Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 06:55 am BST

PDB ID	:	1GVI
Title	:	Thermus maltogenic amylase in complex with beta-CD
Authors	:	Kim, M.-S.; Kim, J.-I.; Oh, B.-H.
Deposited on	:	2002-02-14
Resolution	:	3.30 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:

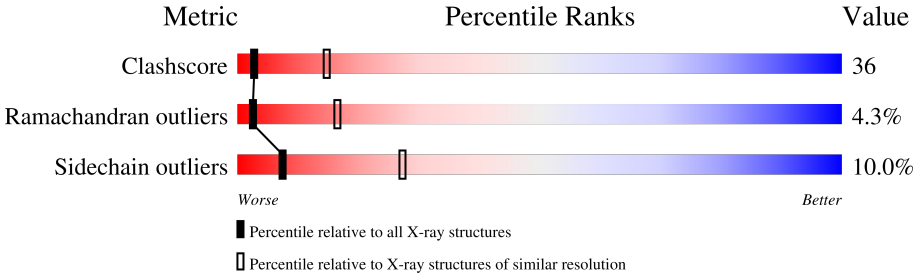
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.30 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))
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	588	43% 48% 9% •
1	B	588	41% 49% 9%
2	C	7	71% 29%
2	D	7	86% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9810 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.

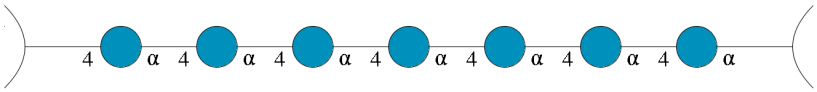
- Molecule 1 is a protein called MALTOGENIC AMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	588	4828	3119	819	869	21	0	0	0
1	B	588	4828	3119	819	869	21	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	LEU	GLU	conflict	UNP O69007
B	357	LEU	GLU	conflict	UNP O69007

- Molecule 2 is an oligosaccharide called Cycloheptakis-(1-4)-(alpha-D-glucopyranose).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	C	7	77	42	35	0	0	0
2	D	7	77	42	35	0	0	0

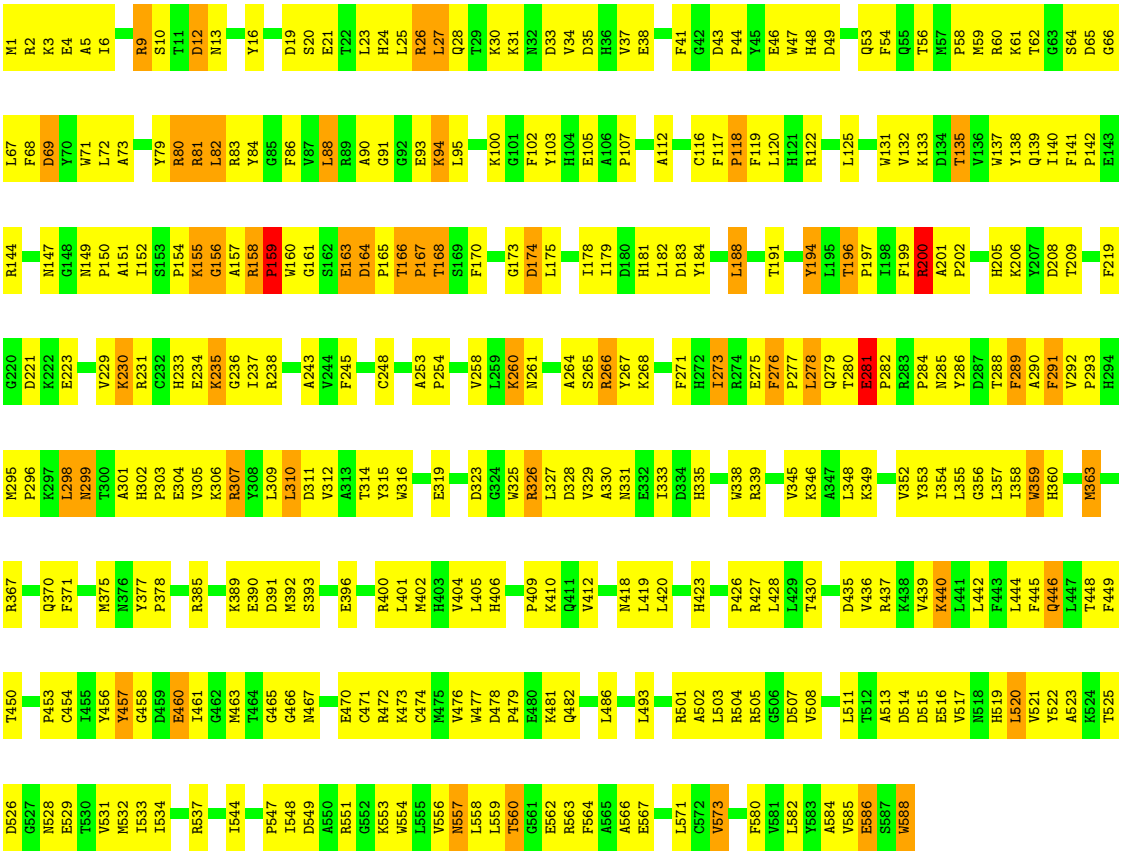
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

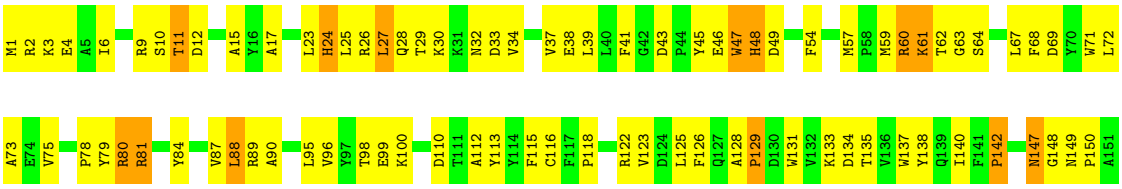
• Molecule 1: MALTOGENIC AMYLASE

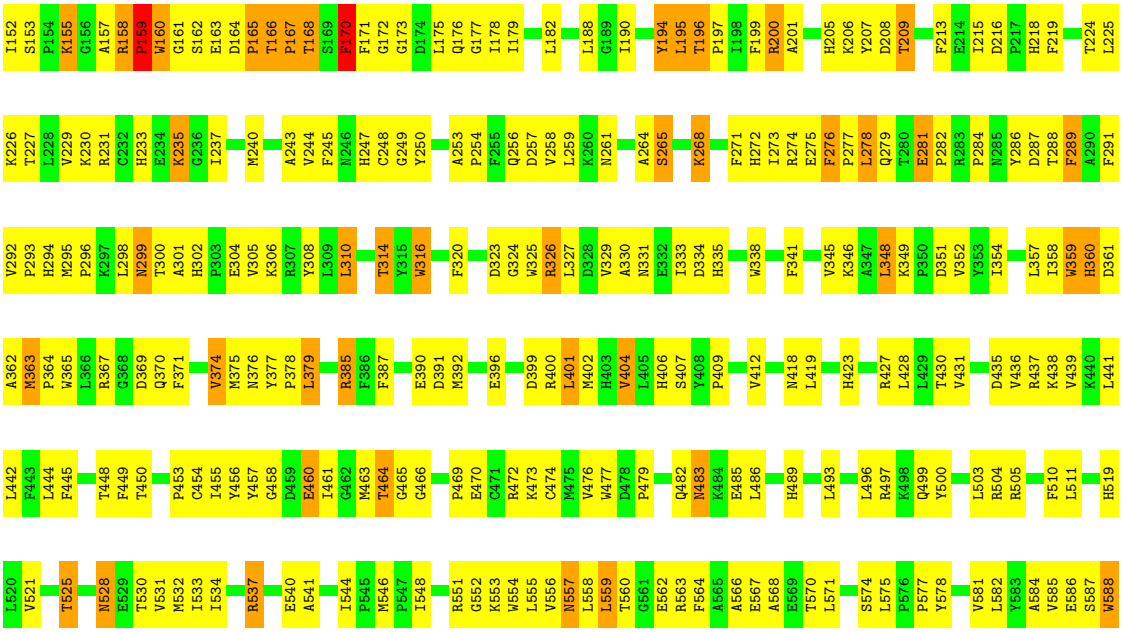
Chain A: 43% 48% 9%



• Molecule 1: MALTOGENIC AMYLASE

Chain B: 41% 49% 9%





- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain C:

- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain D:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	119.09Å 119.09Å 270.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.30	Depositor
% Data completeness (in resolution range)	89.3 (20.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.192 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9810	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

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: GLC

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	0/4982	0.67	0/6770
1	B	0.42	0/4982	0.68	1/6770 (0.0%)
All	All	0.41	0/9964	0.68	1/13540 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	170	PHE	N-CA-C	6.04	127.32	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4828	0	4629	347	0
1	B	4828	0	4629	349	0
2	C	77	0	63	2	0
2	D	77	0	63	3	0
All	All	9810	0	9384	683	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 36.

