C1-C2-C3	-3.23	105.72	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1411	NAG	C1-O5-C5	-3.23	108.16	112.25
2	A	1319	NAG	C1-O5-C5	-3.20	108.19	112.25
3	A	1051	MAN	C2-C3-C4	-3.19	105.62	111.04
4	A	1090	BMA	C1-C2-C3	-3.18	105.78	109.54
4	A	1280	BMA	C3-C4-C5	-3.12	104.75	110.20
2	A	1356	NAG	C2-N2-C7	-3.12	119.03	123.04
3	A	1172	MAN	C1-C2-C3	-3.11	105.86	109.54
3	A	1172	MAN	C2-C3-C4	-3.08	105.81	111.04
6	A	1236	GAL	C1-C2-C3	-3.08	105.90	109.54
3	A	1393	MAN	O5-C5-C6	-3.06	100.73	107.35
2	A	1047	NAG	O4-C4-C3	-3.04	103.50	110.34
3	A	1233	MAN	C1-O5-C5	-2.98	108.47	112.25
3	A	1351	MAN	C1-O5-C5	-2.95	108.50	112.25
3	A	1170	MAN	C1-C2-C3	-2.92	106.09	109.54
3	A	1199	MAN	C3-C4-C5	-2.91	105.13	110.20
3	A	1231	MAN	C2-C3-C4	-2.85	106.19	111.04
3	A	1172	MAN	C3-C4-C5	-2.85	105.23	110.20
3	A	1285	MAN	C1-C2-C3	-2.85	106.17	109.54
3	A	1051	MAN	C3-C4-C5	-2.83	105.27	110.20
3	A	1117	MAN	C2-C3-C4	-2.80	106.29	111.04
3	A	1117	MAN	C1-C2-C3	-2.77	106.27	109.54
3	A	1117	MAN	C1-O5-C5	-2.74	108.77	112.25
2	A	1346	NAG	C6-C5-C4	-2.74	106.26	113.02
4	A	1090	BMA	C2-C3-C4	-2.72	106.42	111.04
4	A	1090	BMA	C3-C4-C5	-2.71	105.47	110.20
3	A	1393	MAN	C6-C5-C4	-2.71	106.34	113.02
2	A	1196	NAG	O3-C3-C2	-2.70	103.77	109.11
5	A	1114	NDG	O4-C4-C3	-2.68	104.30	110.34
3	A	1093	MAN	C1-O5-C5	-2.67	108.85	112.25
2	A	1345	NAG	O5-C5-C6	-2.67	101.57	107.35
3	A	1347	MAN	C6-C5-C4	-2.66	106.46	113.02
2	A	1345	NAG	O7-C7-C8	-2.65	117.20	122.06
6	A	1286	GAL	C1-O5-C5	-2.63	108.91	112.25
4	A	1052	BMA	C1-O5-C5	-2.63	108.92	112.25
2	A	1195	NAG	O3-C3-C2	-2.63	103.91	109.11
3	A	1393	MAN	O3-C3-C2	-2.59	105.32	110.00
3	A	1050	MAN	C1-O5-C5	-2.59	108.96	112.25
3	A	1349	MAN	C3-C4-C5	-2.57	105.71	110.20
2	A	1411	NAG	C2-N2-C7	-2.57	119.74	123.04
2	A	1229	NAG	O4-C4-C3	-2.55	104.59	110.34
4	A	1090	BMA	C1-O5-C5	-2.55	109.02	112.25
3	A	1281	MAN	C1-C2-C3	-2.54	106.53	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1277	NAG	O4-C4-C3	-2.53	104.64	110.34
6	A	1236	GAL	C1-O5-C5	-2.51	109.07	112.25
5	A	1387	NDG	C2-N2-C7	-2.50	119.82	123.04
2	A	1088	NAG	C2-N2-C7	-2.50	119.83	123.04
5	A	1114	NDG	C2-N2-C7	-2.49	119.84	123.04
3	A	1197	MAN	O3-C3-C4	-2.46	104.79	110.34
