



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 11:15 PM BST

PDB ID : 5NV4  
Title : UDP-Glucose Glycoprotein Glucosyltransferase from Chaetomium thermophilum double mutant D611C:G1050C  
Authors : Roversi, P.; Caputo, A.T.; Hill, J.; Alonzi, D.S.; Zitzmann, N.  
Deposited on : 2017-05-03  
Resolution : 2.78 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

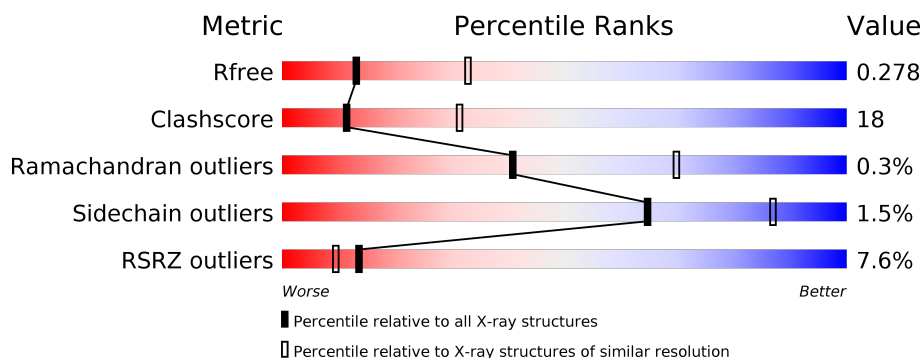
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 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))
$R_{free}$	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	1494	
2	B	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1601	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11198 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 UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1377	Total	C	N	O	S	0	0	0
			11066	7080	1884	2068	34			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	-	expression tag	UNP G0SB58
A	22	THR	-	expression tag	UNP G0SB58
A	23	GLY	-	expression tag	UNP G0SB58
A	611	CYS	ASP	engineered mutation	UNP G0SB58
A	1050	CYS	GLY	engineered mutation	UNP G0SB58
A	1506	GLY	-	expression tag	UNP G0SB58
A	1507	THR	-	expression tag	UNP G0SB58
A	1508	LYS	-	expression tag	UNP G0SB58
A	1509	HIS	-	expression tag	UNP G0SB58
A	1510	HIS	-	expression tag	UNP G0SB58
A	1511	HIS	-	expression tag	UNP G0SB58
A	1512	HIS	-	expression tag	UNP G0SB58
A	1513	HIS	-	expression tag	UNP G0SB58
A	1514	HIS	-	expression tag	UNP G0SB58

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula:  $CH_2O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		

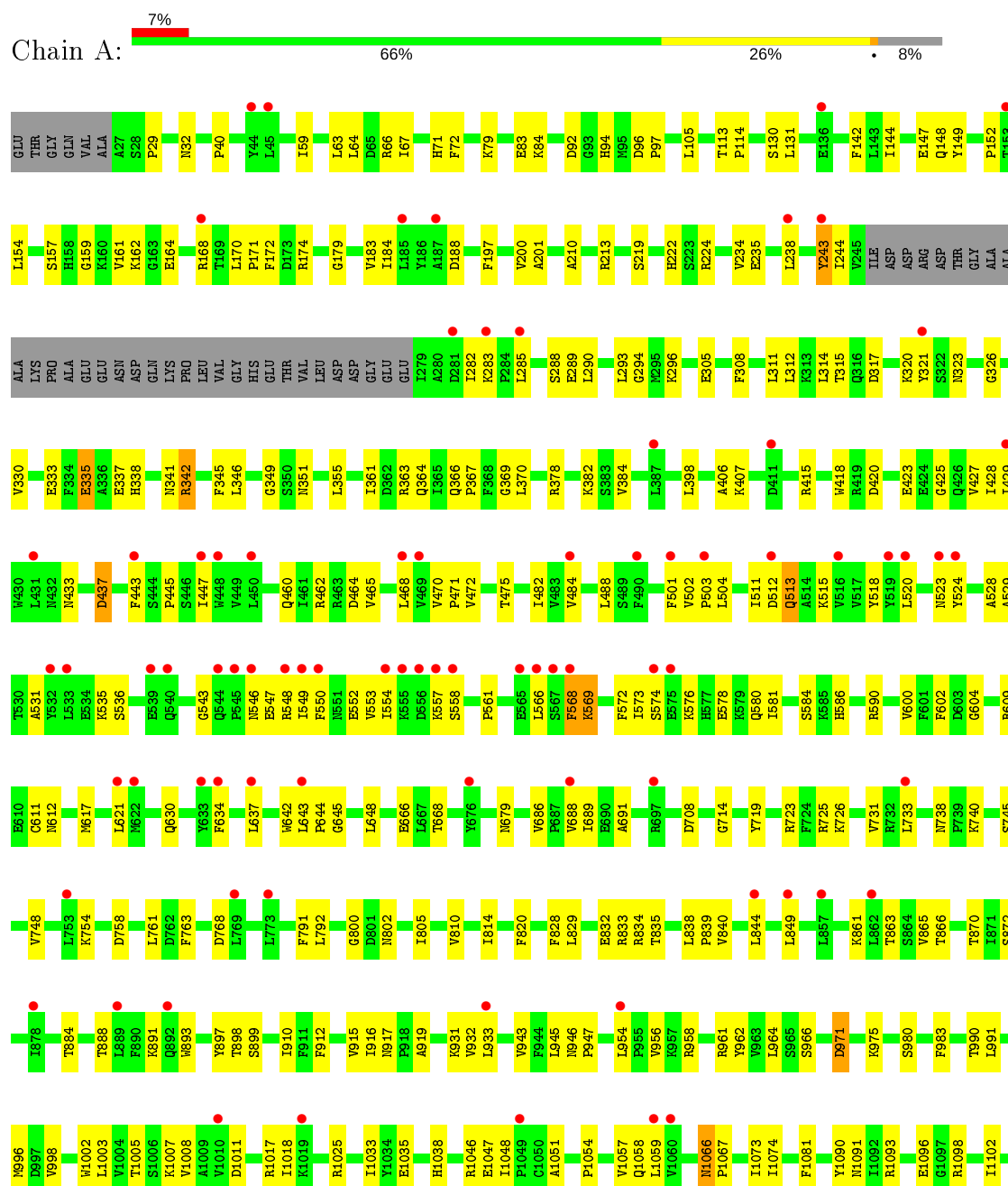
- Molecule 5 is water.