All (683) 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:281:GLU:HB2	1:A:282:PRO:HD3	1.33	1.08
1:B:281:GLU:HB2	1:B:282:PRO:CD	1.93	0.99
1:B:275:GLU:HG3	1:B:277:PRO:HD2	1.46	0.97
1:B:155:LYS:HG3	1:B:170:PHE:HB2	1.47	0.96
1:A:253:ALA:HB3	1:A:254:PRO:HD3	1.44	0.95
1:A:357:LEU:HD22	1:A:375:MET:HG3	1.50	0.93
1:B:29:THR:HG1	1:B:71:TRP:HZ3	1.00	0.93
1:B:558:LEU:HD11	1:B:584:ALA:HB2	1.49	0.92
1:A:31:LYS:HA	1:A:69:ASP:OD1	1.70	0.91
1:A:44:PRO:HD3	1:A:82:LEU:HA	1.53	0.90
1:A:281:GLU:HB2	1:A:282:PRO:CD	2.02	0.89
1:B:281:GLU:HB2	1:B:282:PRO:HD3	1.52	0.88
1:A:160:TRP:HB3	1:A:165:PRO:HB3	1.55	0.88
1:A:158:ARG:HB3	1:A:159:PRO:HD2	1.56	0.87
1:B:253:ALA:HB3	1:B:254:PRO:HD3	1.54	0.87
1:B:133:LYS:HB2	1:B:505:ARG:HH21	1.39	0.87
1:B:557:ASN:HD21	1:B:559:LEU:HD12	1.36	0.87
1:B:64:SER:HB2	1:B:68:PHE:O	1.77	0.85
1:B:430:THR:HG21	1:B:465:GLY:H	1.39	0.85
1:B:333:ILE:HD12	1:B:338:TRP:CZ2	2.12	0.84
1:A:88:LEU:HD23	1:A:88:LEU:N	1.93	0.83
1:A:513:ALA:HB3	1:A:516:GLU:HG2	1.59	0.82
1:B:88:LEU:HD23	1:B:88:LEU:H	1.44	0.82
1:B:291:PHE:O	1:B:293:PRO:HD3	1.80	0.81
1:B:164:ASP:HB2	1:B:165:PRO:HD3	1.63	0.80
1:A:557:ASN:HB3	1:A:560:THR:HG22	1.64	0.80
1:B:87:VAL:HG22	1:B:96:VAL:HG22	1.63	0.80
1:A:401:LEU:HD21	1:A:445:PHE:HZ	1.46	0.80
1:B:556:VAL:HG13	1:B:584:ALA:HB3	1.61	0.79
1:A:554:TRP:H	1:A:586:GLU:HB2	1.46	0.79
1:A:81:ARG:HB2	1:A:118:PRO:O	1.81	0.79
1:B:314:THR:HG22	1:B:348:LEU:HD12	1.63	0.79
1:A:275:GLU:HB3	1:A:285:ASN:HD22	1.48	0.79
1:A:400:ARG:NH2	1:B:100:LYS:HD3	1.98	0.78
1:B:430:THR:CG2	1:B:465:GLY:H	1.96	0.78
1:A:167:PRO:HG2	1:A:168:THR:H	1.49	0.78
1:A:553:LYS:HE3	1:A:554:TRP:NE1	1.98	0.78
1:A:419:LEU:HD23	1:A:419:LEU:H	1.50	0.77
1:A:149:ASN:ND2	1:A:151:ALA:HB2	1.99	0.76
1:A:158:ARG:CB	1:A:159:PRO:HD2	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:MET:HG2	1:A:73:ALA:HB2	1.69	0.75
1:A:291:PHE:O	1:A:293:PRO:HD3	1.87	0.75
1:A:557:ASN:ND2	1:A:559:LEU:H	1.84	0.74
1:B:326:ARG:HD2	1:B:326:ARG:C	2.08	0.74
1:B:261:ASN:HB3	1:B:264:ALA:HB3	1.69	0.74
1:A:30:LYS:HB3	1:A:33:ASP:HB2	1.68	0.74
1:A:243:ALA:HB2	1:A:325:TRP:CE3	2.23	0.74
1:B:345:VAL:HG23	1:B:346:LYS:H	1.53	0.73
1:A:158:ARG:HD3	1:A:159:PRO:HD2	1.70	0.73
1:A:266:ARG:HE	1:A:266:ARG:HA	1.53	0.73
1:B:357:LEU:CD2	1:B:375:MET:HG3	2.19	0.73
1:A:359:TRP:CZ3	1:B:112:ALA:HB2	2.23	0.73
1:A:400:ARG:HG3	1:A:400:ARG:HH11	1.54	0.73
1:B:6:ILE:HD13	1:B:88:LEU:HD11	1.70	0.73
1:A:59:MET:HE1	1:A:86:PHE:HD2	1.52	0.73
1:A:461:ILE:HB	1:A:482:GLN:HB2	1.70	0.73
1:B:450:THR:HG23	1:B:505:ARG:HA	1.72	0.72
1:B:39:LEU:HD12	1:B:57:MET:HE2	1.70	0.72
1:A:158:ARG:CD	1:A:159:PRO:HD2	2.20	0.72
1:B:400:ARG:O	1:B:404:VAL:HG12	1.89	0.72
1:B:557:ASN:ND2	1:B:559:LEU:H	1.87	0.72
1:B:461:ILE:HB	1:B:482:GLN:HB2	1.69	0.72
1:A:88:LEU:HD23	1:A:88:LEU:H	1.53	0.72
1:A:520:LEU:HD12	1:A:521:VAL:N	2.04	0.71
1:A:34:VAL:HG13	1:A:90:ALA:HB2	1.72	0.71
1:A:167:PRO:CG	1:A:168:THR:H	2.02	0.71
1:A:448:THR:OG1	1:A:503:LEU:HD22	1.90	0.71
1:A:560:THR:HG23	1:A:562:GLU:H	1.55	0.71
1:A:3:LYS:HE2	1:A:95:LEU:HD21	1.72	0.71
1:A:158:ARG:HD3	1:A:159:PRO:CD	2.20	0.71
1:A:102:PHE:C	1:A:103:TYR:HD1	1.94	0.71
1:A:175:LEU:HD13	1:A:219:PHE:HB3	1.70	0.71
1:B:196:THR:HG23	1:B:197:PRO:CD	2.21	0.71
1:A:260:LYS:HE3	1:A:260:LYS:HA	1.72	0.70
1:B:554:TRP:HB2	1:B:586:GLU:HB3	1.73	0.70
1:A:160:TRP:HB3	1:A:165:PRO:CB	2.20	0.70
1:A:112:ALA:HB2	1:B:359:TRP:CZ3	2.25	0.70
1:B:345:VAL:HG23	1:B:346:LYS:N	2.07	0.70
1:B:330:ALA:HB1	1:B:371:PHE:CZ	2.27	0.69
1:A:401:LEU:HD21	1:A:445:PHE:CZ	2.27	0.69
1:B:88:LEU:HD23	1:B:88:LEU:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:C	1:A:165:PRO:HD3	2.13	0.69
1:B:196:THR:HG23	1:B:197:PRO:HD2	1.74	0.69
1:B:281:GLU:CB	1:B:282:PRO:HD3	2.22	0.69
1:A:132:VAL:HG11	1:A:353:TYR:CD1	2.27	0.69
1:A:359:TRP:HZ3	1:B:112:ALA:HB2	1.56	0.68
1:B:385:ARG:HH11	1:B:392:MET:HE3	1.58	0.68
1:A:271:PHE:HB2	1:A:273:ILE:HD11	1.75	0.68
1:A:532:MET:C	1:A:533:ILE:HD12	2.13	0.68
1:A:534:ILE:HD13	1:A:573:VAL:HG11	1.76	0.68
1:B:230:LYS:O	1:B:230:LYS:HD3	1.93	0.68
1:B:357:LEU:HD22	1:B:375:MET:HG3	1.76	0.68
1:A:64:SER:HB2	1:A:68:PHE:O	1.93	0.68
1:A:333:ILE:HD12	1:A:338:TRP:CZ2	2.29	0.68
1:B:423:HIS:HB2	1:B:472:ARG:HE	1.58	0.68
1:B:548:ILE:HD11	1:B:568:ALA:O	1.93	0.67
1:B:326:ARG:HD2	1:B:326:ARG:O	1.93	0.67
1:B:63:GLY:HA3	1:B:402:MET:CE	2.25	0.67
1:A:430:THR:CG2	1:A:465:GLY:H	2.08	0.67
1:B:511:LEU:HD12	1:B:511:LEU:N	2.09	0.67
1:B:79:TYR:O	1:B:81:ARG:HD3	1.95	0.67
1:A:112:ALA:HB2	1:B:359:TRP:HZ3	1.58	0.66
1:A:520:LEU:HD11	1:A:522:TYR:HD1	1.60	0.66
1:A:409:PRO:HG2	1:A:412:VAL:HG23	1.78	0.66
1:B:155:LYS:HE3	1:B:170:PHE:HB3	1.77	0.66
1:B:387:PHE:HB2	1:B:442:LEU:HD21	1.78	0.66
1:B:159:PRO:C	1:B:165:PRO:HG2	2.16	0.66
1:A:12:ASP:HB3	1:A:363:MET:SD	2.36	0.65
1:A:44:PRO:HD2	1:A:81:ARG:HG2	1.77	0.65
1:A:142:PRO:HD2	1:A:196:THR:HG22	1.77	0.65
1:B:281:GLU:CB	1:B:282:PRO:CD	2.73	0.65
1:A:436:VAL:CG1	1:A:486:LEU:HD13	2.27	0.65
1:A:31:LYS:HG3	1:A:67:LEU:O	1.97	0.65
1:A:116:CYS:HB3	1:B:360:HIS:CD2	2.31	0.65
1:A:273:ILE:HD12	1:A:273:ILE:N	2.12	0.65
1:A:557:ASN:C	1:A:557:ASN:HD22	2.00	0.65
1:A:160:TRP:CB	1:A:165:PRO:HB3	2.27	0.65
1:A:400:ARG:HH21	1:B:100:LYS:HD3	1.60	0.65
1:A:558:LEU:HD11	1:A:584:ALA:HB2	1.77	0.64
1:B:226:LYS:O	1:B:230:LYS:HB2	1.96	0.64
1:B:537:ARG:HB3	1:B:537:ARG:HH11	1.62	0.64
1:B:553:LYS:HB2	1:B:588:TRP:CE3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASP:OD2	1:A:223:GLU:HB2	1.98	0.64
1:A:377:TYR:N	1:A:378:PRO:HD2	2.13	0.64
1:B:26:ARG:HA	1:B:71:TRP:O	1.97	0.64
1:B:80:ARG:HG2	1:B:80:ARG:HH11	1.61	0.64
1:A:284:PRO:HG3	1:A:293:PRO:HG3	1.79	0.64
1:B:137:TRP:O	1:B:454:CYS:HA	1.97	0.64
1:B:392:MET:HB2	1:B:396:GLU:HB2	1.80	0.64
1:A:155:LYS:HG3	1:A:156:GLY:H	1.63	0.64
1:A:302:HIS:CG	1:A:303:PRO:HD2	2.33	0.64
1:B:3:LYS:HE2	1:B:95:LEU:HD21	1.79	0.64
1:B:166:THR:HG21	1:B:469:PRO:O	1.98	0.64
1:A:253:ALA:HB3	1:A:254:PRO:CD	2.24	0.63
1:A:544:ILE:O	1:A:573:VAL:HG12	1.98	0.63
1:B:64:SER:HB3	1:B:69:ASP:HA	1.80	0.63
1:A:100:LYS:HD3	1:B:400:ARG:NH2	2.13	0.63
1:A:357:LEU:CD2	1:A:375:MET:HG3	2.25	0.63
1:B:532:MET:C	1:B:533:ILE:HD12	2.18	0.63
1:B:556:VAL:CG1	1:B:584:ALA:HB3	2.29	0.63
1:A:253:ALA:CB	1:A:254:PRO:HD3	2.26	0.63
1:B:284:PRO:HB3	1:B:286:TYR:CE1	2.34	0.63
1:B:385:ARG:HD3	1:B:391:ASP:OD2	1.98	0.63
1:A:345:VAL:HG23	1:A:346:LYS:N	2.14	0.62
1:B:357:LEU:HD23	1:B:375:MET:HE2	1.80	0.62
1:B:461:ILE:CD1	1:B:463:MET:HG3	2.30	0.62
1:B:533:ILE:HD12	1:B:533:ILE:N	2.14	0.62
1:A:503:LEU:HD21	1:A:531:VAL:HG11	1.80	0.62
1:A:439:VAL:HG11	1:A:486:LEU:HD21	1.81	0.62
1:A:436:VAL:HG13	1:A:486:LEU:HD13	1.82	0.62
1:A:548:ILE:HD11	1:A:571:LEU:HB2	1.82	0.62
1:A:360:HIS:CD2	1:B:116:CYS:HB3	2.34	0.62
1:A:553:LYS:HE3	1:A:554:TRP:HE1	1.64	0.62
1:B:265:SER:O	1:B:268:LYS:HD3	1.99	0.62
1:B:450:THR:HG23	1:B:504:ARG:O	2.00	0.61
1:B:553:LYS:H	1:B:587:SER:HA	1.65	0.61
1:A:427:ARG:HH12	1:A:458:GLY:H	1.49	0.61
1:A:450:THR:HG23	1:A:504:ARG:O	2.00	0.61
1:B:62:THR:OG1	1:B:406:HIS:HE1	1.83	0.61
1:A:165:PRO:O	1:A:166:THR:CB	2.48	0.61
1:A:167:PRO:O	1:A:168:THR:OG1	2.19	0.61
1:A:423:HIS:CD2	1:A:423:HIS:H	2.17	0.61
1:A:60:ARG:HH12	1:A:72:LEU:HD23	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ILE:HB	1:B:155:LYS:NZ	2.16	0.61
1:B:158:ARG:HB3	1:B:159:PRO:HD2	1.81	0.61
1:B:179:ILE:HA	1:B:182:LEU:HD13	1.82	0.61
1:B:444:LEU:HA	1:B:493:LEU:HD21	1.83	0.61
1:A:238:ARG:HD2	1:A:323:ASP:CG	2.21	0.60
1:B:80:ARG:HG2	1:B:80:ARG:NH1	2.16	0.60