3	A	1388	MAN	C1-O5-C5	-2.46	109.13	112.25
3	A	1231	MAN	C3-C4-C5	-2.46	105.91	110.20
2	A	1047	NAG	O7-C7-N2	-2.45	116.86	121.86
2	A	1196	NAG	C1-O5-C5	-2.45	109.14	112.25
5	A	1357	NDG	O3-C3-C2	-2.43	104.31	109.11
2	A	1318	NAG	O3-C3-C2	-2.39	104.39	109.11
2	A	1167	NAG	C2-N2-C7	-2.36	120.00	123.04
4	A	1280	BMA	C2-C3-C4	-2.35	107.05	111.04
2	A	1435	NAG	O3-C3-C2	-2.31	104.54	109.11
5	A	1387	NDG	C6-C5-C4	-2.30	107.35	113.02
2	A	1087	NAG	C2-N2-C7	-2.29	120.10	123.04
2	A	1436	NAG	C1-O5-C5	-2.29	109.35	112.25
3	A	1173	MAN	C1-C2-C3	-2.28	106.84	109.54
3	A	1049	MAN	C1-C2-C3	-2.28	106.84	109.54
5	A	1357	NDG	O7-C7-C8	-2.27	117.89	122.06
2	A	1345	NAG	C6-C5-C4	-2.27	107.42	113.02
2	A	1196	NAG	C2-N2-C7	-2.24	120.16	123.04
2	A	1436	NAG	C3-C2-N2	-2.24	105.20	110.56
3	A	1050	MAN	C1-C2-C3	-2.24	106.89	109.54
2	A	1392	NAG	O3-C3-C2	-2.24	104.68	109.11
3	A	1169	MAN	O3-C3-C4	-2.24	105.30	110.34
3	A	1235	MAN	C1-C2-C3	-2.23	106.90	109.54
2	A	1319	NAG	O7-C7-C8	-2.22	118.00	122.06
3	A	1089	MAN	C3-C4-C5	-2.20	106.37	110.20
3	A	1120	MAN	C1-O5-C5	-2.18	109.48	112.25
6	A	1204	GAL	C1-C2-C3	-2.18	106.96	109.54
3	A	1283	MAN	C1-O5-C5	-2.17	109.50	112.25
2	A	1436	NAG	O5-C5-C6	-2.16	102.68	107.35
2	A	1166	NAG	C2-N2-C7	-2.15	120.28	123.04
3	A	1391	MAN	O5-C5-C6	-2.15	102.70	107.35
6	A	1237	GAL	C1-C2-C3	-2.14	107.02	109.54
3	A	1116	MAN	C1-O5-C5	-2.12	109.56	112.25
6	A	1286	GAL	O3-C3-C2	-2.12	106.18	110.00
2	A	1329	NAG	C3-C4-C5	-2.11	106.53	110.20
6	A	1237	GAL	C1-O5-C5	-2.11	109.58	112.25
6	A	1204	GAL	C1-O5-C5	-2.08	109.60	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1394	BMA	C3-C4-C5	-2.07	106.58	110.20
2	A	1346	NAG	O7-C7-C8	-2.05	118.29	122.06
3	A	1050	MAN	C3-C4-C5	-2.05	106.62	110.20
3	A	1051	MAN	C1-O5-C5	-2.04	109.65	112.25
3	A	1053	MAN	C1-O5-C5	-2.04	109.65	112.25
2	A	1386	NAG	O7-C7-C8	-2.03	118.33	122.06
4	A	1168	BMA	C1-C2-C3	-2.03	107.14	109.54
2	A	1392	NAG	O7-C7-C8	-2.02	118.35	122.06
2	A	1435	NAG	O7-C7-C8	-2.02	118.35	122.06
2	A	1230	NAG	O7-C7-C8	-2.02	118.35	122.06
4	A	1394	BMA	C1-C2-C3	-2.02	107.16	109.54
3	A	1199	MAN	C2-C3-C4	-2.02	107.62	111.04
3	A	1093	MAN	C1-C2-C3	-2.01	107.16	109.54
2	A	1412	NAG	O7-C7-C8	-2.01	118.37	122.06
