Full wwPDB X-ray Structure Validation Report

Aug 7, 2020 – 11:07 PM BST

PDB ID	:	1CVI
Title	:	CRYSTAL STRUCTURE OF HUMAN PROSTATIC ACID PHOSPHATASE
Authors	:	Jakob, C.G.; Lewinski, K.; Kuciel, R.; Ostrowski, W.; Lebioda, L.
Deposited on	:	1999-08-23
Resolution	:	3.20 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 ⓘ symbol.

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

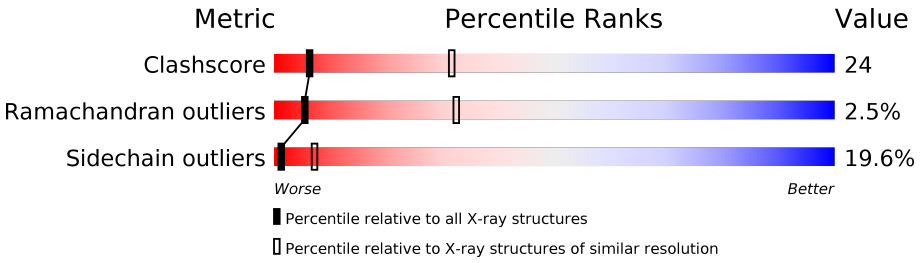
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.20 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	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	342	46% 43% 11%
1	B	342	46% 42% 12%
1	C	342	43% 47% 10%
1	D	342	45% 44% 11%
2	E	8	25% 25% 50%
3	F	4	50% 50%
4	G	3	33% 33% 33%
4	J	3	67% 33%

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Mol	Chain	Length	Quality of chain
4	K	3	33% 67%
4	M	3	33% 67%
5	H	4	25% 75%
5	L	4	25% 75%
6	I	6	33% 50% 17%

2 Entry composition

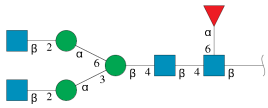
There are 9 unique types of molecules in this entry. The entry contains 12376 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROSTATIC ACID PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2801	1807	461	517	16			
1	B	342	Total	C	N	O	S	0	0	0
			2801	1807	461	517	16			
1	C	342	Total	C	N	O	S	0	0	0
			2801	1807	461	517	16			
1	D	342	Total	C	N	O	S	0	0	0
			2801	1807	461	517	16			

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

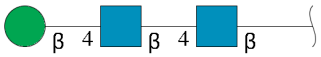


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	0	0	0
			99	56	4	39			

- Molecule 3 is an oligosaccharide called 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
3	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

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

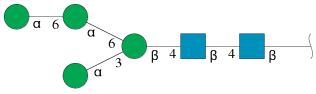


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called 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.

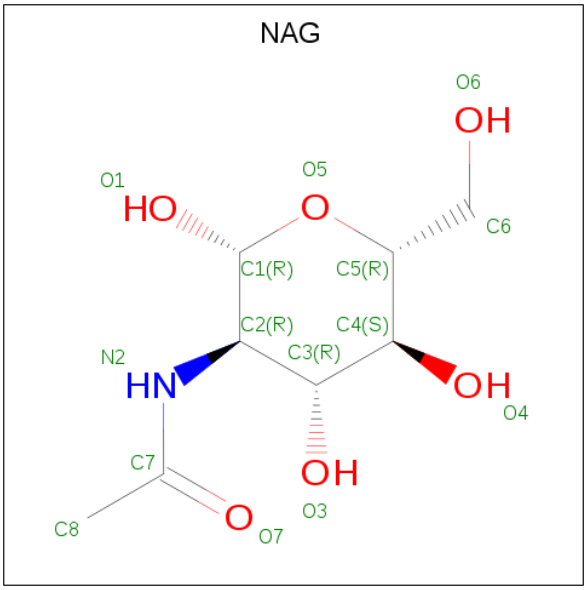
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	L	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is an oligosaccharide called 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.