1:A:133:LYS:HB2	1:A:505:ARG:HH21	1.67	0.60
1:B:449:PHE:O	1:B:497:ARG:NH2	2.35	0.60
1:A:444:LEU:HA	1:A:493:LEU:HD21	1.84	0.60
1:B:525:THR:HG23	1:B:530:THR:HG23	1.83	0.60
1:A:439:VAL:HG12	1:A:486:LEU:HD11	1.83	0.60
1:B:444:LEU:HD11	1:B:582:LEU:HD11	1.83	0.60
1:A:149:ASN:HD21	1:A:151:ALA:HB2	1.66	0.59
1:A:248:CYS:O	1:A:296:PRO:HD2	2.01	0.59
1:A:277:PRO:O	1:A:279:GLN:HG3	2.02	0.59
1:B:39:LEU:HD12	1:B:57:MET:CE	2.32	0.59
1:A:358:ILE:HG23	1:A:360:HIS:CE1	2.38	0.59
1:A:278:LEU:HA	1:A:285:ASN:HD21	1.67	0.59
1:A:349:LYS:HB3	1:A:352:VAL:HG23	1.84	0.59
1:A:449:PHE:CE1	1:A:508:VAL:HG11	2.38	0.59
1:B:419:LEU:HD23	1:B:419:LEU:H	1.67	0.59
1:B:229:VAL:HG11	1:B:320:PHE:O	2.01	0.59
1:B:560:THR:HG22	1:B:562:GLU:H	1.65	0.59
1:B:197:PRO:O	1:B:206:LYS:HB2	2.03	0.59
1:A:557:ASN:HD22	1:A:559:LEU:H	1.50	0.58
1:A:175:LEU:CD1	1:A:219:PHE:HB3	2.32	0.58
1:A:79:TYR:O	1:A:81:ARG:HD2	2.02	0.58
1:A:140:ILE:O	1:A:140:ILE:HG13	2.04	0.58
1:B:131:TRP:O	1:B:135:THR:HG23	2.04	0.58
1:B:175:LEU:HD13	1:B:219:PHE:HB3	1.85	0.58
1:B:160:TRP:HB3	1:B:165:PRO:HD3	1.85	0.58
1:B:250:TYR:HB2	1:B:294:HIS:HB2	1.86	0.58
1:A:402:MET:HE3	1:A:406:HIS:CD2	2.39	0.58
1:A:144:ARG:HG3	1:A:472:ARG:O	2.04	0.58
1:B:161:GLY:HA3	1:B:164:ASP:OD2	2.03	0.58
1:A:94:LYS:C	1:A:94:LYS:HD2	2.24	0.58
1:A:254:PRO:O	1:A:258:VAL:HG23	2.03	0.58
1:B:10:SER:O	1:B:11:THR:HB	2.03	0.58
1:B:64:SER:CB	1:B:69:ASP:HA	2.34	0.58
1:B:557:ASN:ND2	1:B:559:LEU:N	2.52	0.58
1:B:155:LYS:HZ1	1:B:172:GLY:HA2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PRO:O	1:A:155:LYS:HB2	2.02	0.57
1:B:190:ILE:C	1:B:190:ILE:HD12	2.25	0.57
1:A:12:ASP:OD1	1:A:367:ARG:NH1	2.37	0.57
1:B:6:ILE:HA	1:B:28:GLN:O	2.03	0.57
1:B:197:PRO:HB2	1:B:206:LYS:HB3	1.87	0.57
1:B:470:GLU:O	1:B:473:LYS:HG3	2.05	0.57
1:A:513:ALA:C	1:A:515:ASP:H	2.08	0.57
1:B:273:ILE:HD12	1:B:273:ILE:N	2.19	0.57
1:B:302:HIS:CD2	1:B:304:GLU:H	2.23	0.57
1:B:458:GLY:N	1:B:460:GLU:OE2	2.37	0.57
1:A:231:ARG:O	1:A:235:LYS:HD3	2.05	0.57
1:B:358:ILE:HB	1:B:374:VAL:HG11	1.87	0.57
1:A:196:THR:OG1	1:A:197:PRO:HD2	2.05	0.57
1:B:292:VAL:HG12	1:B:292:VAL:O	2.04	0.57
1:A:88:LEU:N	1:A:88:LEU:CD2	2.67	0.57
1:A:331:ASN:HB3	1:A:358:ILE:HG12	1.86	0.57
1:A:557:ASN:CB	1:A:560:THR:HG22	2.34	0.56
1:A:409:PRO:HG2	1:A:412:VAL:CG2	2.35	0.56
1:B:160:TRP:HB3	1:B:165:PRO:CG	2.35	0.56
1:B:205:HIS:CD2	2:D:5:GLC:H2	2.39	0.56
1:B:349:LYS:O	1:B:352:VAL:HG23	2.05	0.56
1:B:333:ILE:HD12	1:B:338:TRP:HZ2	1.68	0.56
1:A:511:LEU:N	1:A:511:LEU:HD12	2.20	0.56
1:B:243:ALA:HB2	1:B:325:TRP:CE3	2.40	0.56
1:A:315:TYR:CE1	1:A:319:GLU:HG3	2.41	0.56
1:B:17:ALA:HA	1:B:23:LEU:HD23	1.87	0.56
1:B:461:ILE:HD11	1:B:463:MET:HG3	1.88	0.56
1:A:19:ASP:OD1	1:A:21:GLU:N	2.38	0.56
1:A:284:PRO:CG	1:A:293:PRO:HG3	2.35	0.56
1:B:567:GLU:O	1:B:568:ALA:HB2	2.06	0.56
1:A:393:SER:HB2	1:A:517:VAL:HG13	1.88	0.56
1:A:588:TRP:CE3	1:A:588:TRP:C	2.78	0.56
1:B:165:PRO:HB3	1:B:171:PHE:HZ	1.71	0.56
1:B:537:ARG:HB3	1:B:537:ARG:NH1	2.21	0.56
1:A:6:ILE:HD13	1:A:88:LEU:HD11	1.87	0.56
1:B:188:LEU:HD23	1:B:188:LEU:O	2.05	0.56
1:A:330:ALA:HB1	1:A:371:PHE:CZ	2.41	0.55
1:B:557:ASN:C	1:B:557:ASN:HD22	2.09	0.55
1:A:167:PRO:CG	1:A:168:THR:N	2.69	0.55
1:A:553:LYS:HB3	1:A:586:GLU:HB3	1.87	0.55
1:A:26:ARG:HA	1:A:71:TRP:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:O	1:A:234:GLU:HB2	2.07	0.55
1:B:521:VAL:HG23	1:B:534:ILE:HD13	1.88	0.55
1:B:548:ILE:HG13	1:B:548:ILE:O	2.05	0.55
1:B:390:GLU:OE2	1:B:438:LYS:HE2	2.07	0.55
1:A:516:GLU:HB2	1:A:519:HIS:HB2	1.89	0.55
1:B:259:LEU:HD23	1:B:278:LEU:HD23	1.89	0.55
1:A:24:HIS:C	1:A:25:LEU:HD22	2.26	0.55
1:B:27:LEU:HD12	1:B:37:VAL:HG21	1.89	0.55
1:B:152:ILE:HB	1:B:155:LYS:HZ3	1.72	0.55
1:B:377:TYR:N	1:B:378:PRO:HD2	2.21	0.54
1:A:23:LEU:HG	1:A:120:LEU:HD12	1.90	0.54
1:A:157:ALA:O	1:A:158:ARG:O	2.26	0.54
1:B:476:VAL:O	1:B:482:GLN:NE2	2.40	0.54
1:A:237:ILE:N	1:A:237:ILE:HD12	2.23	0.54
1:A:470:GLU:O	1:A:473:LYS:HG3	2.07	0.54
1:B:131:TRP:HE1	1:B:351:ASP:HB3	1.73	0.54
1:B:331:ASN:HB3	1:B:358:ILE:HG12	1.89	0.54
1:A:520:LEU:HD12	1:A:520:LEU:C	2.27	0.54
1:A:563:ARG:HD2	1:A:563:ARG:O	2.07	0.54
1:B:155:LYS:HE3	1:B:170:PHE:CB	2.37	0.54
1:B:168:THR:O	1:B:168:THR:HG22	2.07	0.54
1:A:430:THR:HG21	1:A:465:GLY:H	1.72	0.54
1:A:456:TYR:O	1:A:458:GLY:N	2.41	0.54
1:B:167:PRO:CD	1:B:168:THR:H	2.21	0.54
1:A:236:GLY:C	1:A:237:ILE:HD12	2.28	0.54
1:A:554:TRP:H	1:A:586:GLU:CB	2.17	0.54
1:B:288:THR:O	1:B:289:PHE:C	2.46	0.54
1:B:357:LEU:HD23	1:B:375:MET:HG3	1.88	0.54
1:A:10:SER:HB3	1:A:84:TYR:OH	2.08	0.54
1:A:34:VAL:HG11	1:A:88:LEU:HB2	1.89	0.54
1:B:208:ASP:O	1:B:249:GLY:HA3	2.07	0.54
1:A:140:ILE:HD12	1:A:178:ILE:HG12	1.90	0.53
1:A:292:VAL:HG12	1:A:292:VAL:O	2.08	0.53
1:A:80:ARG:HD2	1:A:119:PHE:CE2	2.43	0.53
1:A:537:ARG:HD2	1:A:537:ARG:O	2.08	0.53
1:B:155:LYS:CG	1:B:170:PHE:HB2	2.30	0.53
1:A:559:LEU:HD11	1:A:580:PHE:HE1	1.72	0.53
1:B:254:PRO:O	1:B:258:VAL:HG23	2.09	0.53
1:B:230:LYS:HD3	1:B:230:LYS:C	2.29	0.53
1:B:306:LYS:O	1:B:310:LEU:HB2	2.08	0.53
1:B:329:VAL:HG12	1:B:329:VAL:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TRP:HB2	1:A:454:CYS:HB2	1.91	0.53
1:A:467:ASN:O	1:A:470:GLU:HB2	2.09	0.53
1:B:418:ASN:O	1:B:453:PRO:HA	2.09	0.53
1:A:385:ARG:HG2	1:A:391:ASP:HB2	1.91	0.53
1:A:553:LYS:HD2	1:A:588:TRP:HB3	1.91	0.53
1:A:64:SER:HB3	1:A:69:ASP:HA	1.90	0.53
1:B:98:THR:HB	1:B:113:TYR:O	2.09	0.52
1:B:466:GLY:O	1:B:470:GLU:HB2	2.09	0.52
1:A:144:ARG:HG3	1:A:144:ARG:HH11	1.74	0.52
1:A:428:LEU:HD11	1:A:442:LEU:HD13	1.91	0.52
1:A:1:MET:HE2	1:A:95:LEU:HD22	1.91	0.52
1:A:158:ARG:HD3	1:A:159:PRO:HD3	1.91	0.52
1:B:131:TRP:O	1:B:134:ASP:N	2.41	0.52
1:A:167:PRO:HG2	1:A:168:THR:N	2.22	0.52
1:B:26:ARG:HG3	1:B:26:ARG:NH1	2.25	0.52
1:A:393:SER:OG	1:A:396:GLU:HG3	2.10	0.52
1:A:206:LYS:HE2	1:A:219:PHE:CE1	2.44	0.52
1:B:430:THR:HG21	1:B:465:GLY:N	2.18	0.52
1:A:173:GLY:O	1:A:174:ASP:HB3	2.09	0.52
1:A:254:PRO:HB3	1:A:267:TYR:CD2	2.45	0.52
1:B:60:ARG:NH1	1:B:72:LEU:HD23	2.25	0.52
1:B:201:ALA:HB3	1:B:206:LYS:HG3	1.92	0.52
1:B:557:ASN:HD22	1:B:559:LEU:N	2.08	0.51
1:B:231:ARG:HG3	1:B:231:ARG:HH11	1.75	0.51
1:B:345:VAL:CG2	1:B:346:LYS:H	2.21	0.51
1:B:552:GLY:HA2	1:B:587:SER:HB3	1.92	0.51
1:B:557:ASN:HD22	1:B:558:LEU:N	2.08	0.51
1:A:385:ARG:HB3	1:A:392:MET:CE	2.41	0.51
1:A:516:GLU:CB	1:A:519:HIS:HB2	2.40	0.51
1:A:588:TRP:CD2	1:A:588:TRP:OXT	2.63	0.51
1:B:155:LYS:HG3	1:B:170:PHE:CB	2.30	0.51
1:B:199:PHE:O	1:B:200:ARG:C	2.49	0.51
1:B:362:ALA:CB	1:B:374:VAL:HG21	2.41	0.51
1:B:247:HIS:HA	1:B:298:LEU:HD13	1.91	0.51
1:A:41:PHE:O	1:A:54:PHE:HB2	2.11	0.51
1:A:260:LYS:HE3	1:A:260:LYS:CA	2.41	0.51
1:B:240:MET:HG3	1:B:324:GLY:O	2.10	0.51
1:A:27:LEU:HD22	1:A:28:GLN:N	2.26	0.51
1:B:140:ILE:O	1:B:142:PRO:HD3	2.11	0.51
1:A:94:LYS:HD2	1:A:94:LYS:O	2.10	0.51
1:B:233:HIS:HE1	1:B:323:ASP:OD2	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LYS:HG3	1:A:156:GLY:N	2.25	0.50
1:B:63:GLY:HA3	1:B:402:MET:HE3	1.92	0.50
1:B:197:PRO:HB2	1:B:206:LYS:O	2.11	0.50
1:B:235:LYS:HB3	1:B:237:ILE:HD13	1.91	0.50
1:A:138:TYR:CZ	1:A:457:TYR:HA	2.46	0.50
1:B:500:TYR:HB2	1:B:503:LEU:HD12	1.94	0.50
1:B:10:SER:HA	1:B:15:ALA:HB3	1.92	0.50
1:A:105:GLU:O	1:A:107:PRO:HD3	2.10	0.50
1:B:438:LYS:O	1:B:441:LEU:HB2	2.11	0.50
1:A:165:PRO:O	1:A:166:THR:HB	2.10	0.50
1:A:205:HIS:O	1:A:205:HIS:ND1	2.44	0.50
1:B:32:ASN:N	1:B:69:ASP:OD2	2.36	0.50
1:B:195:LEU:N	1:B:195:LEU:HD23	2.27	0.50
1:B:257:ASP:OD2	1:B:265:SER:HB2	2.12	0.50
