Full wwPDB X-ray Structure Validation Report (i)

Mar 2, 2023 – 03:19 pm GMT

PDB ID	:	5MU1
Title	:	UDP-Glucose Glycoprotein Glucosyltransferase from Chaetomium thermophilum soaked with K2PtI6
Authors	:	Roversi, P.; Caputo, A.T.; Hill, J.; Alonzi, D.S.; Zitzmann, N.
Deposited on	:	2017-01-11
Resolution	:	3.48 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

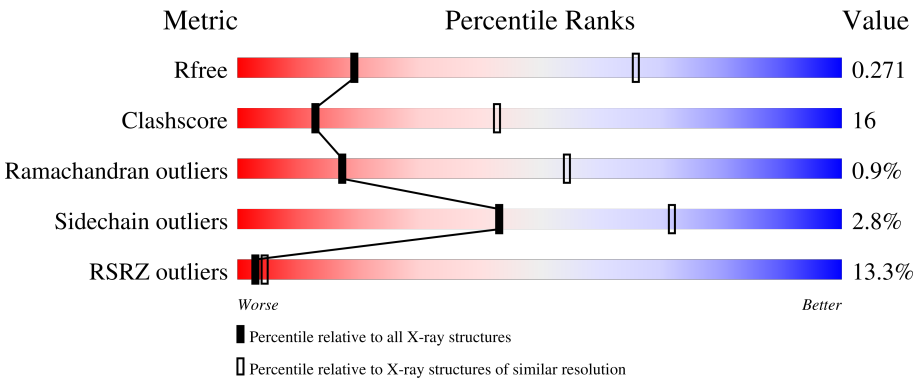
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.48 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	12%, 66%, 25%, • 8%
2	B	7	29%, 43%, 29%
3	C	5	40%, 60%
4	D	5	20%, 60%, 20%
5	E	7	71%, 29%

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	B	2	-	-	-	X
6	IOD	A	1606	-	-	X	-
6	IOD	A	1607	-	-	X	-
6	IOD	A	1614	-	-	X	-
6	IOD	A	1618	-	-	X	-
6	IOD	A	1619	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11720 atoms, of which 345 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.

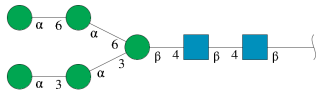
- Molecule 1 is a protein called UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	1377	11411	7080	345	1884	2070	32	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

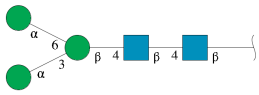
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	-	expression tag	UNP G0SB58
A	22	THR	-	expression tag	UNP G0SB58
A	23	GLY	-	expression tag	UNP G0SB58
A	1506	GLY	-	expression tag	UNP G0SB58
A	1507	THR	-	expression tag	UNP G0SB58
A	1508	LYS	-	expression tag	UNP G0SB58
A	1509	HIS	-	expression tag	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 alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



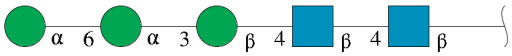
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	7	83	46	2	35	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



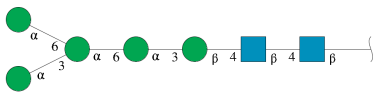
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	5	61	34	2	25	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-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
			Total	C	N	O			
4	D	5	61	34	2	25	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-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
			Total	C	N	O			
5	E	7	83	46	2	35	0	0	0

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
6	A	14	14	14	0	0

- Molecule 7 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Pt		
7	A	6	6	6	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

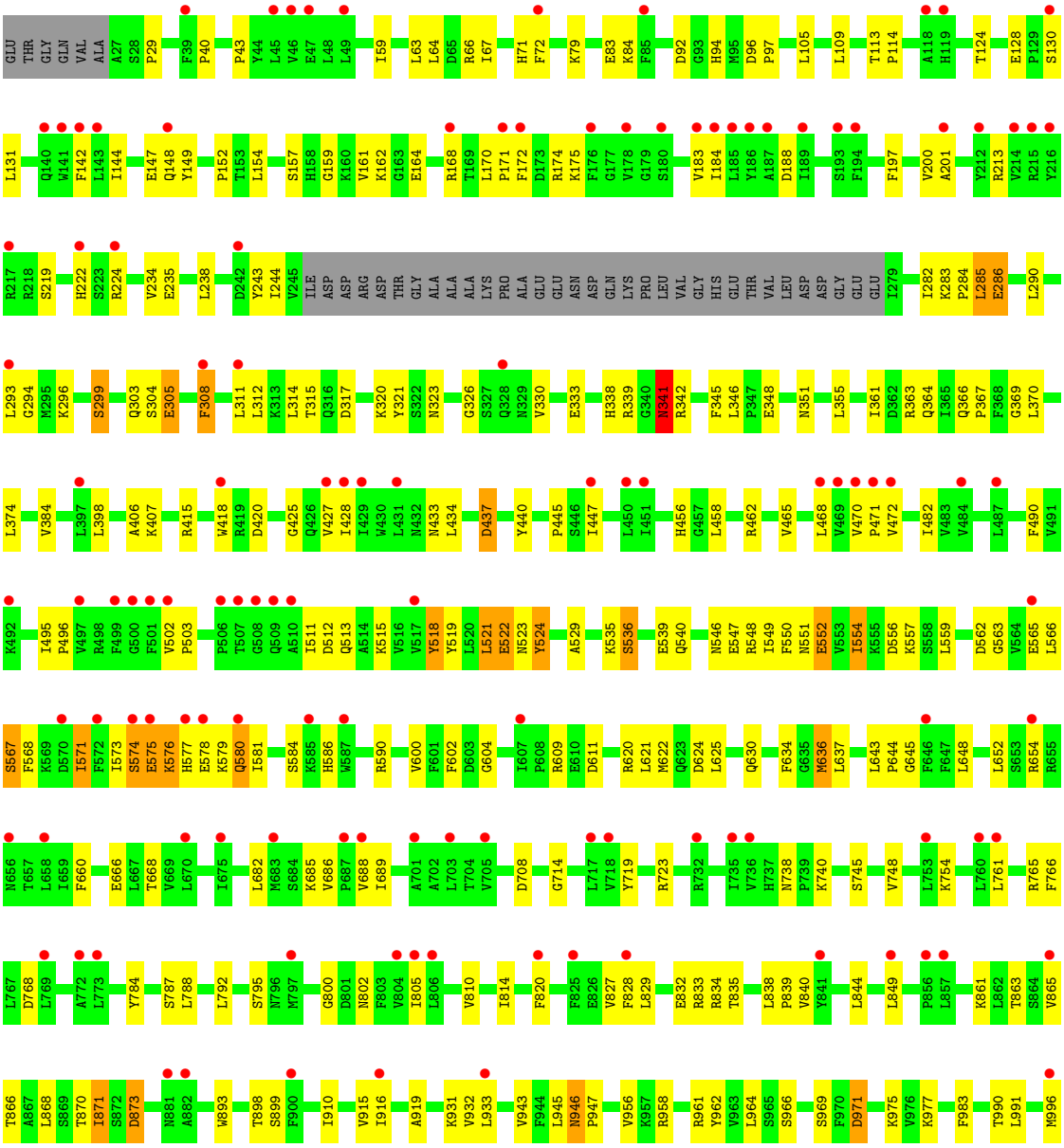
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
8	A	1	1	1	0	0

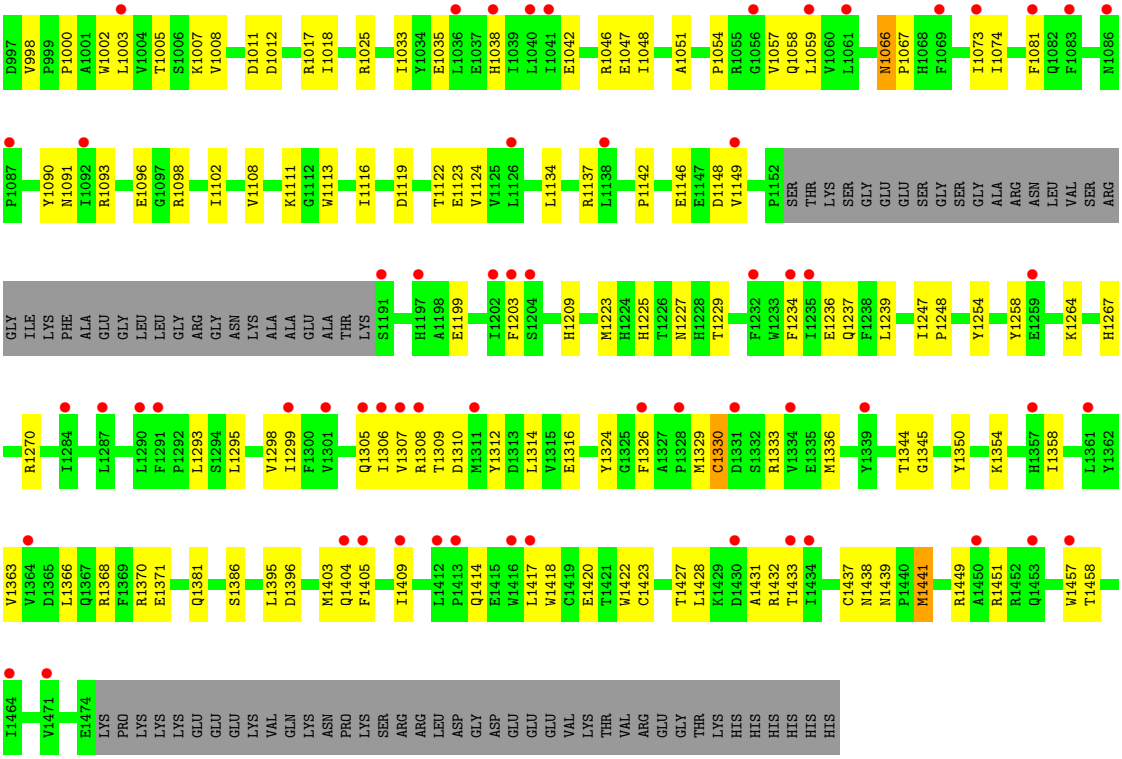
3 Residue-property plots (i)

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

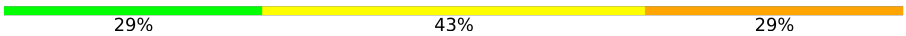
Chain A:

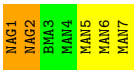




• Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



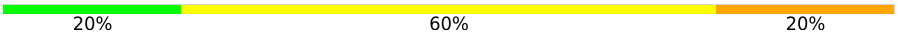


• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 4: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-

D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	116.95Å 116.95Å 301.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	101.28 – 3.48 101.28 – 3.48	Depositor EDS
% Data completeness (in resolution range)	86.8 (101.28-3.48) 86.8 (101.28-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 3.49Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.237 , 0.252 0.254 , 0.271	Depositor DCC
R_{free} test set	1269 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	123.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 94.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.074 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	11720	wwPDB-VP
Average B, all atoms (Å^2)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.47	0/11331	0.77	7/15369 (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	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	522	GLU	C-N-CA	9.11	144.49	121.70
1	A	523	ASN	N-CA-CB	6.74	122.72	110.60
1	A	341	ASN	CB-CA-C	5.90	122.20	110.40
1	A	523	ASN	C-N-CA	5.87	136.38	121.70
1	A	243	TYR	C-N-CA	5.48	135.40	121.70
1	A	285	LEU	N-CA-C	5.21	125.07	111.00
1	A	1441	MET	CB-CG-SD	-5.09	97.14	112.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	518	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11066	345	10936	365	0
2	B	83	0	70	4	0
3	C	61	0	52	0	0
4	D	61	0	52	1	0
5	E	83	0	70	2	0
6	A	14	0	0	12	0
7	A	6	0	0	1	0
8	A	1	0	0	0	0
All	All	11375	345	11180	372	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 16.