3	A	1197	MAN	O4-C4-C3	-2.00	105.83	110.34
3	A	1361	MAN	C3-C4-C5	-2.00	106.71	110.20
3	A	1169	MAN	C6-C5-C4	2.01	117.97	113.02
3	A	1348	MAN	C1-C2-C3	2.03	111.94	109.54
2	A	1230	NAG	C6-C5-C4	2.04	118.04	113.02
3	A	1283	MAN	O3-C3-C2	2.05	113.70	110.00
3	A	1231	MAN	O2-C2-C3	2.05	114.25	110.12
4	A	1168	BMA	C6-C5-C4	2.07	118.11	113.02
3	A	1282	MAN	O5-C1-C2	2.07	114.21	110.86
3	A	1388	MAN	O5-C1-C2	2.07	114.22	110.86
3	A	1050	MAN	O3-C3-C4	2.08	115.02	110.34
3	A	1389	MAN	C1-O5-C5	2.09	114.90	112.25
3	A	1390	MAN	O5-C1-C2	2.10	114.27	110.86
2	A	1329	NAG	C1-O5-C5	2.10	114.92	112.25
3	A	1361	MAN	C1-C2-C3	2.11	112.04	109.54
3	A	1348	MAN	O5-C1-C2	2.14	114.32	110.86
2	A	1277	NAG	C1-O5-C5	2.16	114.98	112.25
2	A	1329	NAG	O3-C3-C2	2.16	113.40	109.11
3	A	1169	MAN	O5-C1-C2	2.17	114.38	110.86
2	A	1435	NAG	C2-N2-C7	2.20	125.86	123.04
3	A	1197	MAN	O2-C2-C1	2.20	113.61	109.21
6	A	1203	GAL	O5-C1-C2	2.20	114.43	110.86
3	A	1171	MAN	O5-C1-C2	2.20	114.43	110.86
2	A	1196	NAG	C4-C3-C2	2.22	114.69	111.23
3	A	1117	MAN	O5-C1-C2	2.23	114.47	110.86
2	A	1048	NAG	C3-C4-C5	2.26	114.13	110.20
3	A	1388	MAN	C2-C3-C4	2.26	114.88	111.04
2	A	1195	NAG	O7-C7-N2	2.26	126.48	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1393	MAN	C2-C3-C4	2.27	114.89	111.04
3	A	1284	MAN	O5-C1-C2	2.28	114.56	110.86
3	A	1050	MAN	O5-C1-C2	2.29	114.57	110.86
3	A	1332	MAN	O5-C1-C2	2.30	114.58	110.86
3	A	1391	MAN	C1-O5-C5	2.30	115.17	112.25
2	A	1328	NAG	O4-C4-C3	2.31	115.53	110.34
2	A	1329	NAG	O7-C7-N2	2.31	126.58	121.86
3	A	1199	MAN	C1-C2-C3	2.31	112.28	109.54
3	A	1201	MAN	C3-C4-C5	2.33	114.27	110.20
3	A	1279	MAN	O5-C1-C2	2.35	114.67	110.86
2	A	1435	NAG	O7-C7-N2	2.37	126.70	121.86
5	A	1114	NDG	C3-C4-C5	2.38	114.34	110.20
3	A	1362	MAN	C1-C2-C3	2.39	112.37	109.54
4	A	1352	BMA	O2-C2-C1	2.41	114.04	109.21
2	A	1356	NAG	O4-C4-C3	2.41	115.77	110.34
2	A	1048	NAG	C6-C5-C4	2.43	119.02	113.02
4	A	1394	BMA	O5-C1-C2	2.44	114.81	110.86
3	A	1350	MAN	C1-C2-C3	2.44	112.43	109.54
3	A	1172	MAN	O5-C1-C2	2.49	114.89	110.86
3	A	1231	MAN	O3-C3-C2	2.51	114.54	110.00
5	A	1387	NDG	C3-C4-C5	2.52	114.58	110.20
2	A	1435	NAG	C4-C3-C2	2.54	115.17	111.23
3	A	1347	MAN	C2-C3-C4	2.57	115.40	111.04