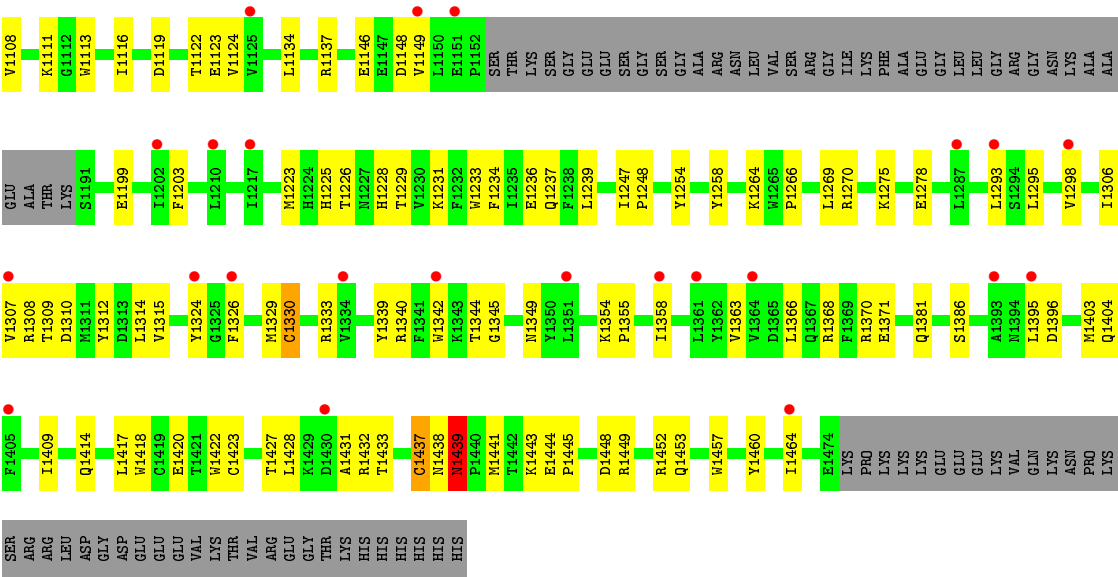
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	34	Total	O	0	0
			34	34		

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: UDP-glucose-glycoprotein glucosyltransferase-like protein





● Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.23Å 142.16Å 186.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.85 – 2.78 77.85 – 2.78	Depositor EDS
% Data completeness (in resolution range)	97.8 (77.85-2.78) 97.8 (77.85-2.78)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.239 , 0.245 0.265 , 0.278	Depositor DCC
$R_{free}$ test set	2526 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	90.7	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 65.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11198	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.41	0/11331	0.73	3/15369 (0.0%)

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	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	568	PHE	C-N-CA	8.46	142.84	121.70
1	A	305	GLU	C-N-CA	8.08	141.90	121.70
1	A	243	TYR	C-N-CA	5.96	136.59	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1439	ASN	Mainchain
1	A	335	GLU	Peptide

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11066	0	10936	392	0
2	B	39	0	34	0	0
3	A	56	0	52	0	0
4	A	3	0	2	0	0
5	A	34	0	0	0	0
All	All	11198	0	11024	392	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 18.