All (372) 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	1.68	1.33
1:A:244:ILE:CA	1:A:285:LEU:HD21	1.73	1.17
1:A:149:TYR:CE1	1:A:157:SER:HB3	1.83	1.13
1:A:1225:HIS:ND1	1:A:1308:ARG:HA	1.62	1.12
1:A:1295:LEU:HD21	1:A:1298:VAL:CG2	1.79	1.12
1:A:244:ILE:HA	1:A:285:LEU:CD2	1.83	1.07
1:A:67:ILE:HG22	1:A:72:PHE:CD2	1.91	1.05
1:A:67:ILE:HG22	1:A:72:PHE:HD2	1.15	1.04
1:A:1149:VAL:HG13	1:A:1371:GLU:O	1.57	1.02
1:A:72:PHE:CE1	1:A:84:LYS:HG3	1.99	0.97
1:A:1225:HIS:CE1	1:A:1308:ARG:HA	1.98	0.97
1:A:1329:MET:SD	1:A:1358:ILE:CD1	2.53	0.95
1:A:149:TYR:HE1	1:A:157:SER:HB3	1.21	0.93
1:A:458:LEU:HD23	1:A:496:PRO:HG2	1.51	0.92
1:A:1324:TYR:CD1	1:A:1326:PHE:HE1	1.86	0.92
1:A:546:ASN:HB3	1:A:549:ILE:HG22	1.50	0.91
1:A:1048:ILE:HD11	1:A:1137:ARG:HD2	1.53	0.89
1:A:1058:GLN:HG2	1:A:1073:ILE:HG22	1.54	0.89
1:A:338:HIS:HD2	1:A:898:THR:HG23	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PHE:HE1	1:A:84:LYS:HG3	1.35	0.88
1:A:1438:ASN:HA	1:A:1449:ARG:HH22	1.39	0.87
1:A:1441:MET:SD	6:A:1618:IOD:I	3.04	0.86
1:A:1441:MET:SD	6:A:1619:IOD:I	3.04	0.85
1:A:244:ILE:HA	1:A:285:LEU:HD21	0.89	0.85
1:A:67:ILE:CG2	1:A:72:PHE:HD2	1.89	0.84
1:A:456:HIS:HB2	6:A:1614:IOD:I	2.46	0.84
1:A:482:ILE:HD12	1:A:609:ARG:HH22	1.43	0.84
1:A:1441:MET:SD	7:A:1620:PT:PT	1.58	0.84
1:A:1422:TRP:CZ3	1:A:1437:CYS:SG	2.71	0.83
1:A:445:PRO:HG3	1:A:462:ARG:NH2	1.95	0.82
1:A:551:ASN:HA	1:A:554:ILE:HD12	1.60	0.81
1:A:686:VAL:O	1:A:754:LYS:HE2	1.79	0.81
2:B:1:NAG:H3	2:B:2:NAG:HN2	1.45	0.81
1:A:1007:LYS:HG3	1:A:1035:GLU:HB2	1.60	0.81
1:A:1324:TYR:CD1	1:A:1326:PHE:CE1	2.70	0.80
5:E:3:BMA:H3	5:E:4:MAN:H5	1.63	0.79
1:A:1059:LEU:HD11	1:A:1074:ILE:HD11	1.62	0.79
1:A:433:ASN:O	1:A:437:ASP:HB2	1.85	0.77
1:A:1350:TYR:CE1	1:A:1405:PHE:HE2	2.02	0.77
1:A:1314:LEU:HG	1:A:1363:VAL:CG2	2.15	0.76
1:A:384:VAL:HG23	1:A:865:VAL:HG11	1.67	0.76
1:A:1225:HIS:ND1	1:A:1308:ARG:CA	2.48	0.75
1:A:285:LEU:O	1:A:286:GLU:HB2	1.87	0.74
1:A:546:ASN:HB3	1:A:549:ILE:CG2	2.17	0.73
1:A:342:ARG:HD2	1:A:348:GLU:HG3	1.68	0.73
1:A:142:PHE:HE1	1:A:197:PHE:HD2	1.35	0.73
1:A:1295:LEU:HD21	1:A:1298:VAL:HG23	1.68	0.73
1:A:67:ILE:CG2	1:A:72:PHE:CD2	2.67	0.73
1:A:519:TYR:CG	1:A:576:LYS:HG2	2.24	0.72
1:A:1267:HIS:CD2	6:A:1606:IOD:I	3.13	0.72
1:A:338:HIS:CD2	1:A:898:THR:HG23	2.23	0.71
1:A:66:ARG:O	1:A:71:HIS:HB3	1.91	0.70
1:A:130:SER:O	1:A:161:VAL:HG13	1.92	0.70
1:A:1295:LEU:HD21	1:A:1298:VAL:HG22	1.73	0.70
1:A:1422:TRP:HZ3	1:A:1437:CYS:SG	2.13	0.69
1:A:420:ASP:HB3	1:A:425:GLY:HA2	1.74	0.69
1:A:1428:LEU:HD12	1:A:1431:ALA:HB3	1.74	0.69
1:A:515:LYS:CG	1:A:581:ILE:HD11	2.21	0.69
1:A:1048:ILE:HD11	1:A:1137:ARG:HB3	1.73	0.69
1:A:282:ILE:HG13	1:A:990:THR:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:PRO:HG3	1:A:462:ARG:HH21	1.55	0.69
1:A:1354:LYS:NZ	1:A:1405:PHE:CE1	2.57	0.69
1:A:188:ASP:OD1	1:A:219:SER:HB3	1.93	0.69
1:A:550:PHE:CD2	1:A:568:PHE:CZ	2.81	0.69
1:A:1324:TYR:CE1	1:A:1326:PHE:HE1	2.12	0.68
1:A:29:PRO:HB2	1:A:1018:ILE:HD13	1.74	0.68
1:A:1307:VAL:HG13	1:A:1433:THR:HG22	1.76	0.68
1:A:834:ARG:O	1:A:839:PRO:HD3	1.95	0.67
1:A:346:LEU:HD12	1:A:893:TRP:HH2	1.58	0.67
1:A:311:LEU:O	1:A:315:THR:HG22	1.93	0.67
1:A:326:GLY:HA2	1:A:330:VAL:HG11	1.75	0.67
1:A:142:PHE:CE1	1:A:197:PHE:HD2	2.12	0.67
1:A:296:LYS:HE2	1:A:330:VAL:HG13	1.77	0.67
1:A:152:PRO:HB3	1:A:200:VAL:HG21	1.76	0.66
1:A:304:SER:O	1:A:305:GLU:HB3	1.94	0.66
1:A:1098:ARG:HH21	1:A:1102:ILE:HD11	1.59	0.66
1:A:1042:GLU:CD	6:A:1606:IOD:I	3.04	0.66
1:A:1418:TRP:HE1	1:A:1427:THR:HB	1.61	0.65
1:A:341:ASN:HB2	1:A:893:TRP:CD1	2.31	0.65
1:A:550:PHE:HD2	1:A:568:PHE:CZ	2.14	0.65
1:A:346:LEU:HD12	1:A:893:TRP:CH2	2.32	0.65
1:A:546:ASN:CB	1:A:549:ILE:HG22	2.23	0.65
1:A:170:LEU:HD11	1:A:172:PHE:CE1	2.32	0.65
1:A:519:TYR:OH	1:A:577:HIS:HA	1.96	0.65
1:A:1366:LEU:O	1:A:1370:ARG:HG3	1.97	0.65
1:A:384:VAL:CG2	1:A:865:VAL:HG11	2.27	0.64
1:A:1324:TYR:CE1	1:A:1326:PHE:CE1	2.86	0.64
1:A:482:ILE:HD12	1:A:609:ARG:NH2	2.10	0.64
1:A:515:LYS:HG2	1:A:581:ILE:HD11	1.80	0.64
1:A:518:TYR:CD1	1:A:580:GLN:HG2	2.33	0.64
1:A:1048:ILE:CD1	1:A:1137:ARG:HB3	2.28	0.64
5:E:3:BMA:H3	5:E:4:MAN:C5	2.27	0.64
1:A:600:VAL:CG2	1:A:609:ARG:HG2	2.29	0.63
1:A:1108:VAL:HG12	1:A:1134:LEU:HD22	1.79	0.63
1:A:96:ASP:HB2	1:A:97:PRO:HD2	1.79	0.63
1:A:1350:TYR:CE1	1:A:1405:PHE:CE2	2.86	0.62
1:A:1042:GLU:OE2	6:A:1606:IOD:I	2.87	0.62
2:B:1:NAG:H3	2:B:2:NAG:N2	2.13	0.62
1:A:124:THR:HA	1:A:128:GLU:OE1	2.00	0.62
1:A:829:LEU:O	1:A:833:ARG:HB2	2.00	0.62
1:A:458:LEU:HD12	1:A:625:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:MET:CG	1:A:1358:ILE:HD11	2.29	0.62
1:A:304:SER:O	1:A:305:GLU:CB	2.46	0.62
1:A:346:LEU:CD1	1:A:893:TRP:HH2	2.13	0.61
1:A:40:PRO:HB3	1:A:224:ARG:HD2	1.83	0.61
1:A:1058:GLN:HG2	1:A:1073:ILE:CG2	2.30	0.61
1:A:1354:LYS:NZ	1:A:1405:PHE:CZ	2.63	0.61
1:A:398:LEU:HD23	1:A:866:THR:HG22	1.82	0.61
1:A:418:TRP:HE1	1:A:648:LEU:HD11	1.66	0.61
1:A:1058:GLN:CG	1:A:1073:ILE:HG22	2.30	0.60
1:A:1247:ILE:HG13	1:A:1248:PRO:HD3	1.82	0.60
1:A:600:VAL:HG23	1:A:609:ARG:CG	2.31	0.60
1:A:420:ASP:OD1	1:A:427:VAL:CG1	2.49	0.60
1:A:470:VAL:HG23	1:A:600:VAL:HG22	1.82	0.60
1:A:345:PHE:HB3	1:A:893:TRP:CZ2	2.37	0.59
1:A:1199:GLU:HB2	1:A:1229:THR:O	2.01	0.59
1:A:634:PHE:CG	6:A:1607:IOD:I	3.26	0.59
1:A:1054:PRO:HB2	1:A:1057:VAL:HG21	1.84	0.59
1:A:1333:ARG:HG2	1:A:1423:CYS:C	2.22	0.59
1:A:515:LYS:HG3	1:A:581:ILE:HD11	1.84	0.59
1:A:482:ILE:CD1	1:A:609:ARG:NH2	2.66	0.59
1:A:899:SER:HA	1:A:943:VAL:O	2.03	0.58
1:A:458:LEU:CD2	1:A:496:PRO:HG2	2.31	0.58
1:A:1422:TRP:CE3	1:A:1437:CYS:SG	2.96	0.58