3	A	1349	MAN	O5-C1-C2	2.58	115.04	110.86
3	A	1116	MAN	O5-C1-C2	2.58	115.05	110.86
3	A	1118	MAN	C3-C4-C5	2.65	114.81	110.20
3	A	1234	MAN	C3-C4-C5	2.67	114.85	110.20
3	A	1282	MAN	C3-C4-C5	2.70	114.90	110.20
3	A	1173	MAN	C3-C4-C5	2.71	114.92	110.20
3	A	1091	MAN	C3-C4-C5	2.71	114.92	110.20
3	A	1170	MAN	C3-C4-C5	2.72	114.95	110.20
3	A	1347	MAN	C1-C2-C3	2.73	112.77	109.54
4	A	1052	BMA	C3-C4-C5	2.73	114.96	110.20
3	A	1358	MAN	C1-C2-C3	2.74	112.78	109.54
3	A	1200	MAN	O5-C1-C2	2.74	115.31	110.86
2	A	1319	NAG	O3-C3-C2	2.76	114.58	109.11
3	A	1389	MAN	C1-C2-C3	2.77	112.81	109.54
2	A	1346	NAG	C4-C3-C2	2.79	115.56	111.23
2	A	1392	NAG	C3-C4-C5	2.80	115.07	110.20
2	A	1319	NAG	C3-C4-C5	2.83	115.12	110.20
3	A	1347	MAN	C3-C4-C5	2.92	115.29	110.20
3	A	1199	MAN	C1-O5-C5	2.92	115.95	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1347	MAN	C1-O5-C5	3.07	116.14	112.25
3	A	1393	MAN	O2-C2-C1	3.11	115.45	109.21
3	A	1358	MAN	C1-O5-C5	3.18	116.28	112.25
3	A	1359	MAN	C1-C2-C3	3.24	113.37	109.54
3	A	1121	MAN	O5-C1-C2	3.24	116.11	110.86
3	A	1393	MAN	C3-C4-C5	3.25	115.86	110.20
3	A	1197	MAN	C1-C2-C3	3.28	113.42	109.54
2	A	1048	NAG	C4-C3-C2	3.46	116.61	111.23
2	A	1386	NAG	C4-C3-C2	3.56	116.76	111.23
3	A	1231	MAN	C1-O5-C5	3.56	116.77	112.25
3	A	1283	MAN	O5-C1-C2	3.65	116.78	110.86
2	A	1346	NAG	O5-C5-C6	3.70	115.35	107.35
2	A	1386	NAG	C3-C4-C5	3.71	116.67	110.20
2	A	1319	NAG	C3-C2-N2	3.73	119.49	110.56
2	A	1412	NAG	C4-C3-C2	3.75	117.06	111.23
5	A	1387	NDG	C1-O-C5	3.76	117.02	112.25
3	A	1284	MAN	C1-C2-C3	3.85	114.10	109.54
2	A	1412	NAG	C3-C4-C5	3.93	117.05	110.20
3	A	1197	MAN	C3-C4-C5	3.96	117.09	110.20
3	A	1233	MAN	O5-C1-C2	4.00	117.35	110.86
3	A	1235	MAN	O5-C1-C2	4.08	117.47	110.86
2	A	1436	NAG	C4-C3-C2	4.08	117.57	111.23
3	A	1320	MAN	O5-C1-C2	4.12	117.54	110.86
2	A	1318	NAG	C3-C4-C5	4.21	117.53	110.20
3	A	1053	MAN	O5-C1-C2	4.29	117.82	110.86
3	A	1120	MAN	O5-C1-C2	4.31	117.84	110.86
2	A	1230	NAG	C3-C4-C5	4.35	117.78	110.20
3	A	1389	MAN	O5-C1-C2	4.41	118.01	110.86
3	A	1093	MAN	O5-C1-C2	4.47	118.11	110.86
3	A	1202	MAN	O5-C1-C2	4.56	118.25	110.86
3	A	1281	MAN	O5-C1-C2	4.64	118.39	110.86
4	A	1168	BMA	O5-C5-C6	4.69	117.51	107.35