All (392) 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:1329:MET:SD	1:A:1358:ILE:HD11	1.60	1.42
1:A:337:GLU:OE1	1:A:897:TYR:HD2	1.03	1.32
1:A:337:GLU:OE1	1:A:897:TYR:CD2	1.93	1.21
1:A:1295:LEU:HD21	1:A:1298:VAL:CG2	1.71	1.20
1:A:1225:HIS:ND1	1:A:1308:ARG:HA	1.54	1.19
1:A:149:TYR:CE1	1:A:157:SER:HB3	1.77	1.17
1:A:67:ILE:HG22	1:A:72:PHE:HD2	1.11	1.11
1:A:524:TYR:OH	1:A:566:LEU:HD22	1.50	1.09
1:A:554:ILE:HG21	1:A:568:PHE:HE1	1.18	1.08
1:A:1149:VAL:HG13	1:A:1371:GLU:O	1.52	1.07
1:A:1329:MET:SD	1:A:1358:ILE:CD1	2.43	1.06
1:A:67:ILE:HG22	1:A:72:PHE:CD2	1.89	1.06
1:A:1225:HIS:CE1	1:A:1308:ARG:HA	1.90	1.05
1:A:149:TYR:HE1	1:A:157:SER:HB3	1.11	1.05
1:A:524:TYR:HE2	1:A:558:SER:HG	1.04	1.02
1:A:72:PHE:CE1	1:A:84:LYS:HG3	1.95	1.01
1:A:338:HIS:O	1:A:341:ASN:HB2	1.61	1.00
1:A:482:ILE:HD12	1:A:609:ARG:HH22	1.25	0.98
1:A:546:ASN:HB3	1:A:549:ILE:HG22	1.42	0.98
1:A:554:ILE:HG21	1:A:568:PHE:CE1	2.00	0.96
1:A:1324:TYR:CD1	1:A:1326:PHE:HE1	1.82	0.95
1:A:1048:ILE:HD11	1:A:1137:ARG:HD2	1.49	0.94
1:A:338:HIS:HD2	1:A:898:THR:HG23	1.32	0.93
1:A:67:ILE:CG2	1:A:72:PHE:HD2	1.83	0.90
1:A:243:TYR:O	1:A:285:LEU:HG	1.70	0.90
1:A:566:LEU:HD13	1:A:568:PHE:CD2	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:PRO:HG3	1:A:462:ARG:NH2	1.88	0.89
1:A:72:PHE:HE1	1:A:84:LYS:HG3	1.27	0.88
1:A:561:PRO:HG3	1:A:566:LEU:HD23	1.55	0.88
1:A:1058:GLN:HG2	1:A:1073:ILE:HG22	1.55	0.88
1:A:311:LEU:O	1:A:315:THR:HG22	1.75	0.86
1:A:1059:LEU:HD11	1:A:1074:ILE:HD11	1.56	0.85
1:A:513:GLN:NE2	1:A:543:GLY:O	2.08	0.85
1:A:482:ILE:HD12	1:A:609:ARG:NH2	1.89	0.85
1:A:445:PRO:HG3	1:A:462:ARG:HH21	1.43	0.84
1:A:554:ILE:HG23	1:A:558:SER:HB2	1.58	0.84
1:A:1225:HIS:ND1	1:A:1308:ARG:CA	2.40	0.83
1:A:1007:LYS:HG3	1:A:1035:GLU:HB2	1.60	0.83
1:A:524:TYR:HE2	1:A:558:SER:OG	1.62	0.83
1:A:1324:TYR:CD1	1:A:1326:PHE:CE1	2.67	0.83
1:A:686:VAL:O	1:A:754:LYS:HE2	1.79	0.82
1:A:244:ILE:HD11	1:A:954:LEU:HD13	1.60	0.82
1:A:546:ASN:HB3	1:A:549:ILE:CG2	2.09	0.82
1:A:244:ILE:HA	1:A:285:LEU:HB3	1.64	0.80
1:A:67:ILE:CG2	1:A:72:PHE:CD2	2.63	0.79
1:A:346:LEU:HD12	1:A:893:TRP:CH2	2.18	0.78
1:A:566:LEU:HD13	1:A:568:PHE:CE2	2.17	0.78
1:A:1295:LEU:HD21	1:A:1298:VAL:HG23	1.63	0.78
1:A:1428:LEU:HD12	1:A:1431:ALA:HB3	1.64	0.78
1:A:243:TYR:HD1	1:A:285:LEU:HD23	1.46	0.78
1:A:523:ASN:OD1	1:A:566:LEU:HA	1.85	0.77
1:A:346:LEU:CD1	1:A:893:TRP:HH2	1.97	0.77
1:A:1295:LEU:HD21	1:A:1298:VAL:HG22	1.66	0.77
1:A:346:LEU:HD12	1:A:893:TRP:HH2	1.49	0.77
1:A:433:ASN:O	1:A:437:ASP:HB2	1.84	0.77
1:A:475:THR:HA	1:A:543:GLY:HA3	1.68	0.76
1:A:96:ASP:HB2	1:A:97:PRO:HD2	1.66	0.76
1:A:130:SER:O	1:A:161:VAL:HG13	1.85	0.76
1:A:546:ASN:CB	1:A:549:ILE:HG22	2.15	0.76
1:A:282:ILE:HG13	1:A:990:THR:HG22	1.68	0.75
1:A:1324:TYR:CE1	1:A:1326:PHE:HE1	2.04	0.75
1:A:296:LYS:HE2	1:A:330:VAL:HG13	1.68	0.75
1:A:566:LEU:O	1:A:566:LEU:HD12	1.87	0.75
1:A:384:VAL:HG23	1:A:865:VAL:HG11	1.67	0.74
1:A:142:PHE:HE1	1:A:197:PHE:HD2	1.34	0.74
1:A:1048:ILE:HD11	1:A:1137:ARG:HB3	1.70	0.74
1:A:515:LYS:CG	1:A:581:ILE:HD11	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LYS:HG3	1:A:581:ILE:HD11	1.70	0.73
1:A:835:THR:O	1:A:839:PRO:HD2	1.87	0.73
1:A:554:ILE:HG23	1:A:558:SER:CB	2.18	0.72
1:A:338:HIS:CD2	1:A:898:THR:HG23	2.20	0.72
1:A:1307:VAL:HG13	1:A:1433:THR:HG22	1.71	0.72
1:A:1295:LEU:HD21	1:A:1298:VAL:HG21	1.69	0.71
1:A:243:TYR:CD1	1:A:285:LEU:HD23	2.25	0.71
1:A:29:PRO:HB2	1:A:1018:ILE:HD13	1.72	0.71
1:A:547:GLU:HA	1:A:550:PHE:HB3	1.73	0.71
1:A:1314:LEU:HG	1:A:1363:VAL:CG2	2.21	0.71
1:A:384:VAL:CG2	1:A:865:VAL:HG11	2.21	0.71
1:A:1199:GLU:HB2	1:A:1229:THR:O	1.91	0.70
1:A:1324:TYR:CE1	1:A:1326:PHE:CE1	2.79	0.70
1:A:535:LYS:HE2	1:A:552:GLU:OE1	1.91	0.70
1:A:573:ILE:HB	1:A:576:LYS:HB3	1.71	0.70
1:A:872:SER:HB2	1:A:884:THR:OG1	1.90	0.70
1:A:66:ARG:O	1:A:71:HIS:HB3	1.92	0.70
1:A:420:ASP:HB3	1:A:425:GLY:HA2	1.74	0.70
1:A:524:TYR:HE2	1:A:558:SER:CB	2.04	0.69
1:A:244:ILE:HG12	1:A:285:LEU:HD12	1.73	0.69
1:A:152:PRO:HB3	1:A:200:VAL:HG21	1.74	0.69
1:A:1295:LEU:CD2	1:A:1298:VAL:CG2	2.63	0.69
1:A:1422:TRP:HZ3	1:A:1437:CYS:HB2	1.59	0.68
1:A:1108:VAL:HG12	1:A:1134:LEU:HD22	1.73	0.68
1:A:188:ASP:OD1	1:A:219:SER:HB3	1.93	0.68
1:A:326:GLY:HA2	1:A:330:VAL:HG11	1.74	0.68
1:A:1438:ASN:HA	1:A:1449:ARG:HH22	1.59	0.68
1:A:600:VAL:CG2	1:A:609:ARG:HG2	2.24	0.68
1:A:1354:LYS:HD2	1:A:1404:GLN:HG3	1.76	0.67
1:A:1048:ILE:CD1	1:A:1137:ARG:HB3	2.24	0.67
1:A:1366:LEU:O	1:A:1370:ARG:HG3	1.95	0.67