1:A:519:TYR:CD1	1:A:576:LYS:HG2	2.39	0.57
2:B:2:NAG:O7	2:B:2:NAG:H3	2.04	0.57
1:A:932:VAL:HG11	1:A:964:LEU:HG	1.86	0.57
1:A:630:GLN:O	1:A:634:PHE:HD1	1.87	0.57
1:A:805:ILE:HG12	1:A:810:VAL:HG22	1.85	0.57
1:A:1438:ASN:HA	1:A:1449:ARG:NH2	2.15	0.57
1:A:144:ILE:HG12	1:A:183:VAL:HG12	1.86	0.57
1:A:420:ASP:OD1	1:A:427:VAL:HG12	2.04	0.56
1:A:600:VAL:HG23	1:A:609:ARG:HG2	1.86	0.56
1:A:174:ARG:O	1:A:213:ARG:HB3	2.04	0.56
1:A:142:PHE:HE1	1:A:197:PHE:CD2	2.21	0.56
1:A:142:PHE:HE2	1:A:201:ALA:HB2	1.71	0.56
1:A:458:LEU:HD22	1:A:621:LEU:HD21	1.88	0.56
1:A:1324:TYR:HD1	1:A:1326:PHE:CE1	2.22	0.56
1:A:602:PHE:HZ	1:A:621:LEU:HD13	1.70	0.56
1:A:1354:LYS:HD2	1:A:1404:GLN:HG3	1.87	0.56
1:A:1199:GLU:HG3	1:A:1229:THR:OG1	2.06	0.55
1:A:998:VAL:HG22	1:A:1002:TRP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:ARG:HB3	1:A:827:VAL:HG21	1.88	0.55
1:A:535:LYS:C	1:A:549:ILE:HD11	2.26	0.55
1:A:294:GLY:HA3	1:A:947:PRO:HB3	1.89	0.55
1:A:551:ASN:HA	1:A:554:ILE:CD1	2.35	0.55
1:A:296:LYS:HG2	1:A:330:VAL:HG22	1.89	0.55
1:A:519:TYR:HA	1:A:576:LYS:NZ	2.21	0.55
1:A:840:VAL:HG21	1:A:863:THR:HA	1.89	0.55
1:A:915:VAL:HG12	1:A:946:ASN:ND2	2.22	0.55
1:A:1295:LEU:HD21	1:A:1298:VAL:HG21	1.78	0.55
1:A:1091:ASN:OD1	1:A:1122:THR:HG23	2.07	0.54
1:A:547:GLU:HA	1:A:550:PHE:HB3	1.90	0.54
1:A:1059:LEU:CD1	1:A:1074:ILE:HD11	2.35	0.54
1:A:370:LEU:HD13	1:A:933:LEU:HD11	1.89	0.54
1:A:374:LEU:HD22	1:A:910:ILE:HG13	1.90	0.54
1:A:465:VAL:HG22	1:A:643:LEU:CD1	2.37	0.54
1:A:682:LEU:HD13	1:A:788:LEU:HG	1.90	0.54
1:A:234:VAL:HG22	1:A:996:MET:CE	2.38	0.54
1:A:536:SER:HA	1:A:549:ILE:HD13	1.89	0.54
1:A:600:VAL:CG2	1:A:609:ARG:CG	2.86	0.53
1:A:835:THR:O	1:A:839:PRO:HD2	2.07	0.53
1:A:546:ASN:O	1:A:549:ILE:HG22	2.08	0.53
1:A:518:TYR:CE1	1:A:580:GLN:HG2	2.43	0.53
1:A:636:MET:CE	6:A:1607:IOD:I	3.27	0.53
1:A:961:ARG:HG2	1:A:983:PHE:CE2	2.44	0.53
1:A:284:PRO:O	1:A:323:ASN:HB2	2.09	0.53
1:A:622:MET:CE	6:A:1614:IOD:I	3.27	0.53
1:A:447:ILE:HD11	1:A:637:LEU:HB3	1.91	0.53
1:A:468:LEU:HD11	1:A:600:VAL:CG1	2.38	0.53
1:A:1306:ILE:HD11	1:A:1457:TRP:HD1	1.74	0.53
1:A:355:LEU:HD11	1:A:910:ILE:HG23	1.90	0.53
1:A:1003:LEU:HD21	1:A:1264:LYS:HB2	1.90	0.52
1:A:1354:LYS:NZ	1:A:1354:LYS:HB2	2.24	0.52
1:A:458:LEU:HD23	1:A:496:PRO:CG	2.32	0.52
1:A:406:ALA:HB2	1:A:839:PRO:HG2	1.91	0.52
1:A:1247:ILE:HD12	1:A:1258:TYR:CD2	2.44	0.52
1:A:652:LEU:CD1	1:A:660:PHE:CZ	2.93	0.52
1:A:745:SER:O	1:A:748:VAL:HG22	2.08	0.52
1:A:689:ILE:HD13	1:A:761:LEU:HD23	1.90	0.52
1:A:147:GLU:HA	1:A:159:GLY:O	2.10	0.52
1:A:238:LEU:HD13	1:A:283:LYS:HE2	1.91	0.52
1:A:685:LYS:HD2	1:A:784:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:CG1	1:A:285:LEU:HD11	2.39	0.51
1:A:512:ASP:HA	1:A:515:LYS:HE3	1.92	0.51
1:A:1048:ILE:HD11	1:A:1137:ARG:CD	2.33	0.51
1:A:738:ASN:HD22	1:A:792:LEU:HD11	1.75	0.51
1:A:1011:ASP:CG	1:A:1025:ARG:HH22	2.14	0.51
1:A:92:ASP:HB2	1:A:94:HIS:CD2	2.46	0.51
1:A:341:ASN:HB2	1:A:893:TRP:HD1	1.75	0.51
1:A:366:GLN:HE21	1:A:369:GLY:HA3	1.75	0.51
1:A:1295:LEU:CD2	1:A:1298:VAL:CG2	2.71	0.51
1:A:535:LYS:HB3	1:A:549:ILE:HD11	1.93	0.51
1:A:244:ILE:HG12	1:A:285:LEU:HD11	1.94	0.50
1:A:290:LEU:HA	1:A:293:LEU:HD13	1.93	0.50
1:A:427:VAL:CG2	1:A:584:SER:HA	2.41	0.50
1:A:445:PRO:HD3	1:A:462:ARG:HH21	1.76	0.50
1:A:1354:LYS:HE2	1:A:1405:PHE:CD1	2.47	0.50
1:A:471:PRO:HA	1:A:502:VAL:O	2.11	0.50
1:A:1336:MET:CE	1:A:1441:MET:SD	3.00	0.50
1:A:296:LYS:HE2	1:A:330:VAL:CG1	2.41	0.50
1:A:366:GLN:OE1	1:A:1000:PRO:HD2	2.11	0.50
1:A:1223:MET:HG3	1:A:1254:TYR:HB3	1.93	0.50
1:A:445:PRO:CG	1:A:462:ARG:HH21	2.22	0.50
1:A:571:ILE:HG23	1:A:573:ILE:H	1.74	0.50
1:A:668:THR:HG23	1:A:810:VAL:HB	1.93	0.50
1:A:522:GLU:HB3	1:A:576:LYS:HZ1	1.76	0.50
1:A:144:ILE:HB	1:A:149:TYR:HE2	1.76	0.50
1:A:844:LEU:HD12	1:A:849:LEU:HB2	1.93	0.50
1:A:919:ALA:O	1:A:956:VAL:HG23	2.12	0.50
1:A:1199:GLU:HG3	1:A:1229:THR:H	1.76	0.50
1:A:1270:ARG:HD2	1:A:1386:SER:OG	2.12	0.50
1:A:174:ARG:O	1:A:213:ARG:CB	2.60	0.50
1:A:521:LEU:HD23	1:A:529:ALA:CB	2.41	0.50
1:A:312:LEU:HD22	1:A:931:LYS:HD3	1.94	0.49
1:A:547:GLU:HB3	1:A:568:PHE:CZ	2.46	0.49
1:A:79:LYS:O	1:A:83:GLU:HG2	2.12	0.49
1:A:1324:TYR:CE1	1:A:1409:ILE:HG12	2.48	0.49
1:A:1005:THR:HG22	1:A:1237:GLN:HA	1.94	0.49
1:A:600:VAL:HG23	1:A:609:ARG:HG3	1.94	0.49
1:A:235:GLU:HB2	1:A:958:ARG:HD2	1.95	0.49
1:A:1247:ILE:HD12	1:A:1258:TYR:CE2	2.48	0.49
1:A:244:ILE:N	1:A:285:LEU:HD21	2.27	0.49
1:A:1008:VAL:HB	1:A:1033:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:MET:HA	6:A:1619:IOD:I	2.82	0.49
1:A:308:PHE:CE2	1:A:931:LYS:HA	2.48	0.49
1:A:1314:LEU:HG	1:A:1363:VAL:HG22	1.91	0.48
1:A:285:LEU:O	1:A:286:GLU:CB	2.61	0.48
1:A:342:ARG:HG2	1:A:346:LEU:O	2.12	0.48
1:A:366:GLN:HG2	1:A:369:GLY:H	1.77	0.48
1:A:415:ARG:HA	1:A:604:GLY:O	2.14	0.48
1:A:511:ILE:HG22	1:A:515:LYS:HE2	1.96	0.48
1:A:1005:THR:HG21	1:A:1236:GLU:HG2	1.95	0.48
1:A:1336:MET:HE1	6:A:1618:IOD:I	2.84	0.48
1:A:1314:LEU:HG	1:A:1363:VAL:HG21	1.93	0.48
1:A:1368:ARG:O	1:A:1368:ARG:HD3	2.14	0.48
1:A:66:ARG:O	1:A:71:HIS:CB	2.61	0.47
1:A:1381:GLN:HG3	1:A:1403:MET:SD	2.53	0.47
1:A:366:GLN:CG	1:A:369:GLY:H	2.28	0.47
1:A:511:ILE:HG23	1:A:581:ILE:HD13	1.96	0.47
1:A:170:LEU:HB2	1:A:171:PRO:HD2	1.95	0.47
1:A:1395:LEU:HD12	1:A:1396:ASP:N	2.29	0.47
1:A:164:GLU:HB3	1:A:168:ARG:HH12	1.78	0.47
1:A:458:LEU:HD21	1:A:621:LEU:HD11	1.97	0.47
1:A:1309:THR:HG22	1:A:1310:ASP:O	2.12	0.47
1:A:511:ILE:HG22	1:A:515:LYS:CE	2.45	0.47
1:A:645:GLY:HA2	1:A:648:LEU:HB2	1.95	0.47
1:A:654:ARG:CB	1:A:827:VAL:HG21	2.44	0.47
1:A:363:ARG:HG2	1:A:1000:PRO:HG3	1.95	0.47