1:B:496:LEU:HD21	1:B:558:LEU:HB3	1.93	0.50
1:A:385:ARG:HB3	1:A:392:MET:HE2	1.94	0.50
1:A:444:LEU:HD11	1:A:582:LEU:HD11	1.94	0.50
1:A:31:LYS:HG3	1:A:67:LEU:C	2.32	0.49
1:A:199:PHE:O	1:A:200:ARG:C	2.50	0.49
1:A:329:VAL:HG12	1:A:329:VAL:O	2.12	0.49
1:B:158:ARG:NH1	1:B:474:CYS:HB3	2.27	0.49
1:A:102:PHE:C	1:A:103:TYR:CD1	2.81	0.49
1:A:163:GLU:O	1:A:164:ASP:HB3	2.12	0.49
1:A:557:ASN:HD21	1:A:559:LEU:HB2	1.77	0.49
1:B:326:ARG:C	1:B:326:ARG:CD	2.80	0.49
1:A:229:VAL:HG12	1:A:233:HIS:CD2	2.47	0.49
1:B:158:ARG:CB	1:B:159:PRO:HD2	2.42	0.49
1:B:157:ALA:O	1:B:158:ARG:O	2.30	0.49
1:A:191:THR:O	1:A:237:ILE:HA	2.13	0.49
1:A:553:LYS:HD2	1:A:588:TRP:CG	2.46	0.49
1:A:400:ARG:HG3	1:A:400:ARG:NH1	2.25	0.49
1:A:557:ASN:HD22	1:A:558:LEU:N	2.10	0.49
1:A:4:GLU:H	1:A:4:GLU:CD	2.16	0.49
1:A:335:HIS:CD2	1:A:370:GLN:OE1	2.66	0.49
1:B:511:LEU:N	1:B:511:LEU:CD1	2.76	0.49
1:A:1:MET:SD	1:A:90:ALA:HB3	2.52	0.49
1:B:279:GLN:HB2	1:B:281:GLU:HG2	1.94	0.49
1:B:464:THR:OG1	1:B:465:GLY:N	2.46	0.49
1:A:167:PRO:CD	1:A:168:THR:H	2.26	0.49
1:A:288:THR:O	1:A:289:PHE:C	2.51	0.49
1:B:271:PHE:CD1	1:B:271:PHE:N	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:PRO:HG2	1:B:412:VAL:CG2	2.43	0.49
1:A:38:GLU:HG3	1:A:58:PRO:HB3	1.94	0.48
1:A:390:GLU:HB3	1:A:537:ARG:NH1	2.28	0.48
1:B:284:PRO:HB3	1:B:286:TYR:CD1	2.48	0.48
1:A:299:ASN:HD21	1:A:301:ALA:HB3	1.78	0.48
1:B:365:TRP:HB3	1:B:371:PHE:CD2	2.48	0.48
1:B:162:SER:C	1:B:163:GLU:HG3	2.33	0.48
1:B:209:THR:O	1:B:249:GLY:HA3	2.13	0.48
1:A:30:LYS:HB3	1:A:33:ASP:CB	2.41	0.48
1:A:48:HIS:HB3	1:A:53:GLN:NE2	2.28	0.48
1:B:137:TRP:O	1:B:455:ILE:N	2.41	0.48
1:A:131:TRP:CE3	1:A:135:THR:HG21	2.49	0.48
1:A:243:ALA:HB3	1:A:327:LEU:HD23	1.94	0.48
1:B:60:ARG:HH12	1:B:72:LEU:HD23	1.78	0.48
1:A:131:TRP:HE3	1:A:135:THR:HG21	1.78	0.48
1:A:302:HIS:ND1	1:A:303:PRO:HD2	2.29	0.48
1:B:345:VAL:CG2	1:B:346:LYS:N	2.75	0.48
1:A:1:MET:HB3	1:A:93:GLU:OE2	2.13	0.48
1:A:549:ASP:OD2	1:A:551:ARG:HB2	2.13	0.48
1:A:560:THR:HG23	1:A:562:GLU:N	2.25	0.48
1:B:147:ASN:C	1:B:147:ASN:HD22	2.16	0.48
1:B:546:MET:CE	1:B:571:LEU:HD23	2.44	0.48
1:B:41:PHE:O	1:B:54:PHE:HB2	2.14	0.48
1:B:540:GLU:C	1:B:577:PRO:HG3	2.34	0.48
1:A:46:GLU:OE1	1:A:46:GLU:HA	2.13	0.48
1:B:128:ALA:O	1:B:129:PRO:O	2.32	0.48
1:B:160:TRP:HB3	1:B:165:PRO:CD	2.43	0.48
1:B:233:HIS:CE1	1:B:323:ASP:OD2	2.67	0.48
1:B:330:ALA:HB1	1:B:371:PHE:HZ	1.73	0.48
1:A:56:THR:HG23	1:A:56:THR:O	2.14	0.48
1:B:99:GLU:HB2	1:B:115:PHE:CD1	2.49	0.48
1:B:213:PHE:HE2	1:B:308:TYR:CE1	2.32	0.48
1:B:444:LEU:CD1	1:B:582:LEU:HD11	2.44	0.48
1:B:61:LYS:HD2	1:B:69:ASP:HB3	1.95	0.47
1:B:409:PRO:HG2	1:B:412:VAL:HG23	1.96	0.47
1:A:330:ALA:HB1	1:A:371:PHE:HZ	1.79	0.47
1:B:304:GLU:O	1:B:305:VAL:C	2.53	0.47
1:B:333:ILE:HB	1:B:338:TRP:NE1	2.29	0.47
1:B:289:PHE:CZ	2:D:4:GLC:H62	2.49	0.47
1:A:122:ARG:O	1:A:125:LEU:HB3	2.15	0.47
1:A:345:VAL:CG2	1:A:346:LYS:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:MET:O	1:A:533:ILE:HD12	2.14	0.47
1:B:237:ILE:HD12	1:B:237:ILE:N	2.29	0.47
1:B:335:HIS:CD2	1:B:370:GLN:OE1	2.67	0.47
1:B:399:ASP:O	1:B:400:ARG:C	2.50	0.47
1:B:401:LEU:HD12	1:B:401:LEU:HA	1.76	0.47
1:A:410:LYS:NZ	1:A:507:ASP:OD1	2.47	0.47
1:B:279:GLN:HB2	1:B:281:GLU:OE2	2.15	0.47
1:A:131:TRP:CZ3	1:A:238:ARG:HG3	2.49	0.47
1:A:188:LEU:O	1:A:188:LEU:HD23	2.14	0.47
1:A:557:ASN:ND2	1:A:557:ASN:C	2.68	0.47
1:A:558:LEU:N	1:A:558:LEU:CD1	2.78	0.47
1:B:271:PHE:HB2	1:B:273:ILE:HD11	1.96	0.47
1:A:426:PRO:HA	1:A:466:GLY:O	2.15	0.47
1:B:276:PHE:C	1:B:278:LEU:H	2.17	0.47
1:B:409:PRO:O	1:B:412:VAL:HB	2.14	0.47
1:A:233:HIS:HE1	1:A:323:ASP:OD2	1.97	0.47
1:A:517:VAL:HG12	1:A:517:VAL:O	2.13	0.47
1:B:209:THR:O	1:B:249:GLY:N	2.48	0.47
1:A:197:PRO:HB2	1:A:206:LYS:HB3	1.97	0.47
1:A:427:ARG:NH1	1:A:456:TYR:CD2	2.83	0.47
1:B:1:MET:SD	1:B:34:VAL:HG22	2.54	0.47
1:A:23:LEU:HD21	1:A:117:PHE:CE1	2.49	0.47
1:B:560:THR:HG22	1:B:562:GLU:HB2	1.96	0.47
1:A:281:GLU:CB	1:A:282:PRO:CD	2.83	0.46
1:B:540:GLU:CA	1:B:577:PRO:HG3	2.46	0.46
1:A:558:LEU:N	1:A:558:LEU:HD12	2.30	0.46
1:B:206:LYS:HE2	1:B:219:PHE:CE2	2.51	0.46
1:B:12:ASP:OD2	1:B:367:ARG:NH1	2.49	0.46
1:B:78:PRO:O	1:B:79:TYR:HB2	2.15	0.46
1:B:167:PRO:CG	1:B:168:THR:H	2.28	0.46
1:A:1:MET:CE	1:A:95:LEU:HD22	2.44	0.46
1:A:523:ALA:HB2	1:A:532:MET:SD	2.55	0.46
1:B:34:VAL:HG13	1:B:89:ARG:O	2.15	0.46
1:B:150:PRO:C	1:B:152:ILE:H	2.17	0.46
1:B:272:HIS:HB2	1:B:287:ASP:HB2	1.97	0.46
1:A:528:ASN:N	1:A:528:ASN:ND2	2.63	0.46
1:A:290:ALA:O	1:A:291:PHE:CG	2.69	0.46
1:A:501:ARG:HD3	1:A:526:ASP:OD2	2.16	0.46
1:B:48:HIS:O	1:B:49:ASP:HB2	2.16	0.46
1:B:166:THR:HG22	1:B:469:PRO:HB2	1.97	0.46
1:A:400:ARG:O	1:A:404:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:HIS:HB2	1:A:472:ARG:HE	1.80	0.46
1:B:341:PHE:O	1:B:345:VAL:HG22	2.16	0.46
1:B:379:LEU:C	1:B:379:LEU:HD23	2.36	0.46
1:A:419:LEU:HD23	1:A:419:LEU:N	2.23	0.46
1:A:5:ALA:HB2	1:B:4:GLU:HB3	1.97	0.45
1:A:27:LEU:CD2	1:A:28:GLN:N	2.79	0.45
1:A:355:LEU:HD12	1:A:356:GLY:N	2.31	0.45
1:B:369:ASP:C	1:B:370:GLN:HG3	2.36	0.45
1:B:558:LEU:HD22	1:B:582:LEU:HB3	1.98	0.45
1:B:26:ARG:HG3	1:B:26:ARG:HH11	1.81	0.45
1:B:155:LYS:HE2	1:B:172:GLY:N	2.31	0.45
1:B:439:VAL:HG11	1:B:486:LEU:HD21	1.98	0.45
1:A:158:ARG:HB3	1:A:159:PRO:CD	2.38	0.45
1:B:188:LEU:HD11	1:B:460:GLU:HG2	1.96	0.45
1:B:195:LEU:HD23	1:B:195:LEU:H	1.82	0.45
1:B:248:CYS:SG	1:B:296:PRO:HG2	2.56	0.45
1:A:448:THR:CG2	1:A:522:TYR:OH	2.64	0.45
1:A:588:TRP:C	1:A:588:TRP:CD2	2.89	0.45
1:B:54:PHE:CD1	1:B:54:PHE:C	2.89	0.45
1:B:341:PHE:HE2	1:B:354:ILE:HG23	1.81	0.45
1:B:486:LEU:O	1:B:489:HIS:HB3	2.15	0.45
1:A:44:PRO:HG3	1:A:83:ARG:HG2	1.98	0.45
1:A:208:ASP:OD2	1:A:208:ASP:N	2.48	0.45
1:A:82:LEU:HD23	1:A:82:LEU:O	2.16	0.45
1:A:261:ASN:HB3	1:A:264:ALA:HB3	1.97	0.45
1:A:404:VAL:HG23	1:A:405:LEU:H	1.82	0.45
1:B:30:LYS:HB3	1:B:33:ASP:CB	2.47	0.45
1:B:256:GLN:O	1:B:259:LEU:HB2	2.17	0.45
1:B:376:ASN:C	1:B:378:PRO:HD2	2.36	0.45
1:A:140:ILE:O	1:A:142:PRO:N	2.49	0.45
1:A:159:PRO:HD3	1:A:474:CYS:HB2	1.99	0.45
1:A:35:ASP:OD2	1:A:91:GLY:N	2.45	0.45
1:B:37:VAL:HG13	1:B:37:VAL:O	2.16	0.45
1:B:159:PRO:HA	1:B:165:PRO:HG2	1.98	0.45
1:B:215:ILE:O	1:B:216:ASP:C	2.54	0.45
1:A:132:VAL:HA	1:A:135:THR:HG23	1.99	0.45
1:A:201:ALA:HB1	1:A:202:PRO:HD2	1.99	0.45
1:A:349:LYS:HB3	1:A:352:VAL:CG2	2.47	0.45
1:A:37:VAL:HG23	1:A:88:LEU:HB3	2.00	0.45
1:A:168:THR:HG22	1:A:168:THR:O	2.17	0.45
1:B:142:PRO:O	1:B:173:GLY:HA3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:PRO:CG	1:B:168:THR:N	2.79	0.45
1:B:552:GLY:HA2	1:B:587:SER:CB	2.47	0.45
1:B:243:ALA:HB3	1:B:327:LEU:HD23	1.98	0.44
1:B:327:LEU:HD13	1:B:338:TRP:CZ3	2.52	0.44
1:A:1:MET:CE	1:A:95:LEU:HB2	2.47	0.44
1:A:16:TYR:CD2	1:A:409:PRO:HB3	2.51	0.44
1:A:82:LEU:HD23	1:A:82:LEU:C	2.37	0.44
1:A:306:LYS:O	1:A:310:LEU:HB2	2.17	0.44
1:B:431:VAL:HG12	1:B:431:VAL:O	2.18	0.44
1:B:483:ASN:OD1	1:B:485:GLU:HB3	2.17	0.44
1:B:1:MET:SD	1:B:90:ALA:HB2	2.56	0.44
1:B:80:ARG:HH11	1:B:80:ARG:CG	2.29	0.44
1:B:153:SER:H	1:B:155:LYS:HZ2	1.64	0.44
1:B:175:LEU:O	1:B:176:GLN:C	2.53	0.44
1:B:557:ASN:CG	1:B:560:THR:HB	2.37	0.44
1:A:6:ILE:HA	1:A:28:GLN:O	2.18	0.44
1:B:167:PRO:HG2	1:B:168:THR:N	2.33	0.44
1:B:555:LEU:CD1	1:B:585:VAL:HG22	2.48	0.44
1:A:328:ASP:OD2	1:A:329:VAL:HG23	2.17	0.44
1:A:444:LEU:O	1:A:448:THR:HG22	2.18	0.44
1:B:164:ASP:HB2	1:B:165:PRO:CD	2.41	0.44
1:A:199:PHE:CE1	1:A:316:TRP:CZ2	3.06	0.44
1:B:279:GLN:HB2	1:B:281:GLU:CG	2.48	0.44