2	A	1392	NAG	C4-C3-C2	4.88	118.81	111.23
3	A	1169	MAN	O5-C5-C6	4.92	118.00	107.35
3	A	1174	MAN	O5-C1-C2	5.05	119.04	110.86
3	A	1359	MAN	O5-C1-C2	5.06	119.06	110.86
3	A	1119	MAN	O5-C1-C2	5.08	119.10	110.86
3	A	1092	MAN	O5-C1-C2	5.20	119.29	110.86
3	A	1331	MAN	O5-C1-C2	5.23	119.33	110.86
3	A	1362	MAN	O5-C1-C2	5.45	119.70	110.86
3	A	1197	MAN	O5-C1-C2	5.47	119.72	110.86
3	A	1391	MAN	O5-C1-C2	5.55	119.85	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1361	MAN	O5-C1-C2	5.55	119.86	110.86
3	A	1285	MAN	O5-C1-C2	5.55	119.86	110.86
4	A	1352	BMA	O5-C1-C2	5.68	120.07	110.86
3	A	1393	MAN	O5-C1-C2	5.89	120.41	110.86
3	A	1347	MAN	O5-C1-C2	5.91	120.44	110.86
3	A	1350	MAN	O5-C1-C2	5.95	120.51	110.86
3	A	1360	MAN	O5-C1-C2	6.01	120.61	110.86
3	A	1320	MAN	C1-C2-C3	6.13	116.79	109.54
3	A	1199	MAN	O5-C1-C2	6.99	122.20	110.86
3	A	1330	MAN	O5-C1-C2	7.31	122.72	110.86
3	A	1358	MAN	O5-C1-C2	8.11	124.01	110.86
3	A	1231	MAN	O5-C1-C2	8.27	124.28	110.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

99 monomers are involved in 257 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1047	NAG	7	0
2	A	1048	NAG	8	0
3	A	1049	MAN	12	0
3	A	1050	MAN	11	0
3	A	1051	MAN	5	0
4	A	1052	BMA	2	0
3	A	1053	MAN	2	0
2	A	1087	NAG	4	0
2	A	1088	NAG	3	0
3	A	1089	MAN	12	0
4	A	1090	BMA	7	0
3	A	1091	MAN	1	0
3	A	1092	MAN	5	0
3	A	1093	MAN	1	0
5	A	1114	NDG	3	0
2	A	1115	NAG	6	0
3	A	1116	MAN	5	0
3	A	1117	MAN	6	0
3	A	1118	MAN	6	0
3	A	1119	MAN	3	0
3	A	1120	MAN	2	0
3	A	1121	MAN	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1166	NAG	10	0
2	A	1167	NAG	5	0
4	A	1168	BMA	8	0
3	A	1169	MAN	5	0
3	A	1170	MAN	1	0
3	A	1171	MAN	6	0
3	A	1173	MAN	5	0
3	A	1174	MAN	4	0
2	A	1195	NAG	4	0
2	A	1196	NAG	3	0
3	A	1197	MAN	3	0
3	A	1198	MAN	3	0
3	A	1199	MAN	1	0
3	A	1200	MAN	1	0
3	A	1201	MAN	2	0
3	A	1202	MAN	1	0
6	A	1203	GAL	3	0
6	A	1204	GAL	2	0
2	A	1229	NAG	3	0
2	A	1230	NAG	8	0
3	A	1231	MAN	9	0
3	A	1232	MAN	4	0
3	A	1233	MAN	2	0
3	A	1234	MAN	5	0
3	A	1235	MAN	7	0
6	A	1236	GAL	6	0
6	A	1237	GAL	2	0
2	A	1277	NAG	3	0
2	A	1278	NAG	2	0
3	A	1279	MAN	7	0
4	A	1280	BMA	6	0
3	A	1281	MAN	3	0
3	A	1283	MAN	7	0
3	A	1284	MAN	10	0
3	A	1285	MAN	5	0
6	A	1286	GAL	4	0