1:A:345:PHE:HB3	1:A:893:TRP:CZ2	2.29	0.67
1:A:834:ARG:O	1:A:839:PRO:HD3	1.94	0.66
1:A:142:PHE:CE1	1:A:197:PHE:HD2	2.13	0.66
1:A:149:TYR:CE1	1:A:157:SER:CB	2.70	0.66
1:A:482:ILE:CD1	1:A:609:ARG:NH2	2.57	0.66
1:A:1329:MET:CG	1:A:1358:ILE:HD11	2.24	0.66
1:A:600:VAL:HG23	1:A:609:ARG:CG	2.25	0.66
1:A:170:LEU:HD11	1:A:172:PHE:CE1	2.30	0.66
1:A:238:LEU:HD13	1:A:283:LYS:HE2	1.76	0.66
1:A:420:ASP:OD1	1:A:427:VAL:CG1	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:TYR:OH	1:A:566:LEU:CD2	2.39	0.66
1:A:512:ASP:HA	1:A:515:LYS:HE3	1.78	0.66
1:A:470:VAL:HG23	1:A:600:VAL:HG22	1.78	0.66
1:A:1418:TRP:HE1	1:A:1427:THR:HB	1.59	0.65
1:A:1247:ILE:HG13	1:A:1248:PRO:HD3	1.79	0.65
1:A:420:ASP:OD1	1:A:427:VAL:HG12	1.97	0.65
1:A:1003:LEU:HD21	1:A:1264:LYS:HB2	1.79	0.65
1:A:1098:ARG:HH21	1:A:1102:ILE:HD11	1.63	0.64
1:A:1333:ARG:HG2	1:A:1423:CYS:C	2.17	0.64
1:A:445:PRO:CG	1:A:462:ARG:HH21	2.11	0.64
1:A:418:TRP:HE1	1:A:648:LEU:HD11	1.62	0.64
1:A:335:GLU:HA	1:A:337:GLU:HG2	1.79	0.64
1:A:294:GLY:HA3	1:A:947:PRO:HB3	1.80	0.63
1:A:829:LEU:O	1:A:833:ARG:HB2	1.98	0.63
1:A:511:ILE:HG23	1:A:581:ILE:HD13	1.79	0.63
1:A:234:VAL:HG22	1:A:996:MET:CE	2.29	0.62
1:A:630:GLN:O	1:A:634:PHE:HD1	1.82	0.62
1:A:554:ILE:O	1:A:558:SER:HB3	1.98	0.62
1:A:835:THR:O	1:A:839:PRO:CD	2.47	0.62
1:A:553:VAL:O	1:A:557:LYS:HB2	2.01	0.61
1:A:398:LEU:CD2	1:A:866:THR:HG22	2.30	0.61
1:A:465:VAL:HG22	1:A:643:LEU:CD1	2.31	0.61
1:A:1091:ASN:OD1	1:A:1122:THR:HG23	2.00	0.61
1:A:524:TYR:CE1	1:A:566:LEU:HB3	2.36	0.61
1:A:1199:GLU:HG3	1:A:1229:THR:OG1	2.01	0.60
1:A:738:ASN:HD22	1:A:792:LEU:HD11	1.66	0.60
1:A:296:LYS:HE2	1:A:330:VAL:CG1	2.32	0.60
1:A:1339:TYR:HE2	1:A:1441:MET:SD	2.23	0.60
1:A:296:LYS:HG2	1:A:330:VAL:HG22	1.82	0.60
1:A:1058:GLN:CG	1:A:1073:ILE:HG22	2.30	0.60
1:A:600:VAL:HG23	1:A:609:ARG:HG2	1.82	0.60
1:A:289:GLU:OE1	1:A:289:GLU:HA	2.01	0.59
1:A:554:ILE:HD13	1:A:568:PHE:CE1	2.37	0.59
1:A:1048:ILE:HD11	1:A:1137:ARG:CD	2.30	0.59
1:A:406:ALA:HB2	1:A:839:PRO:HG2	1.84	0.59
1:A:572:PHE:O	1:A:572:PHE:CD1	2.55	0.59
1:A:805:ILE:HG12	1:A:810:VAL:HG22	1.84	0.59
1:A:40:PRO:HB3	1:A:224:ARG:HD2	1.85	0.58
1:A:899:SER:HA	1:A:943:VAL:O	2.02	0.58
1:A:1324:TYR:HD1	1:A:1326:PHE:CE1	2.20	0.58
1:A:1225:HIS:HE1	1:A:1308:ARG:HG2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:ILE:O	1:A:558:SER:CB	2.52	0.58
1:A:536:SER:HA	1:A:549:ILE:HD13	1.86	0.58
1:A:472:VAL:O	1:A:503:PRO:HA	2.04	0.58
1:A:311:LEU:O	1:A:315:THR:CG2	2.51	0.57
1:A:998:VAL:HG22	1:A:1002:TRP:HB2	1.86	0.57
1:A:600:VAL:CG2	1:A:609:ARG:CG	2.81	0.57
1:A:1054:PRO:HB2	1:A:1057:VAL:HG21	1.87	0.57
1:A:520:LEU:HD23	1:A:529:ALA:HA	1.86	0.57
1:A:1339:TYR:CE2	1:A:1441:MET:SD	2.98	0.57
1:A:283:LYS:HZ3	1:A:285:LEU:HD11	1.70	0.57
1:A:465:VAL:HG22	1:A:643:LEU:HB2	1.87	0.57
1:A:1058:GLN:HG2	1:A:1073:ILE:CG2	2.31	0.56
1:A:524:TYR:CD2	1:A:558:SER:HA	2.39	0.56
1:A:915:VAL:HG12	1:A:946:ASN:ND2	2.20	0.56
1:A:283:LYS:NZ	1:A:285:LEU:HD21	2.20	0.56
1:A:1011:ASP:CG	1:A:1025:ARG:HH22	2.08	0.56
1:A:844:LEU:HD12	1:A:849:LEU:HB2	1.85	0.56
1:A:561:PRO:CG	1:A:566:LEU:HD23	2.31	0.56
1:A:566:LEU:CD1	1:A:568:PHE:CE2	2.89	0.56
1:A:1199:GLU:HG3	1:A:1229:THR:H	1.70	0.55
1:A:468:LEU:HD11	1:A:600:VAL:CG1	2.35	0.55
1:A:1247:ILE:HD12	1:A:1258:TYR:CD2	2.40	0.55
1:A:428:ILE:HA	1:A:502:VAL:HG12	1.88	0.55
1:A:600:VAL:HG23	1:A:609:ARG:HG3	1.88	0.55
1:A:398:LEU:HD23	1:A:866:THR:HG22	1.87	0.55
1:A:142:PHE:HE1	1:A:197:PHE:CD2	2.21	0.55
1:A:961:ARG:HG2	1:A:983:PHE:CE2	2.42	0.55
1:A:1247:ILE:HD12	1:A:1258:TYR:CE2	2.41	0.54
1:A:546:ASN:O	1:A:549:ILE:HG22	2.06	0.54
1:A:919:ALA:O	1:A:956:VAL:HG23	2.07	0.54
1:A:283:LYS:HZ2	1:A:285:LEU:HD21	1.73	0.54
1:A:234:VAL:HG22	1:A:996:MET:HE1	1.88	0.54
1:A:515:LYS:HG2	1:A:581:ILE:HD11	1.88	0.54
1:A:147:GLU:HA	1:A:159:GLY:O	2.07	0.54
1:A:142:PHE:HE2	1:A:201:ALA:HB2	1.72	0.54
1:A:144:ILE:HG12	1:A:183:VAL:HG12	1.89	0.54
1:A:468:LEU:HD11	1:A:600:VAL:HG12	1.90	0.54
1:A:991:LEU:HD23	1:A:1017:ARG:HG3	1.89	0.54
1:A:370:LEU:HD13	1:A:933:LEU:HD11	1.89	0.54
1:A:1309:THR:HG22	1:A:1310:ASP:O	2.08	0.54
1:A:1314:LEU:HG	1:A:1363:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:PRO:O	1:A:648:LEU:HD13	2.08	0.53
1:A:465:VAL:CG2	1:A:643:LEU:CD1	2.87	0.53
1:A:745:SER:O	1:A:748:VAL:HG22	2.08	0.53
1:A:1199:GLU:CG	1:A:1229:THR:OG1	2.57	0.53
1:A:341:ASN:OD1	1:A:893:TRP:CD1	2.61	0.53
1:A:991:LEU:HG	1:A:1017:ARG:HD2	1.90	0.53