1:A:345:VAL:HG23	1:A:346:LYS:H	1.82	0.44
1:A:290:ALA:O	1:B:81:ARG:NH2	2.49	0.44
1:A:585:VAL:HG12	1:A:586:GLU:N	2.32	0.44
1:A:276:PHE:O	1:A:278:LEU:N	2.50	0.44
1:A:531:VAL:HG12	1:A:533:ILE:CD1	2.48	0.44
1:B:160:TRP:HB3	1:B:165:PRO:HG3	1.99	0.44
1:A:179:ILE:O	1:A:182:LEU:HB2	2.18	0.43
1:A:304:GLU:O	1:A:305:VAL:C	2.57	0.43
1:B:165:PRO:O	1:B:166:THR:CB	2.65	0.43
1:A:161:GLY:H	1:A:165:PRO:HG3	1.83	0.43
1:A:534:ILE:HG21	1:A:573:VAL:HG11	1.98	0.43
1:B:30:LYS:HB3	1:B:33:ASP:HB2	1.98	0.43
1:B:37:VAL:HG11	1:B:71:TRP:CG	2.53	0.43
1:B:564:PHE:CD1	1:B:564:PHE:N	2.86	0.43
1:A:25:LEU:HD12	1:A:84:TYR:CE2	2.53	0.43
1:A:253:ALA:CB	1:A:254:PRO:CD	2.92	0.43
1:A:448:THR:HG23	1:A:448:THR:O	2.17	0.43
1:A:559:LEU:HD11	1:A:580:PHE:CE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:GLU:OE2	1:B:89:ARG:NE	2.42	0.43
1:B:155:LYS:HE2	1:B:171:PHE:C	2.39	0.43
1:B:427:ARG:NH1	1:B:457:TYR:O	2.47	0.43
1:A:181:HIS:O	1:A:184:TYR:HB3	2.18	0.43
1:B:362:ALA:HB3	1:B:374:VAL:HG21	2.01	0.43
1:B:327:LEU:HD13	1:B:371:PHE:HE1	1.83	0.43
1:B:365:TRP:HB3	1:B:371:PHE:HD2	1.82	0.43
1:B:377:TYR:N	1:B:378:PRO:CD	2.82	0.43
1:A:327:LEU:HD11	1:A:354:ILE:CG2	2.48	0.43
1:A:335:HIS:O	1:A:339:ARG:HG3	2.18	0.43
1:A:435:ASP:OD1	1:A:437:ARG:HB2	2.17	0.43
1:A:457:TYR:O	1:A:460:GLU:OE2	2.36	0.43
1:B:37:VAL:HG13	1:B:59:MET:HE3	2.01	0.43
1:B:385:ARG:HH11	1:B:392:MET:CE	2.29	0.43
1:B:531:VAL:HG12	1:B:533:ILE:HD11	2.01	0.43
1:B:574:SER:C	1:B:575:LEU:HD12	2.38	0.43
1:A:59:MET:HE1	1:A:86:PHE:CD2	2.42	0.43
1:A:476:VAL:O	1:A:482:GLN:NE2	2.51	0.43
1:B:194:TYR:CD1	1:B:194:TYR:C	2.92	0.43
1:A:161:GLY:H	1:A:165:PRO:CG	2.31	0.43
1:A:194:TYR:CD1	1:A:194:TYR:C	2.92	0.43
1:A:245:PHE:CD1	1:A:309:LEU:HD22	2.54	0.43
1:A:463:MET:SD	1:A:476:VAL:HG23	2.59	0.43
1:B:200:ARG:HA	1:B:216:ASP:HA	2.01	0.43
1:B:333:ILE:HB	1:B:338:TRP:HE1	1.84	0.43
1:B:521:VAL:HG13	1:B:521:VAL:O	2.19	0.43
1:B:534:ILE:HD11	1:B:546:MET:SD	2.58	0.43
1:A:511:LEU:HD23	1:A:547:PRO:HG2	2.01	0.43
1:B:277:PRO:O	1:B:278:LEU:C	2.57	0.43
1:A:43:ASP:OD2	1:A:81:ARG:HD3	2.19	0.43
1:A:564:PHE:CD1	1:A:564:PHE:N	2.86	0.43
1:B:148:GLY:O	1:B:149:ASN:C	2.56	0.43
1:A:2:ARG:HH22	1:B:2:ARG:HD2	1.83	0.42
1:A:150:PRO:C	1:A:152:ILE:H	2.22	0.42
1:A:206:LYS:HE2	1:A:219:PHE:CZ	2.54	0.42
1:A:237:ILE:N	1:A:237:ILE:CD1	2.82	0.42
1:A:273:ILE:HD12	1:A:273:ILE:H	1.82	0.42
1:B:88:LEU:N	1:B:88:LEU:CD2	2.79	0.42
1:B:456:TYR:O	1:B:457:TYR:C	2.57	0.42
1:B:557:ASN:HD21	1:B:559:LEU:H	1.63	0.42
1:A:309:LEU:O	1:A:312:VAL:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ILE:CD1	1:B:178:ILE:HG12	2.50	0.42
1:B:250:TYR:HB2	1:B:294:HIS:CB	2.47	0.42
1:A:30:LYS:HG2	1:A:31:LYS:N	2.35	0.42
1:B:477:TRP:O	1:B:479:PRO:HD3	2.19	0.42
1:B:2:ARG:HG3	1:B:2:ARG:HH11	1.83	0.42
1:B:43:ASP:HB3	1:B:46:GLU:HB2	2.02	0.42
1:B:205:HIS:ND1	1:B:205:HIS:C	2.73	0.42
1:B:326:ARG:HH12	1:B:375:MET:HE2	1.84	0.42
1:B:363:MET:CB	1:B:364:PRO:HD3	2.50	0.42
1:B:460:GLU:CD	1:B:460:GLU:H	2.22	0.42
1:A:478:ASP:O	1:A:481:LYS:N	2.46	0.42
1:A:502:ALA:HB2	1:A:529:GLU:HG2	2.01	0.42
1:B:207:TYR:C	1:B:209:THR:H	2.22	0.42
1:B:450:THR:CG2	1:B:505:ARG:HA	2.46	0.42
1:A:80:ARG:HD2	1:A:119:PHE:CZ	2.55	0.42
1:A:466:GLY:N	1:A:470:GLU:HB3	2.35	0.42
1:B:177:GLY:O	1:B:178:ILE:C	2.58	0.42
1:B:253:ALA:CB	1:B:254:PRO:HD3	2.35	0.42
1:A:1:MET:HE1	1:A:95:LEU:HB2	2.01	0.42
1:A:534:ILE:CD1	1:A:573:VAL:HG11	2.48	0.42
1:B:224:THR:O	1:B:227:THR:HB	2.19	0.42
1:A:273:ILE:HG23	1:A:286:TYR:HB3	2.01	0.42
1:A:326:ARG:HD2	1:A:326:ARG:C	2.40	0.42
1:A:528:ASN:N	1:A:528:ASN:HD22	2.17	0.42
1:B:27:LEU:HD22	1:B:28:GLN:N	2.35	0.42
1:B:435:ASP:OD1	1:B:437:ARG:HB2	2.19	0.42
1:A:304:GLU:O	1:A:307:ARG:N	2.53	0.42
1:A:345:VAL:HG21	1:A:354:ILE:HD11	2.02	0.42
1:A:573:VAL:O	1:A:573:VAL:CG1	2.68	0.42
1:A:62:THR:OG1	1:A:406:HIS:HE1	2.02	0.42
1:A:161:GLY:N	1:A:165:PRO:HG3	2.35	0.42
1:A:293:PRO:C	1:A:295:MET:H	2.24	0.42
1:B:163:GLU:HB3	1:B:473:LYS:HZ1	1.85	0.42
1:B:245:PHE:N	1:B:245:PHE:CD1	2.88	0.42
1:B:288:THR:HG22	1:B:296:PRO:HA	2.02	0.42
1:B:299:ASN:C	1:B:301:ALA:H	2.23	0.42
1:B:302:HIS:CD2	1:B:304:GLU:HB2	2.54	0.42
1:B:528:ASN:HD22	1:B:528:ASN:HA	1.56	0.42
1:A:513:ALA:C	1:A:515:ASP:N	2.74	0.41
1:B:138:TYR:CZ	1:B:457:TYR:HA	2.55	0.41
1:B:147:ASN:ND2	1:B:148:GLY:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:ALA:N	1:B:577:PRO:HG3	2.35	0.41
1:B:575:LEU:HD21	1:B:581:VAL:HG12	2.02	0.41
1:A:182:LEU:HG	1:A:235:LYS:NZ	2.35	0.41
1:A:418:ASN:O	1:A:453:PRO:HA	2.20	0.41
1:B:10:SER:HB3	1:B:84:TYR:OH	2.20	0.41
1:B:349:LYS:HB3	1:B:352:VAL:HG23	2.02	0.41
1:A:289:PHE:CE1	2:C:4:GLC:H62	2.56	0.41
1:B:45:TYR:HD2	2:C:1:GLC:HO6	1.64	0.41
1:B:167:PRO:HG2	1:B:168:THR:H	1.85	0.41
1:A:328:ASP:CG	1:A:329:VAL:HG23	2.40	0.41
1:B:138:TYR:OH	1:B:457:TYR:HA	2.21	0.41
1:B:225:LEU:O	1:B:226:LYS:C	2.58	0.41
1:B:577:PRO:O	1:B:578:TYR:HB2	2.21	0.41
1:A:345:VAL:CG2	1:A:346:LYS:H	2.33	0.41
1:A:466:GLY:H	1:A:470:GLU:HB3	1.85	0.41
1:A:548:ILE:HG21	1:A:566:ALA:HB1	2.01	0.41
1:B:276:PHE:C	1:B:278:LEU:N	2.74	0.41
1:A:281:GLU:O	1:A:282:PRO:C	2.56	0.41
1:A:430:THR:HG21	1:A:465:GLY:O	2.21	0.41
1:A:558:LEU:HD11	1:A:584:ALA:CB	2.49	0.41
1:B:63:GLY:HA3	1:B:402:MET:HE2	1.99	0.41
1:B:295:MET:SD	2:D:5:GLC:H62	2.60	0.41
1:A:197:PRO:HB2	1:A:206:LYS:CB	2.50	0.41
1:A:404:VAL:HG23	1:A:405:LEU:N	2.35	0.41
1:B:24:HIS:C	1:B:25:LEU:HD22	2.41	0.41
1:A:430:THR:HG23	1:A:465:GLY:H	1.81	0.41
1:A:437:ARG:O	1:A:440:LYS:HG3	2.21	0.41
1:A:573:VAL:O	1:A:573:VAL:HG13	2.21	0.41
1:B:47:TRP:O	1:B:48:HIS:HB2	2.21	0.41
1:B:59:MET:HG2	1:B:73:ALA:HB2	2.02	0.41
1:B:122:ARG:O	1:B:125:LEU:HB3	2.21	0.41
1:B:305:VAL:O	1:B:308:TYR:HB3	2.21	0.41
1:B:333:ILE:HG22	1:B:334:ASP:N	2.36	0.41
1:A:137:TRP:O	1:A:454:CYS:HA	2.21	0.41
1:A:158:ARG:CB	1:A:159:PRO:CD	2.95	0.41
1:B:153:SER:N	1:B:155:LYS:HZ2	2.19	0.41
1:B:207:TYR:HD1	1:B:244:VAL:CG2	2.34	0.41
1:B:385:ARG:NH1	1:B:392:MET:HE3	2.32	0.41
1:A:9:ARG:HD3	1:B:361:ASP:OD2	2.21	0.40
1:A:139:GLN:OE1	1:A:423:HIS:HD2	2.03	0.40
1:A:160:TRP:HB3	1:A:165:PRO:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ILE:CD1	1:A:463:MET:HG3	2.51	0.40
1:A:501:ARG:N	1:A:529:GLU:OE2	2.54	0.40
1:B:448:THR:O	1:B:448:THR:HG22	2.21	0.40
1:B:519:HIS:ND1	1:B:544:ILE:HG12	2.35	0.40
1:B:557:ASN:ND2	1:B:559:LEU:HD12	2.19	0.40
1:A:84:TYR:CD1	1:A:84:TYR:N	2.89	0.40
1:A:420:LEU:HG	1:A:446:GLN:OE1	2.21	0.40
1:A:533:ILE:HD12	1:A:533:ILE:N	2.35	0.40
1:B:125:LEU:HD12	1:B:126:PHE:N	2.36	0.40
1:B:158:ARG:HD3	1:B:158:ARG:HA	1.89	0.40
1:B:401:LEU:HD23	1:B:510:PHE:CZ	2.56	0.40
1:A:298:LEU:HD12	1:A:298:LEU:HA	1.90	0.40
1:A:477:TRP:O	1:A:479:PRO:HD3	2.21	0.40
1:A:521:VAL:O	1:A:521:VAL:HG13	2.20	0.40
1:A:585:VAL:O	1:A:586:GLU:OE1	2.39	0.40
1:B:162:SER:O	1:B:163:GLU:HG3	2.21	0.40
1:B:276:PHE:O	1:B:278:LEU:N	2.44	0.40
1:A:65:ASP:HB2	1:A:66:GLY:H	1.70	0.40
1:A:231:ARG:O	1:A:234:GLU:HB3	2.21	0.40
1:B:128:ALA:O	1:B:129:PRO:C	2.60	0.40
1:B:199:PHE:CE1	1:B:316:TRP:CZ2	3.08	0.40
1:A:61:LYS:HD2	1:A:69:ASP:OD2	2.22	0.40
1:A:302:HIS:CD2	1:A:304:GLU:H	2.40	0.40
1:A:419:LEU:H	1:A:419:LEU:CD2	2.27	0.40
1:A:588:TRP:OXT	1:A:588:TRP:CG	2.75	0.40
1:B:57:MET:HE1	1:B:75:VAL:HG23	2.02	0.40
1:B:401:LEU:HD21	1:B:445:PHE:CZ	2.57	0.40
1:B:435:ASP:O	1:B:437:ARG:N	2.54	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	586/588 (100%)	486 (83%)	76 (13%)	24 (4%)	3 17
1	B	586/588 (100%)	467 (80%)	93 (16%)	26 (4%)	2 16
All	All	1172/1176 (100%)	953 (81%)	169 (14%)	50 (4%)	2 16