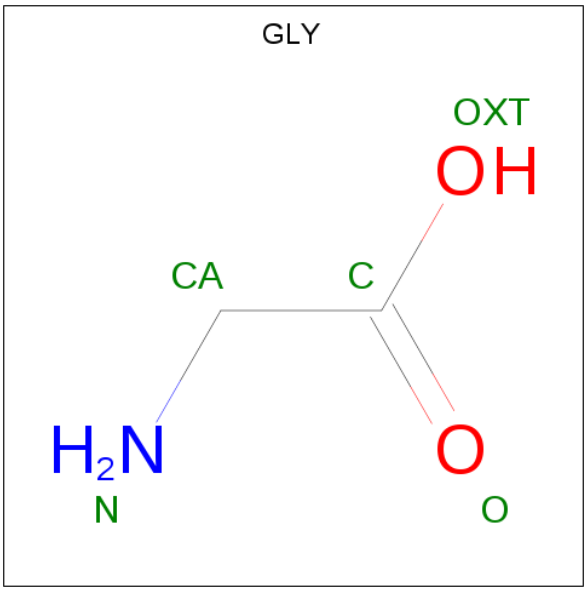
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	163	Total O 163 163	0	0
9	B	188	Total O 188 188	0	0
9	C	144	Total O 144 144	0	0
9	D	138	Total O 138 138	0	0

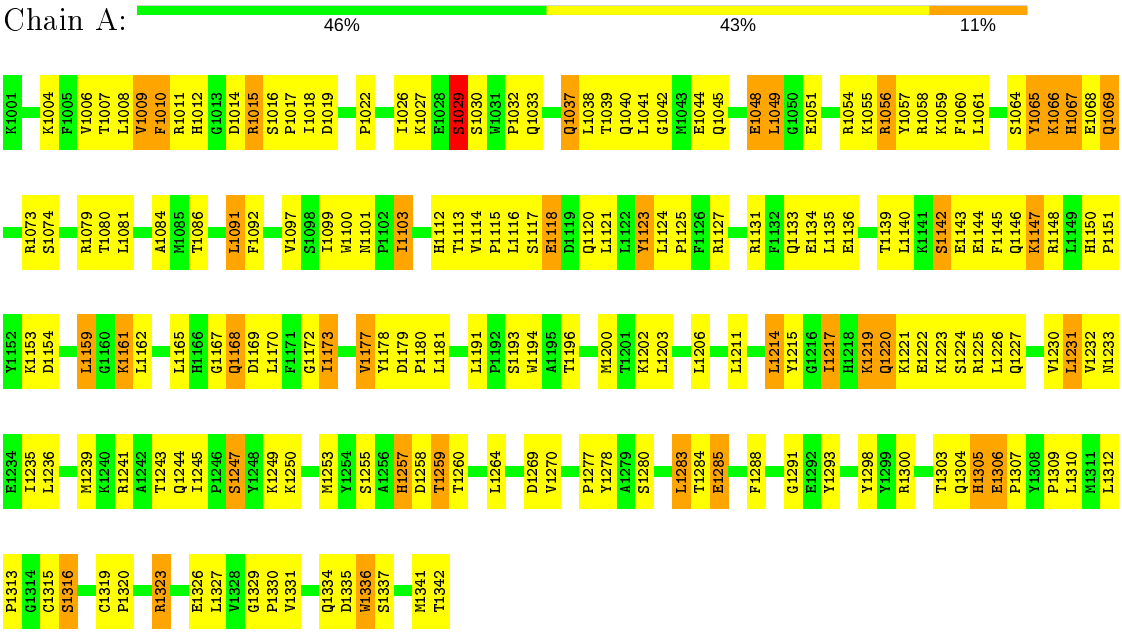
3 Residue-property plots (i)

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.