6	A	1287	GAL	4	0
2	A	1318	NAG	4	0
2	A	1319	NAG	3	0
3	A	1320	MAN	2	0
2	A	1328	NAG	7	0
2	A	1329	NAG	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1330	MAN	7	0
3	A	1331	MAN	4	0
3	A	1332	MAN	1	0
2	A	1345	NAG	11	0
2	A	1346	NAG	3	0
3	A	1347	MAN	6	0
3	A	1348	MAN	6	0
3	A	1349	MAN	9	0
3	A	1350	MAN	3	0
3	A	1351	MAN	3	0
4	A	1352	BMA	3	0
2	A	1356	NAG	9	0
5	A	1357	NDG	5	0
3	A	1358	MAN	5	0
3	A	1359	MAN	6	0
3	A	1360	MAN	5	0
3	A	1361	MAN	1	0
3	A	1362	MAN	4	0
2	A	1363	NAG	4	0
7	A	1364	FUC	2	0
2	A	1386	NAG	7	0
5	A	1387	NDG	1	0
3	A	1388	MAN	4	0
3	A	1389	MAN	3	0
3	A	1390	MAN	5	0
3	A	1391	MAN	7	0
2	A	1392	NAG	6	0
3	A	1393	MAN	4	0
4	A	1394	BMA	2	0
7	A	1395	FUC	3	0
2	A	1411	NAG	7	0
2	A	1412	NAG	9	0
3	A	1413	MAN	3	0
2	A	1435	NAG	4	0
2	A	1436	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	440/470 (93%)	0.02	16 (3%) 46 37	22, 46, 85, 97	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	435	ASN	7.7
1	A	431	SER	5.1
1	A	443	ASN	5.1
1	A	433	THR	4.4
1	A	432	PRO	4.3
1	A	294	GLY	3.4
1	A	440	ALA	3.2
1	A	255	ILE	3.0
1	A	290	PRO	3.0
1	A	441	ALA	3.0
1	A	430	THR	2.7
1	A	258	THR	2.2
1	A	438	GLY	2.2
1	A	289	GLY	2.2
1	A	442	PRO	2.1
1	A	293	SER	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

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^{th} 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	MAN	A	1171	11/12	0.66	1.11	3.99	129,129,129,129	0
7	FUC	A	1364	10/11	0.64	0.48	3.47	129,129,129,129	0
2	NAG	A	1195	14/15	0.65	0.59	1.45	129,129,129,129	0
2	NAG	A	1345	14/15	0.83	0.26	1.42	129,129,129,129	0
2	NAG	A	1278	14/15	0.86	0.26	0.12	129,129,129,129	0
3	MAN	A	1283	11/12	0.61	0.54	-	129,129,129,129	0
3	MAN	A	1350	11/12	0.34	0.89	-	129,129,129,129	0
3	MAN	A	1170	11/12	0.10	0.68	-	129,129,129,129	0
3	MAN	A	1089	11/12	0.29	0.51	-	129,129,129,129	0
4	BMA	A	1090	11/12	0.56	0.57	-	129,129,129,129	0
3	MAN	A	1351	11/12	0.02	1.05	-	129,129,129,129	0
2	NAG	A	1048	14/15	0.85	0.35	-	129,129,129,129	0
3	MAN	A	1118	11/12	0.73	0.89	-	129,129,129,129	0
3	MAN	A	1285	11/12	0.20	0.75	-	129,129,129,129	0
2	NAG	A	1167	14/15	0.82	0.17	-	129,129,129,129	0
3	MAN	A	1235	11/12	0.67	0.59	-	129,129,129,129	0
3	MAN	A	1200	11/12	0.32	0.69	-	129,129,129,129	0