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	118	PRO
1	A	156	GLY
1	A	158	ARG
1	A	159	PRO
1	A	164	ASP
1	A	166	THR
1	A	167	PRO
1	A	168	THR
1	A	281	GLU
1	A	289	PHE
1	A	457	TYR
1	B	158	ARG
1	B	159	PRO
1	B	167	PRO
1	B	168	THR
1	B	170	PHE
1	B	265	SER
1	B	281	GLU
1	B	289	PHE
1	B	360	HIS
1	A	265	SER
1	B	118	PRO
1	B	160	TRP
1	B	209	THR
1	B	483	ASN
1	A	12	ASP
1	A	13	ASN
1	A	20	SER
1	A	174	ASP
1	A	278	LEU
1	A	291	PHE
1	B	129	PRO
1	B	165	PRO
1	B	218	HIS

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Mol	Chain	Res	Type
1	B	278	LEU
1	A	200	ARG
1	B	11	THR
1	B	48	HIS
1	B	166	THR
1	B	566	ALA
1	A	141	PHE
1	A	155	LYS
1	A	514	ASP
1	A	567	GLU
1	B	274	ARG
1	B	436	VAL
1	B	551	ARG
1	B	316	TRP
1	B	142	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	505/505 (100%)	452 (90%)	53 (10%)	7 25
1	B	505/505 (100%)	457 (90%)	48 (10%)	8 29
All	All	1010/1010 (100%)	909 (90%)	101 (10%)	7 27