1:A:535:LYS:C	1:A:549:ILE:HD11	2.28	0.53
1:A:92:ASP:HB2	1:A:94:HIS:CD2	2.43	0.53
1:A:174:ARG:O	1:A:213:ARG:HB3	2.09	0.53
1:A:840:VAL:HG21	1:A:863:THR:HA	1.91	0.53
1:A:1059:LEU:CD1	1:A:1074:ILE:HD11	2.33	0.53
1:A:1381:GLN:HG3	1:A:1403:MET:SD	2.48	0.53
1:A:282:ILE:HG13	1:A:990:THR:CG2	2.37	0.52
1:A:1098:ARG:HG3	1:A:1148:ASP:OD1	2.09	0.52
1:A:1306:ILE:HD11	1:A:1457:TRP:HD1	1.73	0.52
1:A:1439:ASN:HD22	1:A:1443:LYS:HA	1.73	0.52
1:A:566:LEU:CD1	1:A:568:PHE:CD2	2.89	0.52
1:A:235:GLU:HB2	1:A:958:ARG:HD2	1.91	0.52
1:A:1102:ILE:HD13	1:A:1146:GLU:HB2	1.91	0.52
1:A:1270:ARG:HD2	1:A:1386:SER:OG	2.09	0.52
1:A:415:ARG:HA	1:A:604:GLY:O	2.08	0.52
1:A:691:ALA:HB2	1:A:731:VAL:C	2.30	0.52
1:A:1324:TYR:CE1	1:A:1409:ILE:HG12	2.45	0.51
1:A:342:ARG:NE	1:A:342:ARG:O	2.33	0.51
1:A:290:LEU:HA	1:A:293:LEU:HD13	1.92	0.51
1:A:536:SER:HA	1:A:549:ILE:CD1	2.41	0.51
1:A:518:TYR:HB3	1:A:580:GLN:OE1	2.11	0.51
1:A:763:PHE:HD1	1:A:768:ASP:HB3	1.76	0.51
1:A:1368:ARG:O	1:A:1368:ARG:HD3	2.10	0.50
1:A:511:ILE:HG22	1:A:515:LYS:HE2	1.92	0.50
1:A:312:LEU:HD22	1:A:931:LYS:HD3	1.93	0.50
1:A:445:PRO:HD3	1:A:462:ARG:HH21	1.76	0.50
1:A:234:VAL:HG22	1:A:996:MET:HE2	1.94	0.50
1:A:429:ILE:HD11	1:A:501:PHE:CZ	2.46	0.50
1:A:548:ARG:O	1:A:552:GLU:HG3	2.12	0.50
1:A:1344:THR:HG22	1:A:1345:GLY:N	2.26	0.50
1:A:465:VAL:HG22	1:A:643:LEU:HD12	1.93	0.50
1:A:932:VAL:HG11	1:A:964:LEU:HG	1.94	0.50
1:A:415:ARG:HG2	1:A:415:ARG:HH11	1.77	0.50
1:A:484:VAL:O	1:A:488:LEU:HD12	2.11	0.50
1:A:149:TYR:CD2	1:A:154:LEU:CD1	2.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LYS:O	1:A:83:GLU:HG2	2.11	0.50
1:A:349:GLY:HA2	1:A:917:ASN:HB2	1.94	0.50
1:A:668:THR:HG23	1:A:810:VAL:HB	1.94	0.49
1:A:915:VAL:HG12	1:A:946:ASN:HD22	1.77	0.49
1:A:1005:THR:HG21	1:A:1236:GLU:HG2	1.95	0.49
1:A:59:ILE:O	1:A:63:LEU:HG	2.13	0.49
1:A:546:ASN:O	1:A:549:ILE:CG2	2.61	0.49
1:A:174:ARG:O	1:A:213:ARG:CB	2.61	0.49
1:A:566:LEU:C	1:A:566:LEU:HD12	2.32	0.49
1:A:1247:ILE:CG1	1:A:1248:PRO:HD3	2.43	0.49
1:A:471:PRO:HA	1:A:502:VAL:O	2.12	0.49
1:A:1247:ILE:CD1	1:A:1258:TYR:CE2	2.95	0.49
1:A:420:ASP:OD1	1:A:427:VAL:HG13	2.13	0.49
1:A:447:ILE:HD11	1:A:637:LEU:HB3	1.95	0.49
1:A:1295:LEU:CD2	1:A:1298:VAL:HG23	2.38	0.49
1:A:427:VAL:CG2	1:A:584:SER:HA	2.43	0.49
1:A:524:TYR:CE2	1:A:558:SER:HA	2.48	0.48
1:A:290:LEU:O	1:A:293:LEU:HD13	2.13	0.48
1:A:1329:MET:SD	1:A:1358:ILE:CG1	3.01	0.48
1:A:1395:LEU:HD12	1:A:1396:ASP:N	2.27	0.48
1:A:468:LEU:HD22	1:A:617:MET:SD	2.54	0.48
1:A:1108:VAL:CG1	1:A:1134:LEU:HD22	2.40	0.48
1:A:66:ARG:O	1:A:71:HIS:CB	2.60	0.48
1:A:465:VAL:CG2	1:A:643:LEU:HD13	2.44	0.48
1:A:351:ASN:HA	1:A:915:VAL:O	2.13	0.48
1:A:1054:PRO:O	1:A:1074:ILE:CG2	2.62	0.48
1:A:1234:PHE:HB3	1:A:1239:LEU:HD11	1.95	0.48
1:A:130:SER:HB3	1:A:162:LYS:O	2.13	0.48
1:A:1422:TRP:HZ3	1:A:1437:CYS:CB	2.27	0.48
1:A:1444:GLU:OE2	1:A:1452:ARG:NH2	2.47	0.48
1:A:285:LEU:HA	1:A:285:LEU:HD13	1.76	0.48
1:A:691:ALA:HA	1:A:725:ARG:HH21	1.78	0.47
1:A:443:PHE:CD1	1:A:460:GLN:HB3	2.49	0.47
1:A:691:ALA:HB2	1:A:731:VAL:O	2.15	0.47
1:A:445:PRO:CD	1:A:462:ARG:HH21	2.27	0.47
1:A:423:GLU:CD	1:A:590:ARG:HH11	2.18	0.47
1:A:726:LYS:HE3	1:A:761:LEU:HB2	1.95	0.47
1:A:170:LEU:HB2	1:A:171:PRO:HD2	1.96	0.47
1:A:511:ILE:HG22	1:A:515:LYS:CE	2.44	0.47
1:A:1344:THR:HG22	1:A:1345:GLY:H	1.80	0.47
1:A:1008:VAL:HB	1:A:1033:ILE:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1422:TRP:CZ3	1:A:1437:CYS:HB2	2.44	0.46
1:A:991:LEU:CD2	1:A:1017:ARG:HG3	2.45	0.46
1:A:645:GLY:HA2	1:A:648:LEU:HB2	1.96	0.46
1:A:164:GLU:HB3	1:A:168:ARG:HH12	1.80	0.46
1:A:520:LEU:CD2	1:A:529:ALA:HA	2.46	0.46
1:A:838:LEU:HD23	1:A:838:LEU:HA	1.75	0.46
1:A:1307:VAL:HG22	1:A:1433:THR:CG2	2.46	0.46
1:A:465:VAL:HG22	1:A:643:LEU:CB	2.45	0.46
1:A:105:LEU:HD13	1:A:966:SER:HA	1.97	0.46
1:A:1330:CYS:HA	1:A:1414:GLN:OE1	2.16	0.46
1:A:763:PHE:HD1	1:A:768:ASP:CB	2.29	0.46
1:A:1111:LYS:HG3	1:A:1119:ASP:HB3	1.98	0.46
1:A:296:LYS:HG2	1:A:330:VAL:CG2	2.45	0.46
1:A:548:ARG:O	1:A:552:GLU:OE2	2.34	0.46
1:A:916:ILE:O	1:A:945:LEU:HA	2.16	0.46
1:A:170:LEU:HD11	1:A:172:PHE:CZ	2.51	0.45
1:A:406:ALA:CB	1:A:839:PRO:HG2	2.45	0.45
1:A:861:LYS:O	1:A:865:VAL:HG23	2.17	0.45
1:A:361:ILE:HG13	1:A:364:GLN:HG3	1.98	0.45
1:A:1312:TYR:O	1:A:1315:VAL:N	2.49	0.45
1:A:708:ASP:O	1:A:714:GLY:HA3	2.16	0.45
1:A:740:LYS:HB2	1:A:800:GLY:HA3	1.99	0.45
1:A:998:VAL:HG23	1:A:1002:TRP:CE3	2.52	0.45
1:A:1333:ARG:NH2	1:A:1420:GLU:HG2	2.31	0.45