3	MAN	A	1092	11/12	0.80	0.92	-	129,129,129,129	0
3	MAN	A	1121	11/12	0.22	0.70	-	129,129,129,129	0
6	GAL	A	1203	11/12	0.29	0.56	-	129,129,129,129	0
3	MAN	A	1174	11/12	0.38	0.84	-	129,129,129,129	0
3	MAN	A	1202	11/12	0.52	0.56	-	129,129,129,129	0
3	MAN	A	1116	11/12	0.21	0.79	-	129,129,129,129	0
4	BMA	A	1052	11/12	0.40	0.81	-	129,129,129,129	0
3	MAN	A	1120	11/12	0.10	1.43	-	129,129,129,129	0
2	NAG	A	1363	14/15	0.63	0.47	-	129,129,129,129	0
3	MAN	A	1388	11/12	0.54	0.60	-	129,129,129,129	0
3	MAN	A	1389	11/12	0.37	0.42	-	129,129,129,129	0
2	NAG	A	1115	14/15	0.77	0.46	-	129,129,129,129	0
5	NDG	A	1357	14/15	0.57	0.37	-	129,129,129,129	0
3	MAN	A	1349	11/12	0.46	0.79	-	129,129,129,129	0
3	MAN	A	1330	11/12	0.44	0.53	-	129,129,129,129	0
2	NAG	A	1328	14/15	0.47	0.32	-	129,129,129,129	0
3	MAN	A	1119	11/12	0.65	0.70	-	129,129,129,129	0
3	MAN	A	1281	11/12	0.45	0.79	-	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MAN	A	1332	11/12	0.51	0.58	-	129,129,129,129	0
2	NAG	A	1386	14/15	0.81	0.19	-	129,129,129,129	0
3	MAN	A	1361	11/12	0.34	1.04	-	129,129,129,129	0
3	MAN	A	1284	11/12	0.34	0.57	-	129,129,129,129	0
3	MAN	A	1093	11/12	0.48	0.65	-	129,129,129,129	0
2	NAG	A	1230	14/15	0.64	0.37	-	129,129,129,129	0
3	MAN	A	1173	11/12	0.63	0.83	-	129,129,129,129	0
3	MAN	A	1117	11/12	0.42	0.75	-	129,129,129,129	0
3	MAN	A	1231	11/12	0.61	0.65	-	129,129,129,129	0
2	NAG	A	1436	14/15	0.48	1.05	-	129,129,129,129	0
3	MAN	A	1232	11/12	0.25	0.63	-	129,129,129,129	0
2	NAG	A	1088	14/15	0.34	0.50	-	129,129,129,129	0
2	NAG	A	1166	14/15	0.84	0.32	-	129,129,129,129	0
2	NAG	A	1356	14/15	0.65	0.26	-	129,129,129,129	0
3	MAN	A	1091	11/12	0.46	0.58	-	129,129,129,129	0
3	MAN	A	1360	11/12	0.46	0.93	-	129,129,129,129	0
3	MAN	A	1199	11/12	0.68	0.60	-	129,129,129,129	0
3	MAN	A	1393	11/12	0.55	0.66	-	129,129,129,129	0
4	BMA	A	1280	11/12	0.24	0.75	-	129,129,129,129	0
5	NDG	A	1387	14/15	0.84	0.35	-	129,129,129,129	0
3	MAN	A	1348	11/12	0.53	0.69	-	129,129,129,129	0
3	MAN	A	1201	11/12	0.68	0.83	-	129,129,129,129	0
2	NAG	A	1412	14/15	0.16	1.00	-	129,129,129,129	0
3	MAN	A	1169	11/12	0.45	0.60	-	129,129,129,129	0
4	BMA	A	1168	11/12	0.39	0.33	-	129,129,129,129	0