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	26	ARG
1	A	27	LEU
1	A	47	TRP
1	A	49	ASP
1	A	69	ASP
1	A	81	ARG
1	A	82	LEU

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Mol	Chain	Res	Type
1	A	88	LEU
1	A	94	LYS
1	A	135	THR
1	A	147	ASN
1	A	159	PRO
1	A	163	GLU
1	A	170	PHE
1	A	183	ASP
1	A	188	LEU
1	A	194	TYR
1	A	196	THR
1	A	200	ARG
1	A	209	THR
1	A	230	LYS
1	A	235	LYS
1	A	260	LYS
1	A	266	ARG
1	A	268	LYS
1	A	273	ILE
1	A	276	PHE
1	A	280	THR
1	A	281	GLU
1	A	298	LEU
1	A	299	ASN
1	A	307	ARG
1	A	310	LEU
1	A	311	ASP
1	A	314	THR
1	A	326	ARG
1	A	348	LEU
1	A	359	TRP
1	A	363	MET
1	A	389	LYS
1	A	440	LYS
1	A	446	GLN
1	A	460	GLU
1	A	471	CYS
1	A	520	LEU
1	A	525	THR
1	A	556	VAL
1	A	557	ASN
1	A	560	THR

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Mol	Chain	Res	Type
1	A	573	VAL
1	A	586	GLU
1	A	588	TRP
1	B	9	ARG
1	B	24	HIS
1	B	27	LEU
1	B	47	TRP
1	B	60	ARG
1	B	61	LYS
1	B	67	LEU
1	B	80	ARG
1	B	81	ARG
1	B	88	LEU
1	B	110	ASP
1	B	123	VAL
1	B	147	ASN
1	B	155	LYS
1	B	159	PRO
1	B	194	TYR
1	B	195	LEU
1	B	196	THR
1	B	200	ARG
1	B	235	LYS
1	B	268	LYS
1	B	276	PHE
1	B	299	ASN
1	B	300	THR
1	B	310	LEU
1	B	314	THR
1	B	326	ARG
1	B	348	LEU
1	B	359	TRP
1	B	363	MET
1	B	374	VAL
1	B	379	LEU
1	B	385	ARG
1	B	401	LEU
1	B	404	VAL
1	B	407	SER
1	B	428	LEU
1	B	460	GLU
1	B	464	THR

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Mol	Chain	Res	Type
1	B	499	GLN
1	B	525	THR
1	B	528	ASN
1	B	537	ARG
1	B	557	ASN
1	B	559	LEU
1	B	563	ARG
1	B	570	THR
1	B	588	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	32	ASN
1	A	53	GLN
1	A	139	GLN
1	A	147	ASN
1	A	149	ASN
1	A	181	HIS
1	A	233	HIS
1	A	272	HIS
1	A	279	GLN
1	A	299	ASN
1	A	302	HIS
1	A	335	HIS
1	A	360	HIS
1	A	406	HIS
1	A	418	ASN
1	A	423	HIS
1	A	482	GLN
1	A	499	GLN
1	A	518	ASN
1	A	528	ASN
1	A	557	ASN
1	B	7	HIS
1	B	24	HIS
1	B	32	ASN
1	B	139	GLN
1	B	147	ASN
1	B	233	HIS
1	B	299	ASN

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Mol	Chain	Res	Type
1	B	302	HIS
1	B	335	HIS
1	B	343	GLN
1	B	360	HIS
1	B	370	GLN
1	B	406	HIS
1	B	418	ASN
1	B	423	HIS
1	B	482	GLN
1	B	499	GLN
1	B	528	ASN
1	B	557	ASN

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)

14 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	GLC	C	1	2	11,11,12	1.52	3 (27%)	15,15,17	1.33	2 (13%)
2	GLC	C	2	2	11,11,12	1.60	4 (36%)	15,15,17	1.89	3 (20%)
2	GLC	C	3	2	11,11,12	0.86	0	15,15,17	1.83	5 (33%)
2	GLC	C	4	2	11,11,12	1.21	2 (18%)	15,15,17	0.57	0
2	GLC	C	5	2	11,11,12	1.18	1 (9%)	15,15,17	1.06	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLC	C	6	2	11,11,12	1.34	1 (9%)	15,15,17	0.94	1 (6%)
2	GLC	C	7	2	11,11,12	1.60	4 (36%)	15,15,17	1.06	2 (13%)
2	GLC	D	1	2	11,11,12	1.57	2 (18%)	15,15,17	1.32	1 (6%)
2	GLC	D	2	2	11,11,12	1.61	4 (36%)	15,15,17	1.88	3 (20%)
2	GLC	D	3	2	11,11,12	1.08	0	15,15,17	1.81	4 (26%)
2	GLC	D	4	2	11,11,12	1.04	0	15,15,17	0.57	0
2	GLC	D	5	2	11,11,12	1.09	1 (9%)	15,15,17	0.99	1 (6%)
2	GLC	D	6	2	11,11,12	1.31	1 (9%)	15,15,17	1.10	1 (6%)
2	GLC	D	7	2	11,11,12	1.82	5 (45%)	15,15,17	1.03	2 (13%)

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	GLC	C	1	2	-	1/2/19/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	0/2/19/22	0/1/1/1
2	GLC	C	5	2	-	2/2/19/22	0/1/1/1
2	GLC	C	6	2	-	0/2/19/22	0/1/1/1
2	GLC	C	7	2	-	2/2/19/22	0/1/1/1
2	GLC	D	1	2	-	2/2/19/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1
2	GLC	D	4	2	-	0/2/19/22	0/1/1/1
2	GLC	D	5	2	-	2/2/19/22	0/1/1/1
2	GLC	D	6	2	-	1/2/19/22	0/1/1/1
2	GLC	D	7	2	-	0/2/19/22	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	7	GLC	O4-C4	3.01	1.50	1.43
2	D	7	GLC	O5-C5	2.64	1.48	1.43
2	D	1	GLC	O5-C5	2.52	1.48	1.43
2	C	7	GLC	O4-C4	2.50	1.48	1.43
2	D	1	GLC	C4-C5	2.50	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	GLC	C1-C2	2.49	1.57	1.52
2	C	1	GLC	O5-C5	2.46	1.48	1.43
2	C	7	GLC	O5-C5	2.40	1.48	1.43
2	D	7	GLC	C4-C5	2.38	1.58	1.53
2	D	6	GLC	O5-C5	2.38	1.48	1.43
2	C	2	GLC	C2-C3	2.37	1.56	1.52
2	C	5	GLC	O5-C5	2.36	1.48	1.43
2	D	5	GLC	O5-C5	2.28	1.48	1.43
2	C	2	GLC	C1-C2	2.27	1.57	1.52
2	C	2	GLC	O5-C5	2.26	1.48	1.43
2	D	2	GLC	O5-C5	2.15	1.47	1.43
2	D	2	GLC	C2-C3	2.13	1.55	1.52
2	C	2	GLC	O5-C1	2.10	1.47	1.43
2	C	1	GLC	C4-C5	2.09	1.57	1.53
2	C	4	GLC	O5-C5	2.09	1.47	1.43
2	C	7	GLC	C4-C5	2.09	1.57	1.53
2	C	7	GLC	O5-C1	2.07	1.47	1.43
2	C	4	GLC	C1-C2	2.07	1.56	1.52
2	D	2	GLC	O5-C1	2.06	1.47	1.43
2	C	1	GLC	C1-C2	2.06	1.56	1.52
2	C	6	GLC	O5-C5	2.05	1.47	1.43
2	D	7	GLC	O5-C1	2.03	1.47	1.43
2	D	7	GLC	C1-C2	2.02	1.56	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	GLC	O4-C4-C3	-5.48	97.69	110.35
2	C	2	GLC	O4-C4-C3	-5.40	97.86	110.35
2	D	3	GLC	O4-C4-C5	-4.14	99.02	109.30
2	D	1	GLC	C1-O5-C5	4.00	117.61	112.19
2	C	3	GLC	O4-C4-C5	-3.99	99.39	109.30
2	C	1	GLC	C1-O5-C5	3.92	117.50	112.19
2	C	3	GLC	C1-O5-C5	3.69	117.19	112.19
2	D	3	GLC	C1-O5-C5	3.44	116.85	112.19
2	C	2	GLC	O4-C4-C5	3.32	117.55	109.30
2	D	2	GLC	O4-C4-C5	3.22	117.29	109.30
2	D	6	GLC	C1-O5-C5	3.02	116.28	112.19
2	D	7	GLC	O4-C4-C3	-2.86	103.75	110.35
2	C	7	GLC	O4-C4-C3	-2.77	103.95	110.35
2	C	6	GLC	C1-O5-C5	2.60	115.72	112.19
2	D	2	GLC	C1-O5-C5	2.48	115.55	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	5	GLC	O4-C4-C3	-2.48	104.62	110.35
2	D	3	GLC	C1-C2-C3	2.45	112.68	109.67
2	C	7	GLC	C1-O5-C5	2.41	115.46	112.19
2	C	2	GLC	C1-O5-C5	2.34	115.36	112.19
2	C	1	GLC	O5-C1-C2	-2.29	107.23	110.77
2	D	5	GLC	C1-O5-C5	2.21	115.19	112.19
2	C	3	GLC	O6-C6-C5	-2.18	103.80	111.29
2	D	7	GLC	C1-O5-C5	2.13	115.08	112.19
2	C	3	GLC	O5-C1-C2	-2.12	107.51	110.77
2	C	3	GLC	C1-C2-C3	2.05	112.19	109.67
2	D	3	GLC	O6-C6-C5	-2.02	104.35	111.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	5	GLC	C4-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	D	5	GLC	O5-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	C	7	GLC	C4-C5-C6-O6
2	D	6	GLC	O5-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	C	5	GLC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	C	7	GLC	O5-C5-C6-O6
2	C	5	GLC	O5-C5-C6-O6