1:A:420:ASP:OD1	1:A:427:VAL:HG13	2.15	0.47
1:A:472:VAL:O	1:A:503:PRO:HA	2.15	0.47
1:A:861:LYS:O	1:A:865:VAL:HG23	2.15	0.47
1:A:342:ARG:CZ	1:A:946:ASN:HB2	2.45	0.47
1:A:398:LEU:CD2	1:A:866:THR:HG22	2.45	0.46
1:A:792:LEU:O	1:A:795:SER:O	2.32	0.46
1:A:428:ILE:HA	1:A:502:VAL:HG12	1.97	0.46
1:A:1354:LYS:HB2	1:A:1354:LYS:HZ3	1.79	0.46
1:A:571:ILE:O	1:A:577:HIS:HB2	2.15	0.46
1:A:1074:ILE:HD13	1:A:1081:PHE:HB3	1.97	0.46
1:A:835:THR:O	1:A:839:PRO:HG2	2.16	0.46
1:A:149:TYR:CE1	1:A:157:SER:CB	2.77	0.46
1:A:573:ILE:HG22	1:A:575:GLU:HG2	1.98	0.46
1:A:1073:ILE:HG23	1:A:1293:LEU:HD21	1.98	0.46
1:A:1108:VAL:CG1	1:A:1134:LEU:HD22	2.46	0.46
1:A:130:SER:HB3	1:A:162:LYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PHE:HZ	1:A:197:PHE:O	1.99	0.45
1:A:427:VAL:HG23	1:A:584:SER:HA	1.97	0.45
1:A:644:PRO:O	1:A:648:LEU:HD13	2.16	0.45
1:A:686:VAL:O	1:A:688:VAL:HG23	2.16	0.45
1:A:351:ASN:HA	1:A:915:VAL:O	2.16	0.45
1:A:1344:THR:HG22	1:A:1345:GLY:N	2.31	0.45
1:A:234:VAL:HG22	1:A:996:MET:HE2	1.99	0.45
1:A:1247:ILE:CG1	1:A:1248:PRO:HD3	2.45	0.45
1:A:234:VAL:HG22	1:A:996:MET:HE1	1.99	0.45
1:A:521:LEU:CD2	1:A:529:ALA:CB	2.95	0.45
1:A:838:LEU:HD23	1:A:838:LEU:HA	1.72	0.45
1:A:515:LYS:HG2	1:A:519:TYR:OH	2.16	0.45
1:A:154:LEU:HG	1:A:154:LEU:O	2.16	0.45
1:A:575:GLU:O	1:A:579:LYS:HB2	2.17	0.45
1:A:1111:LYS:HG3	1:A:1119:ASP:HB3	1.99	0.45
1:A:465:VAL:HG22	1:A:643:LEU:HB2	1.98	0.45
1:A:1098:ARG:HG3	1:A:1148:ASP:OD1	2.16	0.45
1:A:1102:ILE:HD13	1:A:1146:GLU:HB2	1.99	0.45
1:A:370:LEU:HD13	1:A:933:LEU:CD1	2.47	0.44
1:A:468:LEU:HD11	1:A:600:VAL:HG12	1.97	0.44
1:A:105:LEU:HD13	1:A:966:SER:HA	2.00	0.44
1:A:550:PHE:CD2	1:A:568:PHE:CE1	3.05	0.44
1:A:170:LEU:HD11	1:A:172:PHE:CZ	2.53	0.44
1:A:765:ARG:HH21	1:A:766:PHE:HE1	1.65	0.44
1:A:991:LEU:HG	1:A:1017:ARG:HD2	1.99	0.44
1:A:1225:HIS:HE1	1:A:1308:ARG:HG2	1.81	0.44
1:A:142:PHE:HA	1:A:184:ILE:O	2.18	0.44
1:A:311:LEU:O	1:A:315:THR:CG2	2.64	0.44
1:A:548:ARG:O	1:A:552:GLU:OE2	2.35	0.44
1:A:1305:GLN:HE22	1:A:1417:LEU:HD11	1.83	0.44
1:A:1306:ILE:HD11	1:A:1457:TRP:CD1	2.53	0.44
1:A:317:ASP:O	1:A:320:LYS:HB3	2.17	0.44
1:A:361:ILE:HG13	1:A:364:GLN:HG3	2.00	0.44
1:A:915:VAL:HG12	1:A:946:ASN:HD22	1.82	0.43
1:A:1438:ASN:CA	1:A:1449:ARG:HH22	2.20	0.43
1:A:299:SER:O	1:A:303:GLN:HG3	2.19	0.43
1:A:835:THR:O	1:A:839:PRO:CD	2.65	0.43
1:A:1417:LEU:HD12	1:A:1417:LEU:HA	1.93	0.43
1:A:1354:LYS:CE	1:A:1405:PHE:CE1	3.02	0.43
1:A:43:PRO:HB3	1:A:222:HIS:CE1	2.53	0.43
4:D:1:NAG:H61	4:D:2:NAG:C7	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:PRO:CD	1:A:462:ARG:HH21	2.32	0.43
1:A:519:TYR:HH	1:A:577:HIS:HA	1.80	0.43
1:A:802:ASN:HB2	1:A:814:ILE:HB	2.00	0.43
1:A:1054:PRO:O	1:A:1074:ILE:CG2	2.67	0.43
1:A:1439:ASN:OD1	6:A:1618:IOD:I	3.06	0.43
1:A:1054:PRO:HB2	1:A:1057:VAL:CG2	2.49	0.43
1:A:1309:THR:OG1	1:A:1432:ARG:HB3	2.19	0.43
1:A:308:PHE:HE2	1:A:931:LYS:HA	1.81	0.43
1:A:550:PHE:CD2	1:A:554:ILE:HD11	2.54	0.43
1:A:969:SER:HB2	1:A:977:LYS:HD2	2.01	0.43
1:A:1333:ARG:NH2	1:A:1420:GLU:HG2	2.33	0.43
1:A:131:LEU:HD11	1:A:148:GLN:OE1	2.19	0.42
1:A:282:ILE:HG13	1:A:990:THR:CG2	2.45	0.42
1:A:1199:GLU:CG	1:A:1229:THR:OG1	2.67	0.42
1:A:1451:ARG:HH21	1:A:1458:THR:HG22	1.85	0.42
1:A:244:ILE:HG13	1:A:285:LEU:HD11	2.02	0.42
1:A:312:LEU:HD22	1:A:931:LYS:CD	2.49	0.42
1:A:418:TRP:NE1	1:A:648:LEU:HD11	2.33	0.42
1:A:566:LEU:O	1:A:567:SER:CB	2.67	0.42
1:A:574:SER:O	1:A:578:GLU:HB3	2.20	0.42
1:A:740:LYS:HB2	1:A:800:GLY:HA3	2.01	0.42
1:A:828:PHE:O	1:A:832:GLU:HB2	2.20	0.42
1:A:971:ASP:HB2	1:A:975:LYS:O	2.20	0.42
1:A:339:ARG:NE	1:A:342:ARG:CZ	2.83	0.42
1:A:434:LEU:HD23	1:A:440:TYR:CE2	2.55	0.42
1:A:916:ILE:O	1:A:945:LEU:HA	2.20	0.42
1:A:1003:LEU:HD12	1:A:1038:HIS:HB2	2.01	0.42
1:A:1234:PHE:HB3	1:A:1239:LEU:HD11	2.01	0.42
1:A:1312:TYR:CE1	1:A:1316:GLU:HG3	2.55	0.41
1:A:868:LEU:HD23	1:A:871:ILE:HD12	2.02	0.41
1:A:1073:ILE:CG2	1:A:1293:LEU:HD21	2.50	0.41
1:A:1330:CYS:HA	1:A:1414:GLN:OE1	2.19	0.41
1:A:991:LEU:HD23	1:A:1017:ARG:HG3	2.01	0.41
1:A:1066:ASN:HA	1:A:1067:PRO:HD3	1.79	0.41
1:A:521:LEU:CD2	1:A:529:ALA:HB3	2.51	0.41
1:A:565:GLU:OE2	1:A:571:ILE:HD11	2.20	0.41
1:A:1046:ARG:NH2	1:A:1113:TRP:O	2.54	0.41
1:A:1295:LEU:CD2	1:A:1298:VAL:HG23	2.44	0.41
1:A:1093:ARG:NH1	1:A:1096:GLU:HG3	2.36	0.41
1:A:708:ASP:O	1:A:714:GLY:HA3	2.21	0.41
1:A:1111:LYS:HG3	1:A:1119:ASP:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PRO:HD3	1:A:962:TYR:OH	2.20	0.41
1:A:546:ASN:O	1:A:549:ILE:CG2	2.68	0.41
1:A:1111:LYS:HB3	1:A:1116:ILE:HD12	2.03	0.41
1:A:519:TYR:CD1	1:A:519:TYR:N	2.86	0.41
1:A:719:TYR:O	1:A:723:ARG:HG3	2.20	0.41
1:A:149:TYR:CD2	1:A:154:LEU:CD1	3.04	0.41
1:A:415:ARG:NH2	1:A:624:ASP:OD1	2.54	0.41
1:A:490:PHE:HA	1:A:495:ILE:HD12	2.03	0.41
1:A:512:ASP:O	1:A:515:LYS:HB2	2.21	0.41
1:A:1047:GLU:O	1:A:1051:ALA:HA	2.21	0.41
1:A:113:THR:OG1	1:A:114:PRO:HD3	2.21	0.40
1:A:1299:ILE:HG12	1:A:1363:VAL:HG22	2.03	0.40
1:A:1307:VAL:HG22	1:A:1433:THR:CG2	2.51	0.40
2:B:1:NAG:H3	2:B:2:NAG:C2	2.52	0.40
1:A:59:ILE:O	1:A:63:LEU:HG	2.22	0.40
1:A:465:VAL:HG22	1:A:643:LEU:HD12	2.02	0.40
1:A:1012:ASP:HB2	1:A:1209:HIS:ND1	2.36	0.40
1:A:361:ILE:CG1	1:A:364:GLN:HG3	2.51	0.40
1:A:407:LYS:HD2	1:A:870:THR:OG1	2.21	0.40
1:A:586:HIS:O	1:A:590:ARG:HB2	2.22	0.40
1:A:64:LEU:HD12	1:A:67:ILE:HD11	2.04	0.40
1:A:142:PHE:CE2	1:A:201:ALA:HB2	2.54	0.40
1:A:109:LEU:HD21	1:A:964:LEU:CD1	2.52	0.40
1:A:314:LEU:HD12	1:A:321:TYR:HD2	1.87	0.40
1:A:1090:TYR:HB2	1:A:1124:VAL:HG23	2.03	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%)	1288 (94%)	71 (5%)	12 (1%)	17 54