1:A:317:ASP:O	1:A:320:LYS:HB3	2.17	0.45
1:A:355:LEU:HD11	1:A:910:ILE:HG23	1.98	0.45
1:A:131:LEU:HD11	1:A:148:GLN:OE1	2.16	0.45
1:A:1439:ASN:OD1	1:A:1439:ASN:N	2.50	0.45
1:A:1046:ARG:NH2	1:A:1113:TRP:O	2.50	0.45
1:A:314:LEU:HD12	1:A:321:TYR:HD2	1.82	0.45
1:A:802:ASN:HB2	1:A:814:ILE:HB	1.98	0.45
1:A:1223:MET:HG3	1:A:1254:TYR:HB3	1.98	0.45
1:A:1275:LYS:O	1:A:1278:GLU:HB2	2.16	0.45
1:A:1340:ARG:HD3	1:A:1342:TRP:CZ2	2.51	0.45
1:A:423:GLU:OE1	1:A:590:ARG:NH1	2.50	0.45
1:A:524:TYR:CE2	1:A:558:SER:CB	2.94	0.45
1:A:349:GLY:HA2	1:A:946:ASN:O	2.17	0.44
1:A:554:ILE:HD13	1:A:568:PHE:HE1	1.78	0.44
1:A:602:PHE:HZ	1:A:621:LEU:HD13	1.82	0.44
1:A:406:ALA:HB2	1:A:839:PRO:CG	2.47	0.44
1:A:536:SER:N	1:A:549:ILE:HD11	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1093:ARG:NH1	1:A:1096:GLU:HG3	2.32	0.44
1:A:1306:ILE:HD11	1:A:1457:TRP:CD1	2.51	0.44
1:A:355:LEU:HD13	1:A:912:PHE:CZ	2.53	0.44
1:A:144:ILE:HB	1:A:149:TYR:HE2	1.83	0.44
1:A:738:ASN:HD22	1:A:792:LEU:CD1	2.30	0.44
1:A:998:VAL:CG2	1:A:1002:TRP:HE3	2.31	0.44
1:A:1111:LYS:HB3	1:A:1116:ILE:HD12	2.00	0.44
1:A:971:ASP:HB2	1:A:975:LYS:O	2.18	0.44
1:A:835:THR:O	1:A:839:PRO:HG2	2.17	0.44
1:A:1449:ARG:HB3	1:A:1453:GLN:OE1	2.19	0.43
1:A:465:VAL:CG2	1:A:643:LEU:HD12	2.47	0.43
1:A:471:PRO:HB2	1:A:504:LEU:HD21	1.99	0.43
1:A:465:VAL:HG21	1:A:643:LEU:HD13	2.00	0.43
1:A:888:THR:O	1:A:891:LYS:HG2	2.18	0.43
1:A:142:PHE:HZ	1:A:197:PHE:O	2.02	0.43
1:A:576:LYS:O	1:A:580:GLN:HB2	2.19	0.43
1:A:1005:THR:HG22	1:A:1237:GLN:HA	2.01	0.43
1:A:1417:LEU:HD12	1:A:1417:LEU:HA	1.88	0.43
1:A:346:LEU:HD11	1:A:893:TRP:HH2	1.81	0.43
1:A:1066:ASN:HA	1:A:1067:PRO:HD3	1.70	0.43
1:A:1428:LEU:HD12	1:A:1431:ALA:CB	2.42	0.43
1:A:443:PHE:CE1	1:A:460:GLN:CB	3.02	0.43
1:A:1003:LEU:HD12	1:A:1038:HIS:HB2	1.99	0.43
1:A:113:THR:OG1	1:A:114:PRO:HD3	2.19	0.43
1:A:1266:PRO:HD2	1:A:1269:LEU:HD23	2.00	0.43
1:A:154:LEU:O	1:A:154:LEU:HG	2.19	0.43
1:A:179:GLY:HA3	1:A:210:ALA:HA	2.01	0.43
1:A:828:PHE:O	1:A:832:GLU:HB2	2.18	0.43
1:A:1074:ILE:HD13	1:A:1081:PHE:HB3	2.00	0.43
1:A:1098:ARG:HG2	1:A:1148:ASP:HA	2.01	0.43
1:A:418:TRP:NE1	1:A:648:LEU:HD11	2.30	0.43
1:A:142:PHE:HA	1:A:184:ILE:O	2.19	0.42
1:A:719:TYR:O	1:A:723:ARG:HG3	2.20	0.42
1:A:998:VAL:CG2	1:A:1002:TRP:CE3	3.02	0.42
1:A:335:GLU:HG3	1:A:335:GLU:O	2.19	0.42
1:A:524:TYR:HD2	1:A:558:SER:HA	1.84	0.42
1:A:1231:LYS:HD3	1:A:1233:TRP:CZ2	2.54	0.42
1:A:244:ILE:CG1	1:A:285:LEU:HD12	2.43	0.42
1:A:345:PHE:CD1	1:A:345:PHE:C	2.92	0.42
1:A:679:ASN:ND2	1:A:791:PHE:HB2	2.35	0.42
1:A:1093:ARG:HH12	1:A:1096:GLU:HG3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:HD13	1:A:933:LEU:CD1	2.48	0.42
1:A:1054:PRO:HB2	1:A:1057:VAL:CG2	2.50	0.42
1:A:998:VAL:HG23	1:A:1002:TRP:HE3	1.85	0.42
1:A:528:ALA:O	1:A:531:ALA:HB3	2.20	0.41
1:A:961:ARG:HD3	1:A:961:ARG:HA	1.93	0.41
1:A:1309:THR:OG1	1:A:1432:ARG:HB3	2.19	0.41
1:A:573:ILE:HB	1:A:576:LYS:CB	2.46	0.41
1:A:686:VAL:O	1:A:688:VAL:HG23	2.20	0.41
1:A:835:THR:O	1:A:839:PRO:CG	2.69	0.41
1:A:407:LYS:HD2	1:A:870:THR:OG1	2.21	0.41
1:A:243:TYR:CD1	1:A:285:LEU:CD2	2.99	0.41
1:A:366:GLN:CG	1:A:369:GLY:H	2.34	0.41
1:A:378:ARG:O	1:A:382:LYS:HG3	2.21	0.41
1:A:568:PHE:HB3	1:A:569:LYS:H	1.45	0.41
1:A:367:PRO:HD3	1:A:962:TYR:OH	2.20	0.41
1:A:1047:GLU:O	1:A:1051:ALA:HA	2.21	0.41
1:A:1445:PRO:HD2	1:A:1448:ASP:OD2	2.20	0.41
1:A:427:VAL:HG23	1:A:584:SER:HA	2.03	0.41
1:A:1111:LYS:HG3	1:A:1119:ASP:CB	2.49	0.41
1:A:574:SER:O	1:A:578:GLU:HB2	2.21	0.41
1:A:586:HIS:O	1:A:590:ARG:HB2	2.21	0.41
1:A:366:GLN:HG2	1:A:369:GLY:H	1.85	0.41
1:A:691:ALA:HA	1:A:725:ARG:NH2	2.36	0.41
1:A:689:ILE:HD12	1:A:733:LEU:HD23	2.02	0.41
1:A:1226:THR:OG1	1:A:1228:HIS:HB2	2.20	0.41
1:A:1438:ASN:CA	1:A:1449:ARG:HH22	2.29	0.41
1:A:294:GLY:CA	1:A:947:PRO:HB3	2.50	0.41
1:A:1354:LYS:HA	1:A:1355:PRO:HD3	1.94	0.41
1:A:333:GLU:O	1:A:333:GLU:HG2	2.21	0.41
1:A:464:ASP:OD2	1:A:642:TRP:NE1	2.52	0.41
1:A:1090:TYR:HB2	1:A:1124:VAL:HG23	2.02	0.40
1:A:1073:ILE:HG23	1:A:1293:LEU:HD21	2.03	0.40
1:A:1345:GLY:O	1:A:1349:ASN:CG	2.60	0.40
1:A:345:PHE:HB3	1:A:893:TRP:CE2	2.56	0.40
1:A:32:ASN:OD1	1:A:980:SER:HB3	2.22	0.40
1:A:1247:ILE:HG13	1:A:1248:PRO:CD	2.50	0.40
1:A:1460:TYR:O	1:A:1464:ILE:HG12	2.21	0.40
1:A:64:LEU:HA	1:A:64:LEU:HD12	1.92	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	1371/1494 (92%)	1311 (96%)	56 (4%)	4 (0%)	41 70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	569	LYS
1	A	288	SER
1	A	1439	ASN
1	A	666	GLU