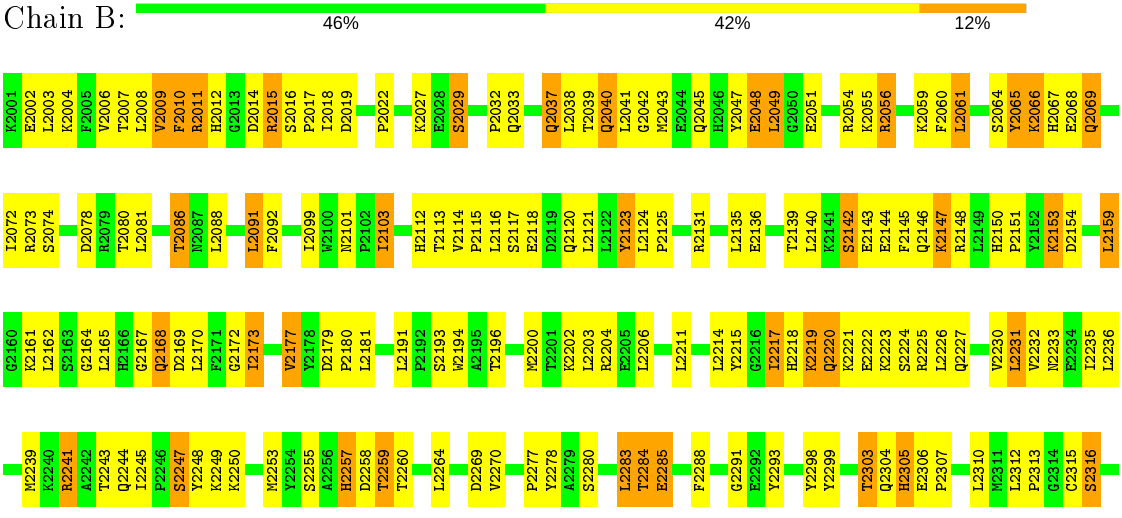
- Molecule 1: PROSTATIC ACID PHOSPHATASE

Chain A:



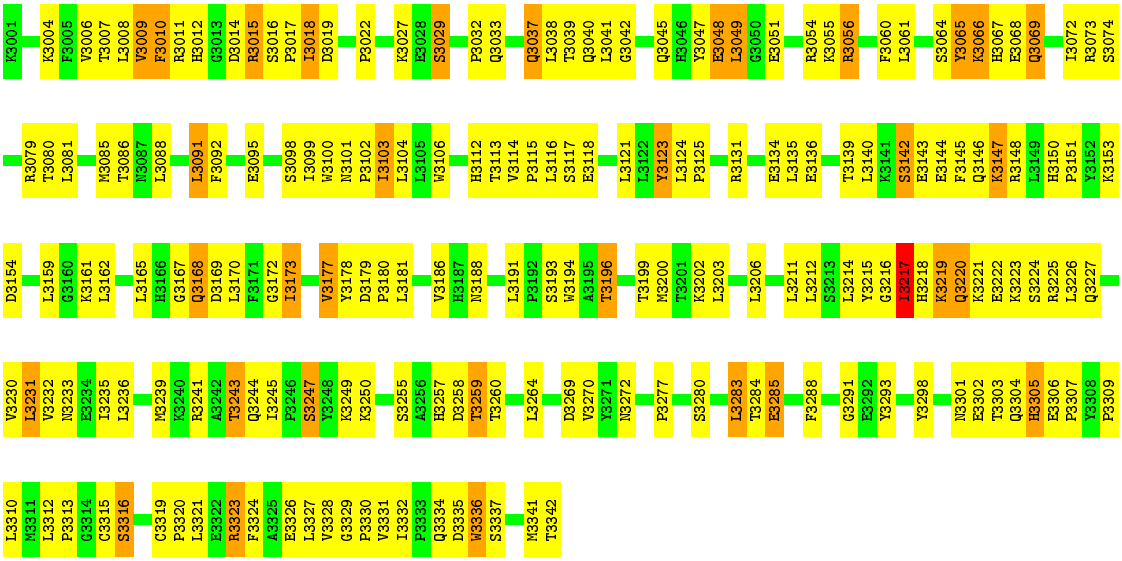
- Molecule 1: PROSTATIC ACID PHOSPHATASE

Chain B:



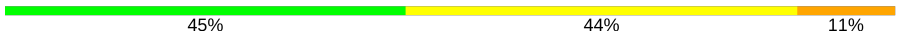
• Molecule 1: PROSTATIC ACID PHOSPHATASE