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	GLU
1	A	333	GLU
1	A	562	ASP
1	A	567	SER
1	A	305	GLU
1	A	524	TYR
1	A	563	GLY
1	A	611	ASP
1	A	539	GLU
1	A	666	GLU
1	A	873	ASP
1	A	1142	PRO

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	1203/1297 (93%)	1169 (97%)	34 (3%)	43 72

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	LYS
1	A	299	SER
1	A	308	PHE
1	A	341	ASN
1	A	437	ASP
1	A	513	GLN
1	A	521	LEU
1	A	524	TYR
1	A	536	SER
1	A	540	GLN
1	A	552	GLU
1	A	554	ILE
1	A	556	ASP

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Mol	Chain	Res	Type
1	A	557	LYS
1	A	559	LEU
1	A	571	ILE
1	A	574	SER
1	A	575	GLU
1	A	576	LYS
1	A	580	GLN
1	A	620	ARG
1	A	636	MET
1	A	768	ASP
1	A	787	SER
1	A	820	PHE
1	A	871	ILE
1	A	873	ASP
1	A	946	ASN
1	A	971	ASP
1	A	1066	ASN
1	A	1123	GLU
1	A	1203	PHE
1	A	1227	ASN
1	A	1330	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	A	513	GLN
1	A	577	HIS
1	A	582	HIS
1	A	619	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

24 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	0.38	0	17,19,21	1.13	1 (5%)
2	NAG	B	2	2	14,14,15	0.40	0	17,19,21	2.20	3 (17%)
2	BMA	B	3	2	11,11,12	0.31	0	15,15,17	0.53	0
2	MAN	B	4	2	11,11,12	0.35	0	15,15,17	0.78	0
2	MAN	B	5	2	11,11,12	0.41	0	15,15,17	0.97	1 (6%)
2	MAN	B	6	2	11,11,12	0.35	0	15,15,17	0.78	1 (6%)
2	MAN	B	7	2	11,11,12	0.37	0	15,15,17	0.97	1 (6%)
3	NAG	C	1	3,1	14,14,15	0.28	0	17,19,21	0.50	0
3	NAG	C	2	3	14,14,15	0.36	0	17,19,21	0.88	1 (5%)
3	BMA	C	3	3	11,11,12	0.28	0	15,15,17	0.42	0
3	MAN	C	4	3	11,11,12	0.36	0	15,15,17	0.83	1 (6%)
3	MAN	C	5	3	11,11,12	0.31	0	15,15,17	0.99	1 (6%)
4	NAG	D	1	1,4	14,14,15	0.34	0	17,19,21	1.01	1 (5%)
4	NAG	D	2	4	14,14,15	0.33	0	17,19,21	0.64	0
4	BMA	D	3	4	11,11,12	0.40	0	15,15,17	0.92	1 (6%)
4	MAN	D	4	4	11,11,12	0.40	0	15,15,17	0.73	0
4	MAN	D	5	4	11,11,12	0.40	0	15,15,17	0.92	1 (6%)
5	NAG	E	1	5,1	14,14,15	0.29	0	17,19,21	2.22	3 (17%)
5	NAG	E	2	5	14,14,15	0.35	0	17,19,21	1.21	2 (11%)
5	BMA	E	3	5	11,11,12	0.29	0	15,15,17	0.88	1 (6%)
5	MAN	E	4	5	11,11,12	0.57	0	15,15,17	1.43	2 (13%)
5	MAN	E	5	5	11,11,12	0.48	0	15,15,17	1.50	1 (6%)
5	MAN	E	6	5	11,11,12	0.40	0	15,15,17	0.94	2 (13%)
5	MAN	E	7	5	11,11,12	0.51	0	15,15,17	1.34	1 (6%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	MAN	B	6	2	-	2/2/19/22	0/1/1/1
2	MAN	B	7	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	MAN	E	4	5	-	2/2/19/22	0/1/1/1
5	MAN	E	5	5	-	2/2/19/22	1/1/1/1
5	MAN	E	6	5	-	0/2/19/22	0/1/1/1
5	MAN	E	7	5	-	0/2/19/22	1/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	O5-C1-C2	-6.84	100.49	111.29
5	E	1	NAG	C1-O5-C5	6.33	120.77	112.19
5	E	1	NAG	O5-C1-C2	5.50	119.97	111.29
5	E	5	MAN	C1-O5-C5	5.41	119.52	112.19
5	E	4	MAN	C1-O5-C5	4.77	118.66	112.19
5	E	7	MAN	C1-O5-C5	4.44	118.21	112.19
2	B	2	NAG	C3-C4-C5	3.95	117.28	110.24
5	E	2	NAG	O5-C1-C2	3.64	117.04	111.29
2	B	1	NAG	C1-C2-N2	3.56	116.56	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	7	MAN	C1-O5-C5	3.36	116.75	112.19
3	C	5	MAN	C1-O5-C5	3.20	116.53	112.19
2	B	2	NAG	C2-N2-C7	3.18	127.44	122.90
4	D	5	MAN	C1-O5-C5	3.13	116.43	112.19
4	D	1	NAG	O5-C1-C2	-3.00	106.55	111.29
2	B	5	MAN	C1-O5-C5	2.88	116.10	112.19
5	E	1	NAG	C3-C4-C5	2.84	115.31	110.24
4	D	3	BMA	O3-C3-C2	2.77	115.30	109.99
5	E	6	MAN	C1-O5-C5	2.67	115.81	112.19
2	B	6	MAN	C1-O5-C5	2.59	115.70	112.19
5	E	4	MAN	C1-C2-C3	2.39	112.60	109.67
3	C	4	MAN	C1-O5-C5	2.34	115.36	112.19
3	C	2	NAG	C2-N2-C7	2.31	126.19	122.90
5	E	3	BMA	C1-O5-C5	2.27	115.27	112.19
5	E	6	MAN	C1-C2-C3	2.11	112.27	109.67
5	E	2	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C3-C2-N2-C7
2	B	6	MAN	C4-C5-C6-O6
5	E	5	MAN	O5-C5-C6-O6
2	B	6	MAN	O5-C5-C6-O6
5	E	5	MAN	C4-C5-C6-O6
5	E	4	MAN	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
2	B	1	NAG	C1-C2-N2-C7
2	B	3	BMA	C4-C5-C6-O6
5	E	4	MAN	C4-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C1-C2-N2-C7
4	D	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C3-C2-N2-C7
3	C	2	NAG	C1-C2-N2-C7
2	B	2	NAG	C4-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7
5	E	2	NAG	O7-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2

All (2) ring outliers are listed below:

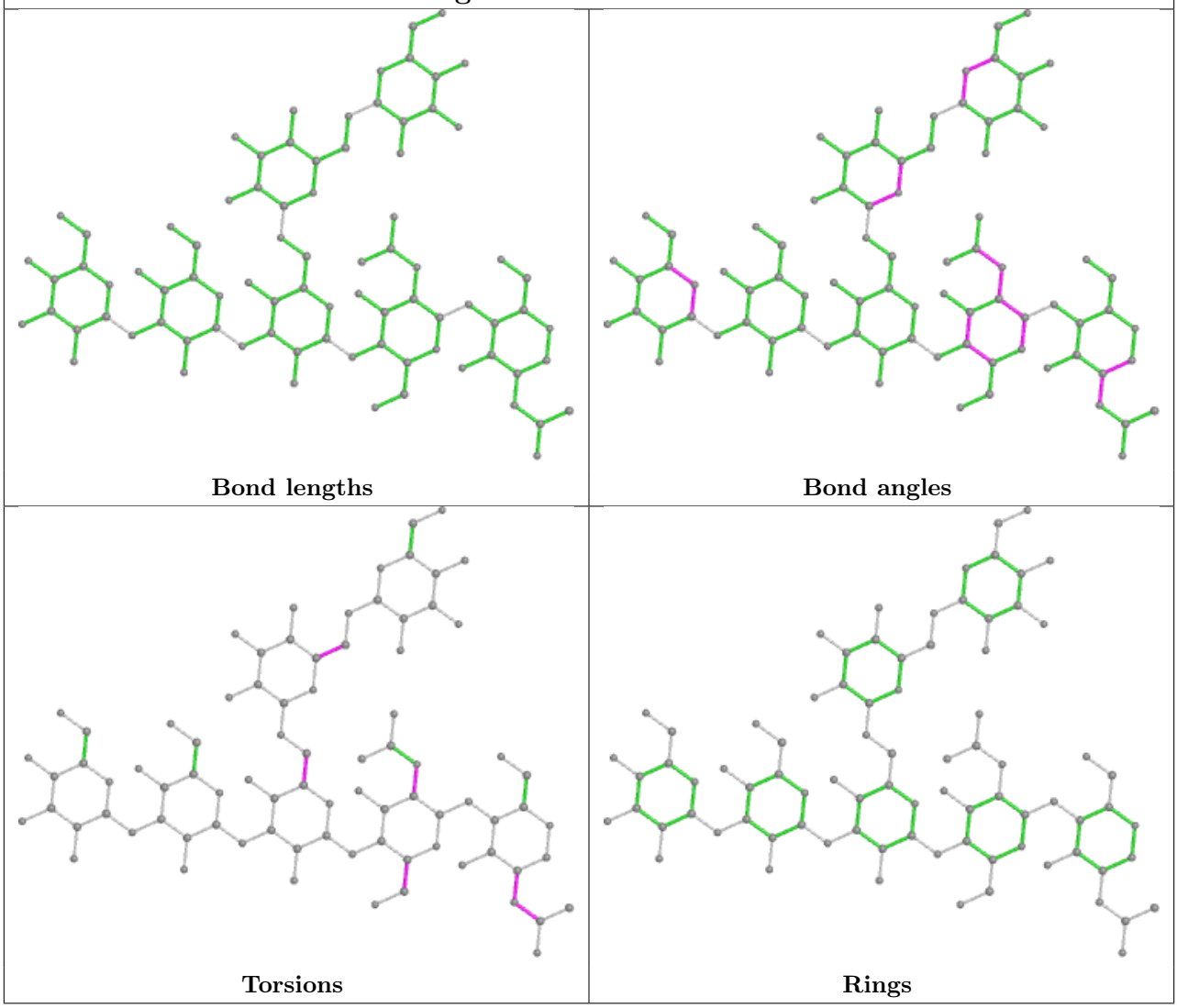
Mol	Chain	Res	Type	Atoms
5	E	7	MAN	C1-C2-C3-C4-C5-O5
5	E	5	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 7 short contacts:

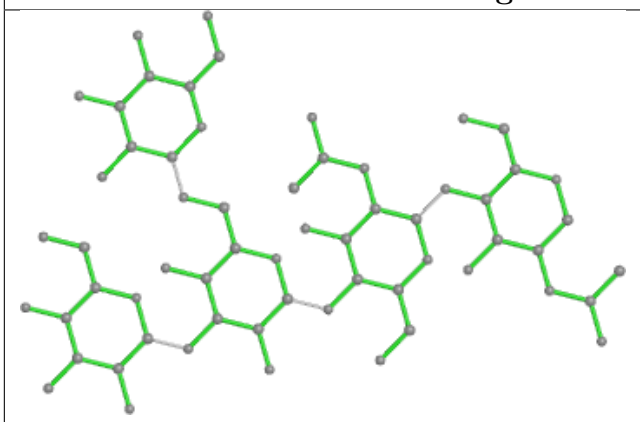
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	4	0
4	D	1	NAG	1	0
2	B	1	NAG	3	0
5	E	4	MAN	2	0
5	E	3	BMA	2	0
4	D	2	NAG	1	0