### 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	1204/1298 (93%)	1186 (98%)	18 (2%)	65 87

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	A	308	PHE
1	A	323	ASN
1	A	342	ARG
1	A	363	ARG
1	A	437	ASP
1	A	513	GLN

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Mol	Chain	Res	Type
1	A	611	CYS
1	A	612	ASN
1	A	758	ASP
1	A	820	PHE
1	A	971	ASP
1	A	1066	ASN
1	A	1123	GLU
1	A	1203	PHE
1	A	1330	CYS
1	A	1437	CYS
1	A	1439	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

3 monosaccharides 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	B	1	1,2	14,14,15	0.34	0	17,19,21	0.98	1 (5%)
2	NAG	B	2	2	14,14,15	0.33	0	17,19,21	0.65	0
2	BMA	B	3	2	11,11,12	0.36	0	15,15,17	0.36	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
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	BMA	B	3	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O5-C1-C2	-3.24	106.17	111.29

There are no chirality outliers.

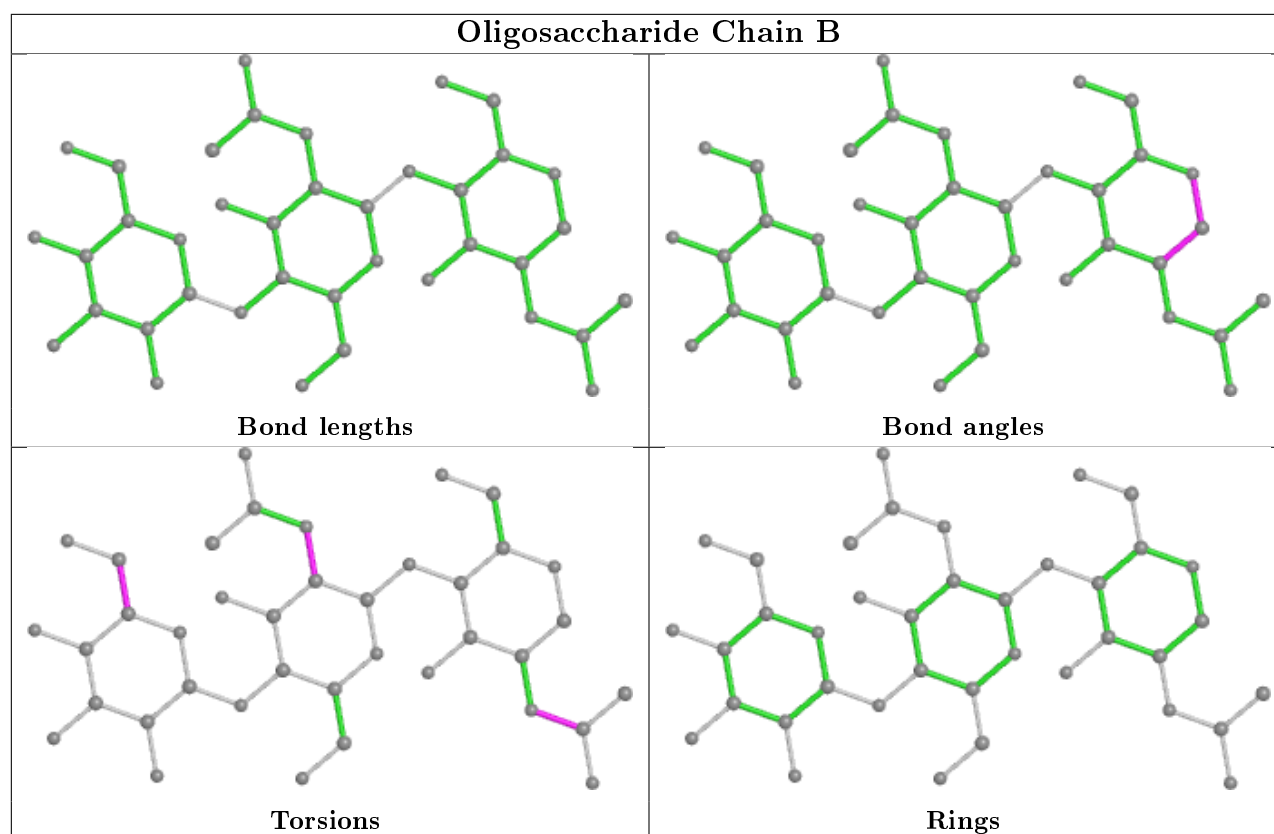
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	3	BMA	O5-C5-C6-O6
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	1607	1	14,14,15	0.28	0	17,19,21	0.53	0
3	NAG	A	1606	1	14,14,15	0.40	0	17,19,21	1.04	1 (5%)
3	NAG	A	1601	1	14,14,15	0.40	0	17,19,21	0.87	0
3	NAG	A	1602	1	14,14,15	0.32	0	17,19,21	0.64	0
4	FMT	A	1608	-	0,2,2	0.00	-	0,1,1	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.