3	MAN	A	1233	11/12	0.67	0.51	-	129,129,129,129	0
4	BMA	A	1352	11/12	0.11	0.85	-	129,129,129,129	0
6	GAL	A	1286	11/12	0.65	0.75	-	129,129,129,129	0
2	NAG	A	1392	14/15	0.60	0.58	-	129,129,129,129	0
3	MAN	A	1279	11/12	0.52	0.35	-	129,129,129,129	0
3	MAN	A	1331	11/12	0.70	0.58	-	129,129,129,129	0
3	MAN	A	1198	11/12	0.32	0.66	-	129,129,129,129	0
2	NAG	A	1087	14/15	0.69	0.67	-	129,129,129,129	0
3	MAN	A	1050	11/12	0.44	0.63	-	129,129,129,129	0
2	NAG	A	1229	14/15	0.81	0.42	-	129,129,129,129	0
2	NAG	A	1196	14/15	0.59	0.87	-	129,129,129,129	0
3	MAN	A	1053	11/12	0.62	0.88	-	129,129,129,129	0
6	GAL	A	1204	11/12	0.48	0.46	-	129,129,129,129	0
3	MAN	A	1390	11/12	0.45	0.53	-	129,129,129,129	0
3	MAN	A	1413	11/12	0.52	0.42	-	129,129,129,129	0
6	GAL	A	1287	11/12	0.57	0.54	-	129,129,129,129	0
2	NAG	A	1277	14/15	0.81	0.37	-	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	GAL	A	1237	11/12	0.41	0.64	-	129,129,129,129	0
5	NDG	A	1114	14/15	0.57	0.33	-	129,129,129,129	0
2	NAG	A	1435	14/15	0.17	1.23	-	129,129,129,129	0
3	MAN	A	1391	11/12	0.51	0.66	-	129,129,129,129	0
7	FUC	A	1395	10/11	0.65	0.44	-	129,129,129,129	0
6	GAL	A	1236	11/12	0.68	0.54	-	129,129,129,129	0
3	MAN	A	1172	11/12	0.04	0.71	-	129,129,129,129	0
2	NAG	A	1047	14/15	0.87	0.22	-	129,129,129,129	0
2	NAG	A	1319	14/15	0.64	0.41	-	129,129,129,129	0
3	MAN	A	1359	11/12	0.20	0.52	-	129,129,129,129	0
3	MAN	A	1051	11/12	0.61	0.65	-	129,129,129,129	0
3	MAN	A	1358	11/12	0.56	0.81	-	129,129,129,129	0
2	NAG	A	1329	14/15	0.73	0.37	-	129,129,129,129	0
3	MAN	A	1347	11/12	0.38	0.30	-	129,129,129,129	0
3	MAN	A	1234	11/12	0.01	0.77	-	129,129,129,129	0
2	NAG	A	1411	14/15	0.65	0.51	-	129,129,129,129	0
3	MAN	A	1362	11/12	0.38	0.83	-	129,129,129,129	0
2	NAG	A	1346	14/15	0.78	0.18	-	129,129,129,129	0
4	BMA	A	1394	11/12	0.45	0.64	-	129,129,129,129	0
3	MAN	A	1320	11/12	0.49	0.51	-	129,129,129,129	0
3	MAN	A	1282	11/12	0.35	0.95	-	129,129,129,129	0
3	MAN	A	1197	11/12	0.54	0.81	-	129,129,129,129	0
2	NAG	A	1318	14/15	0.69	0.39	-	129,129,129,129	0
3	MAN	A	1049	11/12	0.63	0.44	-	129,129,129,129	0

6.5 Other polymers (i)

There are no such residues in this entry.