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

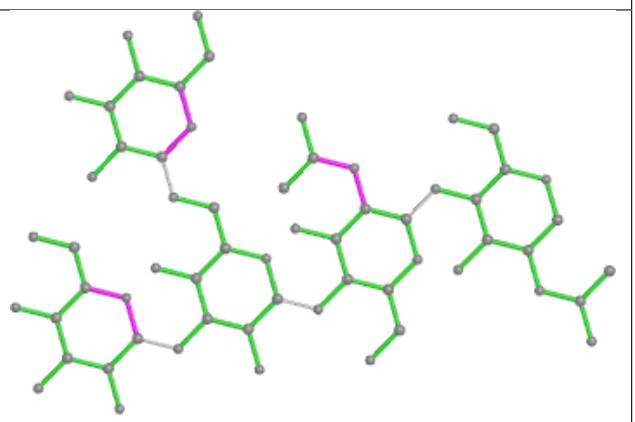
Oligosaccharide Chain B



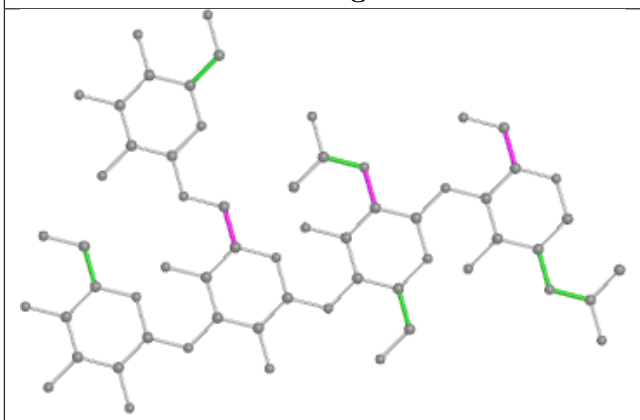
Oligosaccharide Chain C



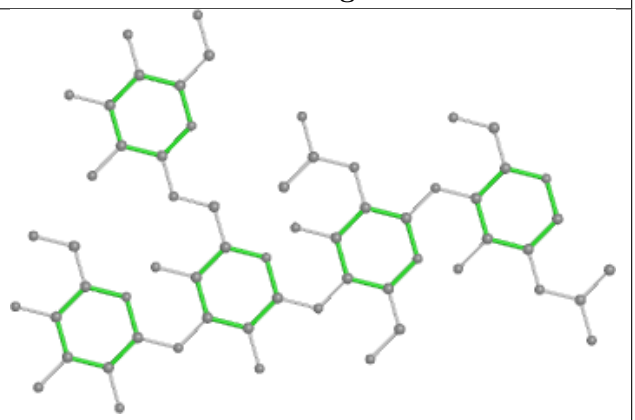
Bond lengths



Bond angles

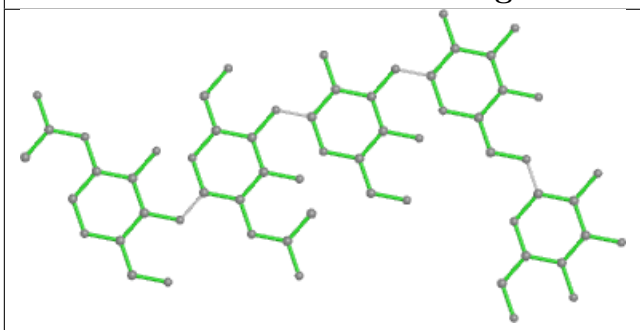


Torsions

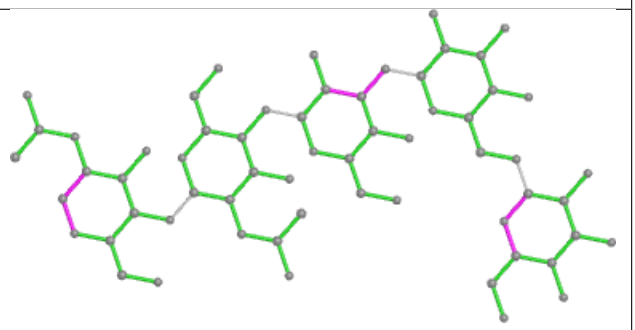


Rings

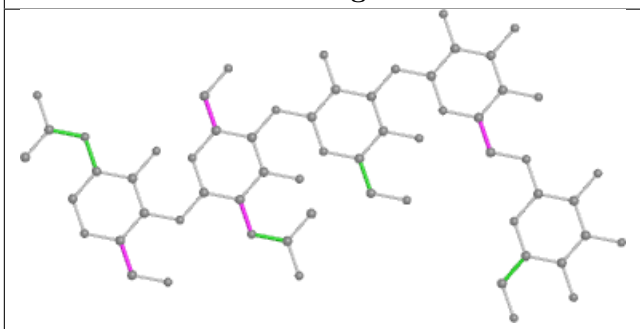
Oligosaccharide Chain D



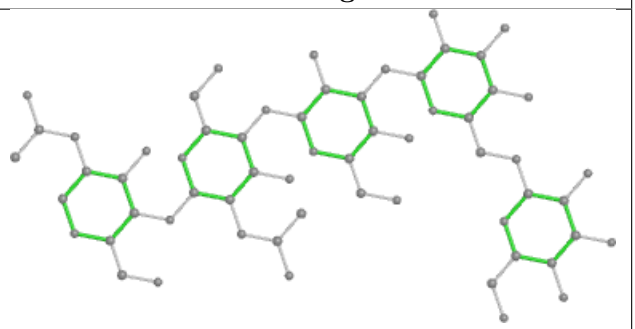
Bond lengths



Bond angles

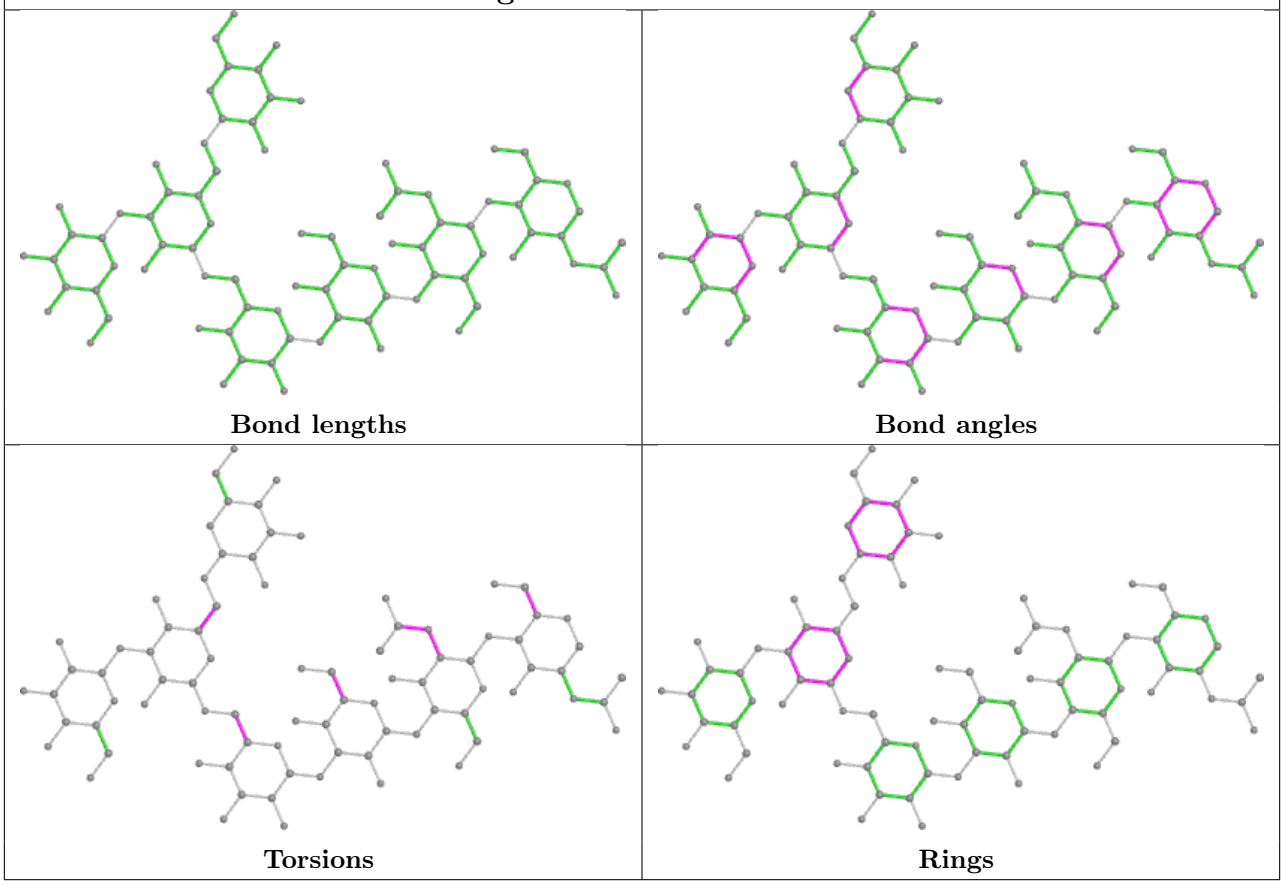


Torsions



Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 21 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1377/1494 (92%)	0.77	183 (13%)	3	4	71, 136, 258, 289	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	PHE	6.2
1	A	328	GLN	6.1
1	A	470	VAL	5.4
1	A	500	GLY	5.3
1	A	184	ILE	4.6
1	A	45	LEU	4.5
1	A	1430	ASP	4.5
1	A	683	MET	4.5
1	A	580	GLN	4.4
1	A	1083	PHE	4.4
1	A	242	ASP	4.3
1	A	216	TYR	4.3
1	A	1339	TYR	4.3
1	A	201	ALA	4.2
1	A	143	LEU	4.2
1	A	499	PHE	4.1
1	A	186	TYR	4.1
1	A	1417	LEU	4.1
1	A	215	ARG	4.0
1	A	185	LEU	4.0
1	A	180	SER	3.9
1	A	187	ALA	3.7
1	A	119	HIS	3.7
1	A	508	GLY	3.7
1	A	1197	HIS	3.6
1	A	468	LEU	3.6
1	A	72	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	570	ASP	3.6
1	A	507	THR	3.6
1	A	141	TRP	3.5
1	A	856	PRO	3.5
1	A	1003	LEU	3.5
1	A	506	PRO	3.5
1	A	820	PHE	3.4
1	A	502	VAL	3.4
1	A	1235	ILE	3.4
1	A	1041	ILE	3.4
1	A	735	ILE	3.3
1	A	769	LEU	3.3
1	A	189	ILE	3.3
1	A	732	ARG	3.3
1	A	1191	SER	3.3
1	A	1305	GLN	3.3
1	A	1450	ALA	3.3
1	A	587	TRP	3.3
1	A	1331	ASP	3.3
1	A	214	VAL	3.3
1	A	517	VAL	3.2
1	A	469	VAL	3.2
1	A	1038	HIS	3.2
1	A	761	LEU	3.2
1	A	1056	GLY	3.2
1	A	224	ARG	3.2
1	A	1361	LEU	3.1
1	A	1301	VAL	3.1
1	A	46	VAL	3.1
1	A	1287	LEU	3.1
1	A	472	VAL	3.1
1	A	471	PRO	3.0
1	A	429	ILE	3.0
1	A	849	LEU	3.0
1	A	1204	SER	3.0
1	A	118	ALA	2.9
1	A	428	ILE	2.9
1	A	418	TRP	2.9
1	A	916	ILE	2.9
1	A	1434	ILE	2.9
1	A	773	LEU	2.9
1	A	509	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	293	LEU	2.9
1	A	172	PHE	2.9
1	A	1234	PHE	2.8
1	A	933	LEU	2.8
1	A	447	ILE	2.8
1	A	574	SER	2.8
1	A	670	LEU	2.8
1	A	171	PRO	2.8
1	A	140	GLN	2.8
1	A	1040	LEU	2.7
1	A	701	ALA	2.7
1	A	705	VAL	2.7
1	A	1073	ILE	2.7
1	A	1357	HIS	2.7
1	A	497	VAL	2.7
1	A	703	LEU	2.7
1	A	646	PHE	2.7
1	A	193	SER	2.7
1	A	717	LEU	2.7
1	A	1433	THR	2.7
1	A	806	LEU	2.6
1	A	900	PHE	2.6
1	A	1291	PHE	2.6
1	A	1149	VAL	2.6
1	A	881	ASN	2.6
1	A	572	PHE	2.6
1	A	176	PHE	2.6
1	A	1464	ILE	2.6
1	A	49	LEU	2.6
1	A	1081	PHE	2.6
1	A	1404	GLN	2.6
1	A	753	LEU	2.6
1	A	1290	LEU	2.6
1	A	575	GLU	2.5
1	A	857	LEU	2.5
1	A	578	GLU	2.5
1	A	492	LYS	2.5
1	A	1307	VAL	2.5
1	A	1061	LEU	2.5
1	A	487	LEU	2.5
1	A	736	VAL	2.5
1	A	882	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	760	LEU	2.4
1	A	1092	ILE	2.4
1	A	217	ARG	2.4
1	A	397	LEU	2.4
1	A	1069	PHE	2.4
1	A	797	MET	2.4
1	A	1232	PHE	2.4
1	A	1086	ASN	2.4
1	A	130	SER	2.4
1	A	996	MET	2.4
1	A	1326	PHE	2.3
1	A	1059	LEU	2.3
1	A	565	GLU	2.3
1	A	450	LEU	2.3
1	A	1412	LEU	2.3
1	A	1409	ILE	2.3
1	A	510	ALA	2.3
1	A	1308	ARG	2.3
1	A	1405	PHE	2.3
1	A	39	PHE	2.3
1	A	222	HIS	2.3
1	A	1453	GLN	2.3
1	A	1306	ILE	2.2
1	A	1413	PRO	2.2
1	A	825	PHE	2.2
1	A	718	VAL	2.2
1	A	1364	VAL	2.2
1	A	1087	PRO	2.2
1	A	1457	TRP	2.2
1	A	1202	ILE	2.2
1	A	212	TYR	2.2
1	A	1311	MET	2.2
1	A	431	LEU	2.2
1	A	194	PHE	2.2
1	A	1471	VAL	2.2
1	A	178	VAL	2.2
1	A	654	ARG	2.2
1	A	841	TYR	2.2
1	A	1259	GLU	2.2
1	A	1416	TRP	2.2
1	A	85	PHE	2.1
1	A	607	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1126	LEU	2.1
1	A	828	PHE	2.1
1	A	47	GLU	2.1
1	A	308	PHE	2.1
1	A	1036	LEU	2.1
1	A	427	VAL	2.1
1	A	688	VAL	2.1
1	A	1138	LEU	2.1
1	A	168	ARG	2.1
1	A	148	GLN	2.1
1	A	675	ILE	2.1
1	A	142	PHE	2.1
1	A	1328	PRO	2.1
1	A	805	ILE	2.1
1	A	804	VAL	2.1
1	A	1299	ILE	2.1
1	A	1334	VAL	2.1
1	A	451	ILE	2.1
1	A	687	PRO	2.1
1	A	311	LEU	2.1
1	A	658	LEU	2.1
1	A	656	ASN	2.0
1	A	183	VAL	2.0
1	A	865	VAL	2.0
1	A	484	VAL	2.0
1	A	1203	PHE	2.0
1	A	772	ALA	2.0
1	A	1284	ILE	2.0
1	A	577	HIS	2.0
1	A	585	LYS	2.0