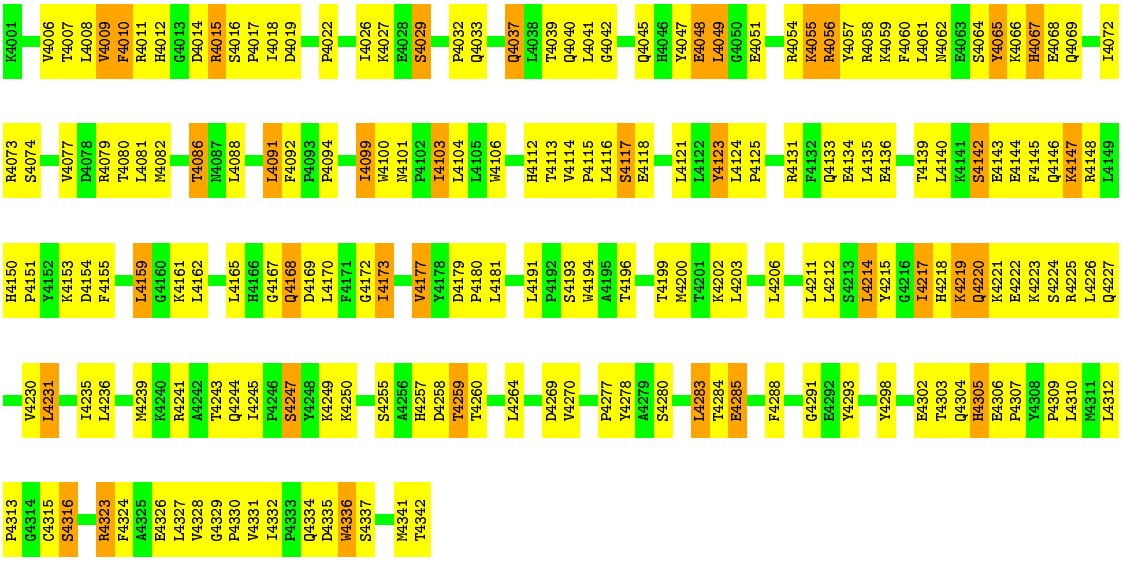
Chain C:



• Molecule 1: PROSTATIC ACID PHOSPHATASE

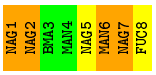
Chain D:





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

Chain E:

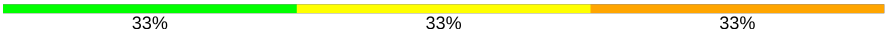


• Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

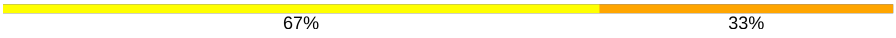
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain J:

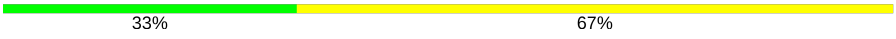


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

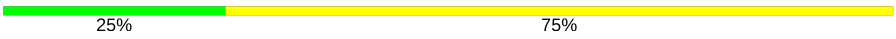
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



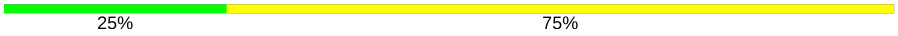
• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 5: 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 L:



• Molecule 6: 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 I:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	126.33Å 207.96Å 73.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	91.7 (8.00-3.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.157 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12376	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.33	0/2883	0.53	0/3914
1	B	0.32	0/2883	0.53	0/3914
1	C	0.33	0/2883	0.53	0/3914
1	D	0.33	0/2883	0.54	0/3914
All	All	0.33	0/11532	0.53	0/15656

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2801	0	2745	141	0
1	B	2801	0	2745	139	0
1	C	2801	0	2745	154	0
1	D	2801	0	2745	135	0
2	E	99	0	85	9	0
3	F	50	0	43	1	0
4	G	39	0	34	4	0
4	J	39	0	34	3	0
4	K	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	39	0	34	1	0
5	H	50	0	43	3	0
5	L	50	0	43	2	0
6	I	72	0	61	2	0
7	A	14	0	13	0	0
7	C	14	0	13	0	0
7	D	14	0	13	0	0
8	A	5	0	2	1	0
8	B	5	0	2	0	0
8	C	5	0	2	1	0
8	D	5	0	2	2	0
9	A	163	0	0	11	0
9	B	188	0	0	12	0
9	C	144	0	0	10	0
9	D	138	0	0	11	0
All	All	12376	0	11438	561	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 24.