'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1606	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1601	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1602	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1607	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1606	NAG	C1-O5-C5	3.76	117.28	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1606	NAG	C8-C7-N2-C2
3	A	1606	NAG	O7-C7-N2-C2
3	A	1601	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1377/1494 (92%)	0.69	104 (7%) <b>13</b> <b>9</b>	61, 103, 155, 264	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	549	ILE	7.3
1	A	519	TYR	5.6
1	A	1351	LEU	5.5
1	A	567	SER	5.3
1	A	524	TYR	5.2
1	A	281	ASP	4.5
1	A	1151	GLU	4.5
1	A	568	PHE	4.3
1	A	450	LEU	4.0
1	A	540	GLN	4.0
1	A	544	GLN	4.0
1	A	546	ASN	3.8
1	A	575	GLU	3.8
1	A	676	TYR	3.8
1	A	1217	ILE	3.7
1	A	574	SER	3.7
1	A	136	GLU	3.6
1	A	484	VAL	3.6
1	A	283	LYS	3.6
1	A	539	GLU	3.5
1	A	1059	LEU	3.4
1	A	1334	VAL	3.4
1	A	1149	VAL	3.4
1	A	1287	LEU	3.1
1	A	550	PHE	3.1
1	A	557	LYS	3.1
1	A	545	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1324	TYR	3.1
1	A	753	LEU	3.0
1	A	565	GLU	3.0
1	A	933	LEU	3.0
1	A	849	LEU	2.9
1	A	862	LEU	2.9
1	A	643	LEU	2.9
1	A	548	ARG	2.9
1	A	520	LEU	2.9
1	A	878	ILE	2.8
1	A	769	LEU	2.8
1	A	243	TYR	2.8
1	A	621	LEU	2.8
1	A	637	LEU	2.8
1	A	892	GLN	2.8
1	A	857	LEU	2.7
1	A	469	VAL	2.7
1	A	532	TYR	2.7
1	A	1361	LEU	2.7
1	A	1395	LEU	2.7
1	A	238	LEU	2.7
1	A	1210	LEU	2.7
1	A	468	LEU	2.7
1	A	501	PHE	2.7
1	A	554	ILE	2.6
1	A	633	TYR	2.6
1	A	185	LEU	2.6
1	A	566	LEU	2.6
1	A	954	LEU	2.6
1	A	1358	ILE	2.6
1	A	168	ARG	2.5
1	A	429	ILE	2.5
1	A	1202	ILE	2.5
1	A	387	LEU	2.5
1	A	411	ASP	2.5
1	A	1293	LEU	2.5
1	A	490	PHE	2.5
1	A	1326	PHE	2.5
1	A	1405	PHE	2.5
1	A	523	ASN	2.5
1	A	44	TYR	2.4
1	A	558	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	697	ARG	2.4
1	A	447	ILE	2.4
1	A	516	VAL	2.4
1	A	889	LEU	2.4
1	A	443	PHE	2.4
1	A	503	PRO	2.4
1	A	555	LYS	2.4
1	A	285	LEU	2.3
1	A	688	VAL	2.3
1	A	1364	VAL	2.3
1	A	431	LEU	2.3
1	A	512	ASP	2.3
1	A	556	ASP	2.3
1	A	45	LEU	2.2
1	A	1060	VAL	2.2
1	A	1298	VAL	2.2
1	A	187	ALA	2.2
1	A	321	TYR	2.2
1	A	1342	TRP	2.2
1	A	153	THR	2.2
1	A	1125	VAL	2.1
1	A	1049	PRO	2.1
1	A	622	MET	2.1
1	A	1019	LYS	2.1
1	A	844	LEU	2.1
1	A	1010	VAL	2.1
1	A	448	TRP	2.1
1	A	1307	VAL	2.1
1	A	1430	ASP	2.1
1	A	634	PHE	2.1
1	A	533	LEU	2.1
1	A	1393	ALA	2.0
1	A	733	LEU	2.0
1	A	1464	ILE	2.0
1	A	773	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

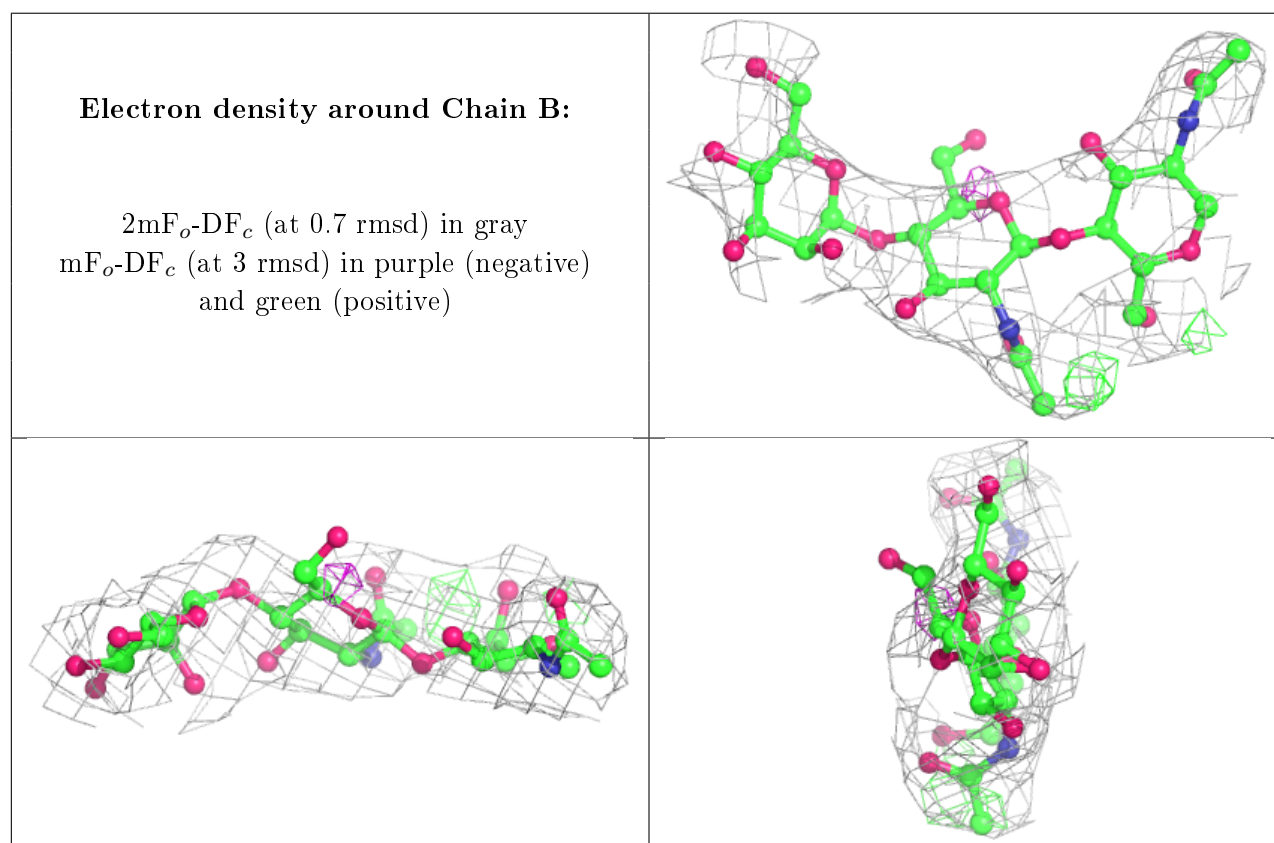
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BMA	B	3	11/12	0.67	0.22	144,147,153,154	0
2	NAG	B	2	14/15	0.78	0.21	127,131,139,142	0
2	NAG	B	1	14/15	0.88	0.14	107,111,119,123	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	1606	14/15	0.61	0.22	150,155,163,163	0
3	NAG	A	1601	14/15	0.70	0.46	150,155,158,158	0
3	NAG	A	1602	14/15	0.75	0.17	148,153,161,162	0
3	NAG	A	1607	14/15	0.78	0.21	215,221,224,226	0
4	FMT	A	1608	3/3	0.90	0.20	72,72,72,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.