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

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

6.3 Carbohydrates (i)

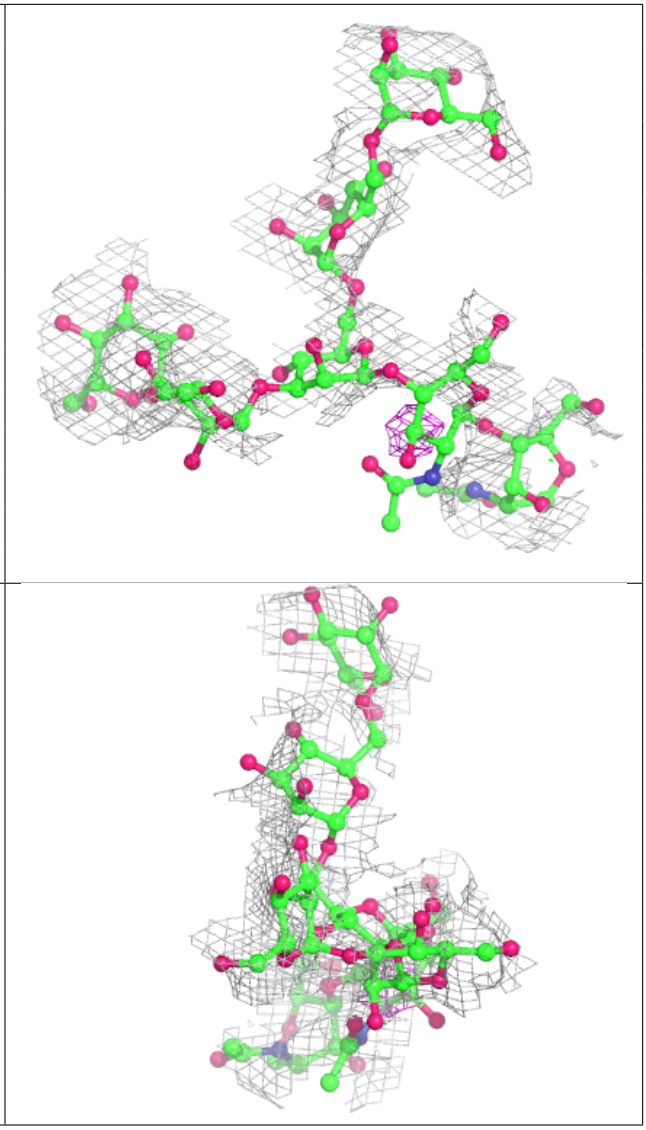
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	B	2	14/15	0.19	0.55	276,281,284,285	0
2	MAN	B	7	11/12	0.32	0.32	273,276,278,278	0
2	BMA	B	3	11/12	0.43	0.17	280,281,283,283	0
2	MAN	B	4	11/12	0.55	0.26	275,279,281,282	0
2	MAN	B	5	11/12	0.56	0.26	275,275,278,279	0
2	NAG	B	1	14/15	0.57	0.28	280,282,288,288	0
3	NAG	C	2	14/15	0.57	0.25	245,259,277,278	0
4	MAN	D	5	11/12	0.57	0.25	249,250,251,252	0
4	MAN	D	4	11/12	0.59	0.21	248,249,250,250	0
3	MAN	C	4	11/12	0.61	0.23	250,256,260,264	0
5	MAN	E	7	11/12	0.61	0.26	185,209,229,229	0
5	MAN	E	4	11/12	0.62	0.22	230,235,241,242	0
3	BMA	C	3	11/12	0.62	0.17	229,247,256,257	0
4	BMA	D	3	11/12	0.67	0.18	237,244,247,247	0
5	BMA	E	3	11/12	0.67	0.27	230,240,249,250	0
5	MAN	E	6	11/12	0.72	0.26	242,256,265,266	0
5	MAN	E	5	11/12	0.72	0.17	189,216,230,231	0
2	MAN	B	6	11/12	0.73	0.16	277,279,281,282	0
5	NAG	E	2	14/15	0.81	0.18	248,252,256,257	0
5	NAG	E	1	14/15	0.81	0.16	255,259,262,264	0
3	MAN	C	5	11/12	0.82	0.34	261,274,278,279	0
4	NAG	D	2	14/15	0.82	0.20	191,198,214,226	0
3	NAG	C	1	14/15	0.91	0.22	188,213,232,252	0
4	NAG	D	1	14/15	0.93	0.18	140,157,168,180	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.

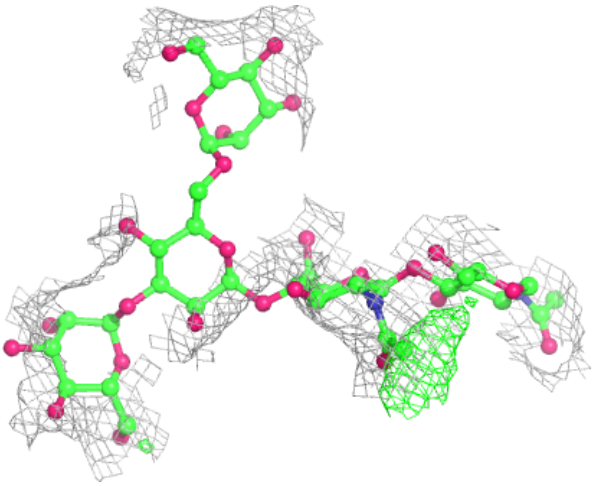
Electron density around Chain B:

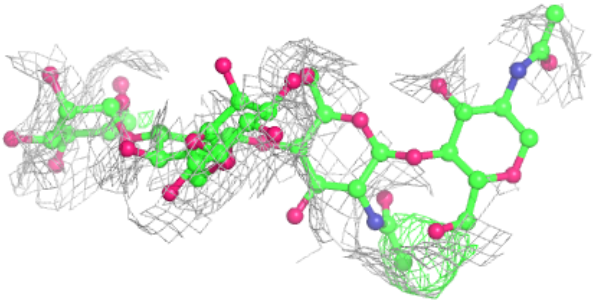
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

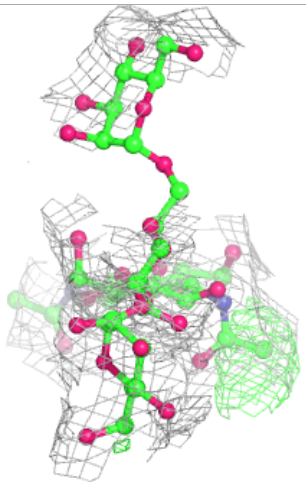


Electron density around Chain C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

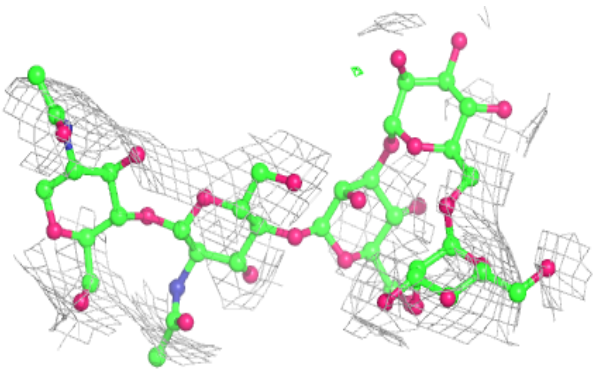


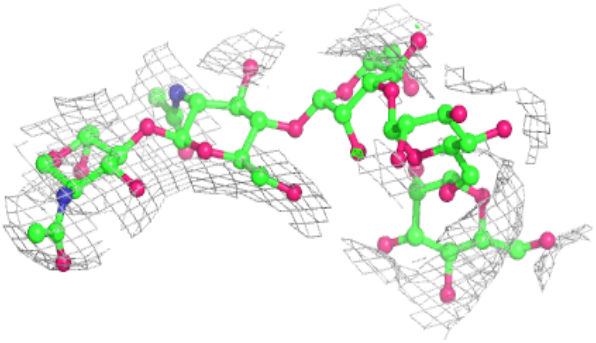


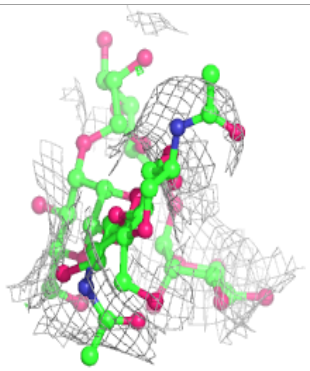


Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

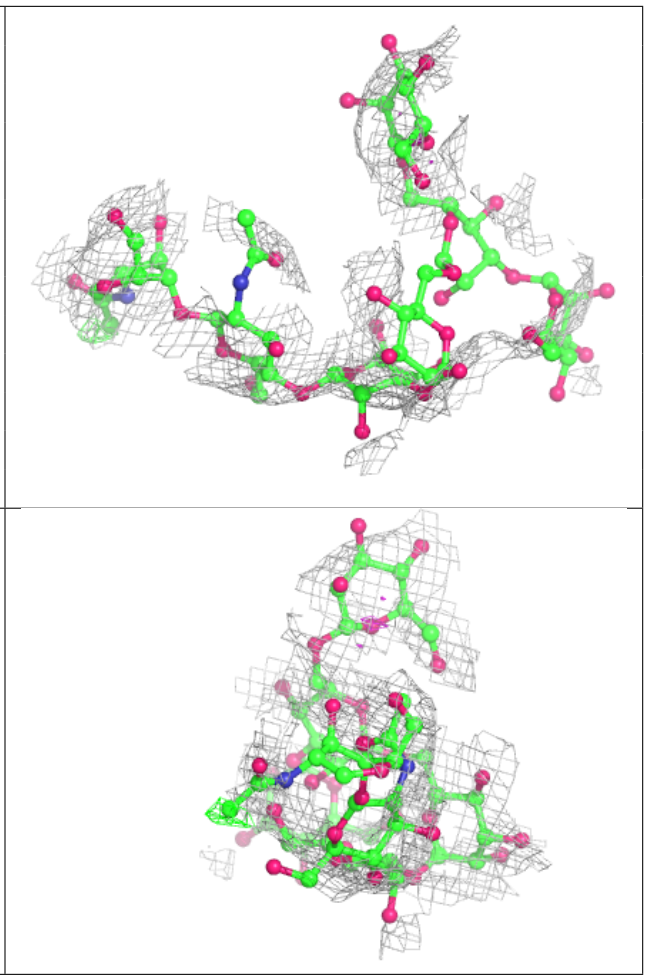






Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	IOD	A	1609	1/1	0.69	0.35	180,180,180,180	1
8	CA	A	1645	1/1	0.75	0.12	141,141,141,141	1
7	PT	A	1604	1/1	0.81	0.12	169,169,169,169	1
6	IOD	A	1608	1/1	0.83	0.34	178,178,178,178	1
7	PT	A	1610	1/1	0.84	0.12	180,180,180,180	1
6	IOD	A	1612	1/1	0.89	0.16	140,140,140,140	1
6	IOD	A	1611	1/1	0.89	0.22	143,143,143,143	1
7	PT	A	1613	1/1	0.90	0.07	142,142,142,142	1
6	IOD	A	1603	1/1	0.90	0.26	168,168,168,168	1
7	PT	A	1617	1/1	0.92	0.15	134,134,134,134	1
6	IOD	A	1618	1/1	0.92	0.11	203,203,203,203	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	IOD	A	1602	1/1	0.94	0.11	175,175,175,175	1
6	IOD	A	1601	1/1	0.94	0.21	180,180,180,180	1
6	IOD	A	1614	1/1	0.95	0.10	149,149,149,149	1
7	PT	A	1620	1/1	0.95	0.08	213,213,213,213	1
7	PT	A	1605	1/1	0.95	0.12	125,125,125,125	1
6	IOD	A	1619	1/1	0.96	0.08	220,220,220,220	1
6	IOD	A	1607	1/1	0.96	0.10	178,178,178,178	1
6	IOD	A	1615	1/1	0.98	0.08	140,140,140,140	1
6	IOD	A	1616	1/1	0.99	0.29	130,130,130,130	1
6	IOD	A	1606	1/1	0.99	0.12	125,125,125,125	1

6.5 Other polymers (i)

There are no such residues in this entry.