All (561) 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:C:3159:LEU:HD11	1:C:3203:LEU:HD21	1.39	1.05
1:D:4159:LEU:HD11	1:D:4203:LEU:HD21	1.42	1.02
1:B:2200:MET:HA	1:B:2200:MET:HE2	1.44	0.99
1:A:1159:LEU:HD11	1:A:1203:LEU:HD21	1.44	0.99
1:B:2159:LEU:HD11	1:B:2203:LEU:HD21	1.41	0.98
1:D:4200:MET:HE2	1:D:4200:MET:HA	1.50	0.93
1:C:3200:MET:HA	1:C:3200:MET:HE2	1.53	0.89
1:A:1181:LEU:HD12	1:A:1200:MET:HE1	1.56	0.88
1:C:3113:THR:HG22	1:D:4113:THR:HG22	1.59	0.84
1:A:1074:SER:HB2	1:A:1255:SER:HB3	1.60	0.83
5:H:2:NAG:H62	5:H:3:BMA:H2	1.60	0.83
1:B:2022:PRO:HD2	1:B:2165:LEU:HD23	1.61	0.82
2:E:6:MAN:O3	2:E:7:NAG:H2	1.79	0.82
1:C:3022:PRO:HD2	1:C:3165:LEU:HD23	1.63	0.81
1:D:4022:PRO:HD2	1:D:4165:LEU:HD23	1.63	0.81
1:A:1200:MET:HA	1:A:1200:MET:HE2	1.64	0.80
1:A:1022:PRO:HD2	1:A:1165:LEU:HD23	1.63	0.79
1:A:1044:GLU:OE1	2:E:7:NAG:H82	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2074:SER:HB2	1:B:2255:SER:HB3	1.65	0.78
1:B:2312:LEU:HD12	1:B:2313:PRO:HD2	1.65	0.78
1:D:4135:LEU:HD11	1:D:4222:GLU:HG2	1.65	0.77
1:D:4074:SER:HB2	1:D:4255:SER:HB3	1.66	0.77
1:A:1312:LEU:HD12	1:A:1313:PRO:HD2	1.66	0.77
1:C:3018:ILE:HB	9:C:6203:HOH:O	1.85	0.77
1:B:2135:LEU:HD11	1:B:2222:GLU:HG2	1.67	0.76
6:I:1:NAG:H61	6:I:2:NAG:C7	2.15	0.75
1:B:2150:HIS:O	1:B:2153:LYS:HB2	1.87	0.75
1:A:1135:LEU:HD11	1:A:1222:GLU:HG2	1.69	0.75
1:D:4312:LEU:HD12	1:D:4313:PRO:HD2	1.69	0.73
1:D:4181:LEU:HD12	1:D:4200:MET:HE1	1.68	0.72
1:C:3312:LEU:HD12	1:C:3313:PRO:HD2	1.70	0.71
1:C:3181:LEU:HD12	1:C:3200:MET:HE1	1.71	0.71
1:B:2115:PRO:HB2	1:B:2118:GLU:HG3	1.73	0.71
1:C:3008:LEU:HD23	1:C:3283:LEU:HB3	1.73	0.71
1:C:3135:LEU:HD11	1:C:3222:GLU:HG2	1.71	0.71
1:C:3270:VAL:HG21	1:C:3310:LEU:HD13	1.73	0.71
1:B:2114:VAL:HG13	1:B:2115:PRO:HD2	1.72	0.71
1:C:3074:SER:HB2	1:C:3255:SER:HB3	1.70	0.71
1:A:1115:PRO:HB2	1:A:1118:GLU:HG3	1.73	0.71
1:B:2181:LEU:HD12	1:B:2200:MET:HE1	1.72	0.70
5:H:2:NAG:C6	5:H:3:BMA:H2	2.21	0.70
1:C:3186:VAL:O	4:J:1:NAG:H82	1.90	0.70
1:A:1114:VAL:HG13	1:A:1115:PRO:HD2	1.73	0.70
1:B:2073:ARG:NH2	9:B:5463:HOH:O	2.25	0.70
1:D:4150:HIS:O	1:D:4153:LYS:HB2	1.91	0.69
1:A:1150:HIS:O	1:A:1153:LYS:HB2	1.92	0.69
1:A:1304:GLN:O	1:A:1305:HIS:HB2	1.93	0.68
1:C:3114:VAL:HG13	1:C:3115:PRO:HD2	1.75	0.68
1:D:4283:LEU:HD23	1:D:4283:LEU:N	2.08	0.68