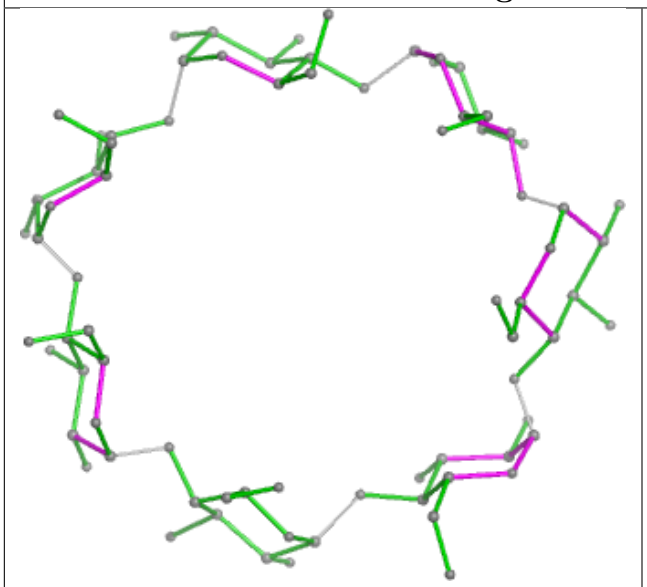
There are no ring outliers.

4 monomers are involved in 5 short contacts:

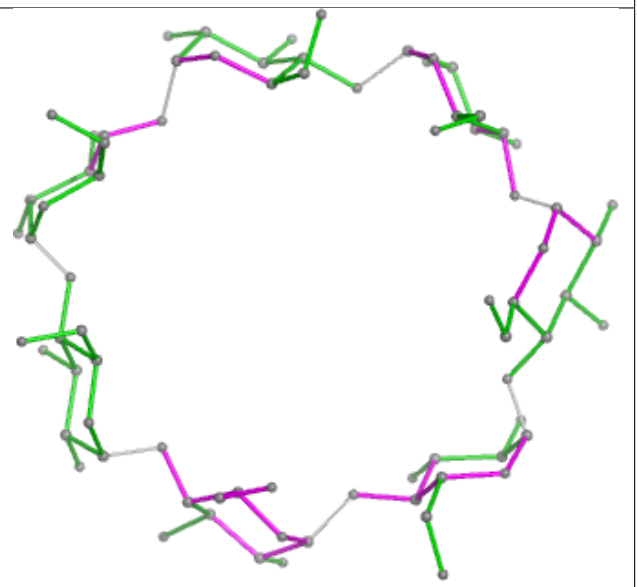
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GLC	1	0
2	C	4	GLC	1	0
2	D	5	GLC	2	0
2	D	4	GLC	1	0

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

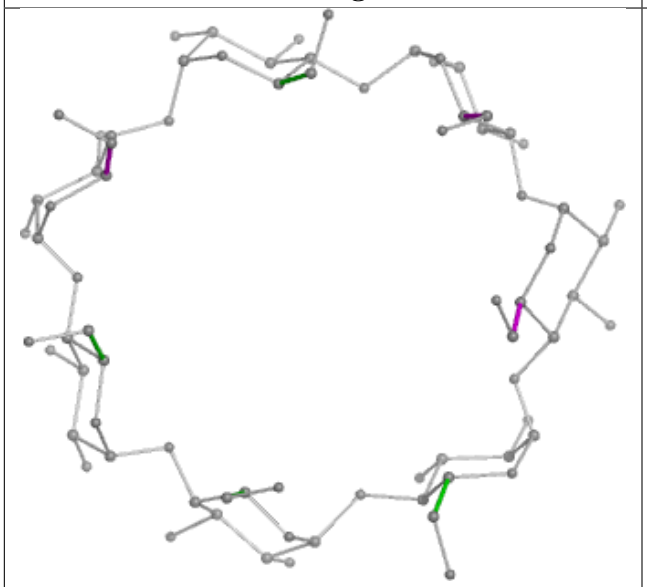
Oligosaccharide Chain C



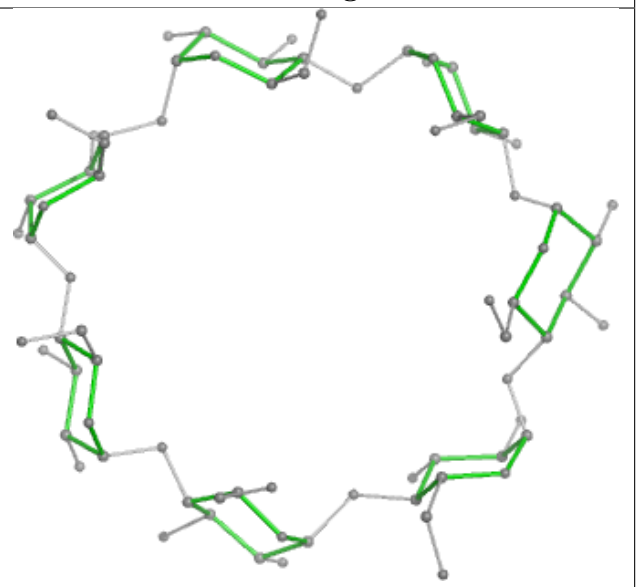
Bond lengths



Bond angles

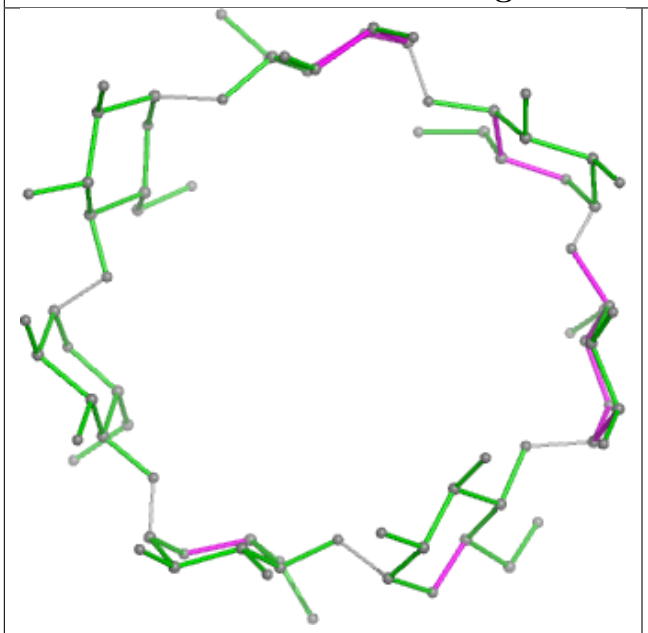


Torsions

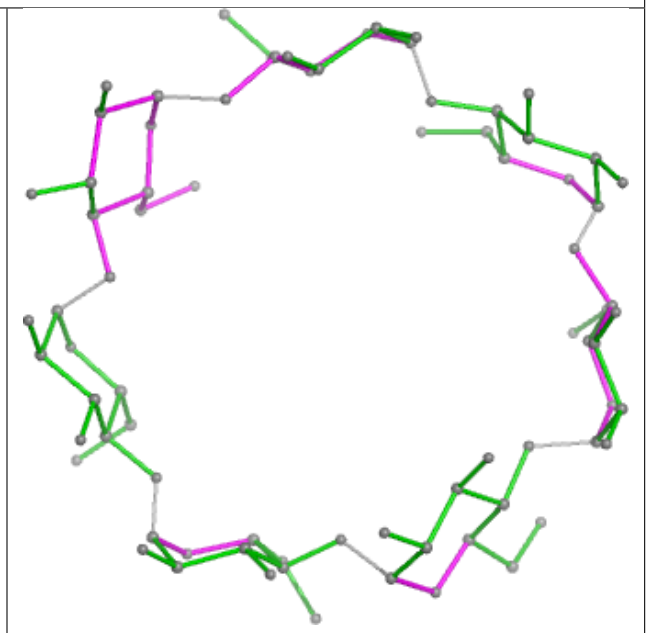


Rings

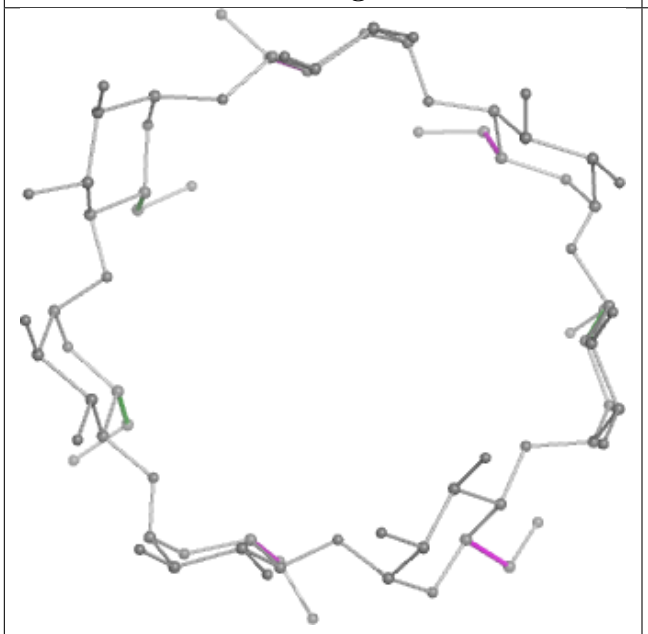
Oligosaccharide Chain D



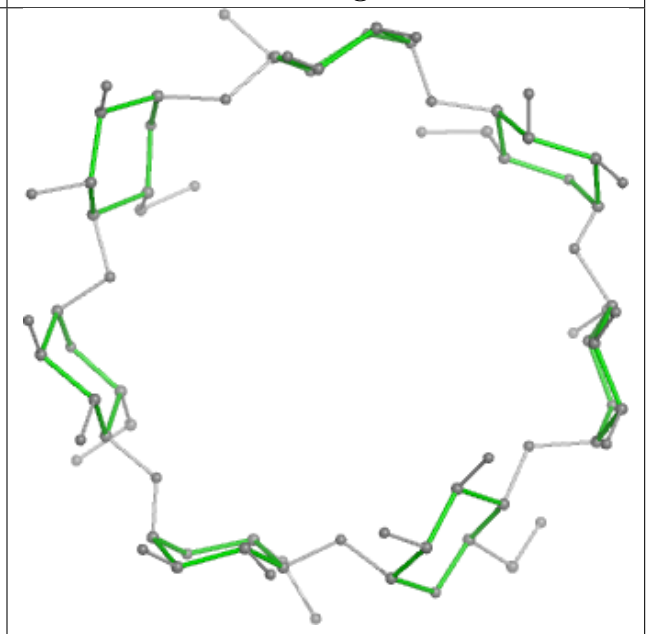
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.