1:A:1115:PRO:HA	9:A:5023:HOH:O	1.93	0.68
1:C:3150:HIS:O	1:C:3153:LYS:HB2	1.93	0.68
1:C:3104:LEU:HD11	1:D:4106:TRP:HB2	1.76	0.68
1:C:3270:VAL:CG2	1:C:3310:LEU:HD13	2.24	0.67
1:C:3283:LEU:HD23	1:C:3283:LEU:N	2.10	0.67
1:C:3106:TRP:HB2	1:D:4104:LEU:HD11	1.75	0.67
1:A:1120:GLN:HG3	9:A:5764:HOH:O	1.93	0.67
1:D:4008:LEU:HD23	1:D:4283:LEU:HB3	1.75	0.66
1:D:4115:PRO:HB2	1:D:4118:GLU:HG3	1.77	0.66
1:A:1116:LEU:HD22	1:A:1123:TYR:CD2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3224:SER:HB3	1:C:3331:VAL:HG13	1.76	0.66
1:C:3245:ILE:HG22	1:C:3247:SER:H	1.60	0.66
1:A:1161:LYS:HA	1:D:4117:SER:HB3	1.78	0.66
1:D:4304:GLN:O	1:D:4305:HIS:HB2	1.96	0.66
1:B:2061:LEU:HB2	9:B:5821:HOH:O	1.95	0.66
1:D:4179:ASP:HB3	1:D:4180:PRO:HD3	1.78	0.66
1:C:3304:GLN:O	1:C:3305:HIS:HB2	1.96	0.65
1:D:4270:VAL:CG2	1:D:4310:LEU:HD13	2.26	0.65
1:C:3115:PRO:HB2	1:C:3118:GLU:HG3	1.79	0.65
1:A:1008:LEU:HD23	1:A:1283:LEU:HB3	1.79	0.65
1:B:2304:GLN:O	1:B:2305:HIS:HB2	1.97	0.65
1:A:1030:SER:OG	1:C:3245:ILE:HG21	1.97	0.65
1:A:1283:LEU:HD23	1:A:1283:LEU:N	2.13	0.64
1:A:1179:ASP:HB3	1:A:1180:PRO:HD3	1.79	0.64
1:B:2270:VAL:CG2	1:B:2310:LEU:HD13	2.27	0.64
1:C:3341:MET:O	1:C:3342:THR:HB	1.98	0.64
1:B:2200:MET:HA	1:B:2200:MET:CE	2.24	0.64
1:B:2283:LEU:HD23	1:B:2283:LEU:N	2.13	0.64
1:D:4224:SER:HB3	1:D:4331:VAL:HG13	1.78	0.64
1:D:4114:VAL:HG13	1:D:4115:PRO:HD2	1.79	0.64
1:A:1181:LEU:HD12	1:A:1200:MET:CE	2.26	0.64
1:D:4270:VAL:HG21	1:D:4310:LEU:HD13	1.80	0.64
8:D:4350:GLY:HA2	9:D:5378:HOH:O	1.97	0.64
4:J:2:NAG:O3	4:J:3:BMA:H2	1.99	0.63
1:B:2224:SER:HB3	1:B:2331:VAL:HG13	1.79	0.63
1:B:2048:GLU:HG3	1:B:2049:LEU:N	2.14	0.63
1:B:2270:VAL:HG21	1:B:2310:LEU:HD13	1.80	0.63
1:C:3048:GLU:HG3	1:C:3049:LEU:N	2.13	0.63
1:C:3179:ASP:HB3	1:C:3180:PRO:HD3	1.80	0.63
1:B:2008:LEU:HD23	1:B:2283:LEU:HB3	1.78	0.62
1:A:1026:ILE:HD12	1:C:3245:ILE:HD11	1.82	0.62
1:A:1121:LEU:HD11	1:A:1231:LEU:HD23	1.80	0.62
1:B:2041:LEU:HD21	9:B:5247:HOH:O	1.99	0.62
1:C:3121:LEU:HD11	1:C:3231:LEU:HD23	1.82	0.62
1:D:4150:HIS:HB3	1:D:4151:PRO:HD3	1.80	0.62
1:A:1097:VAL:O	1:B:2040:GLN:NE2	2.32	0.62
1:B:2150:HIS:HB3	1:B:2151:PRO:HD3	1.80	0.62
1:B:2236:LEU:HA	1:B:2239:MET:HE2	1.81	0.62
1:C:3200:MET:HA	1:C:3200:MET:CE	2.28	0.62
1:A:1224:SER:HB3	1:A:1331:VAL:HG13	1.81	0.61
1:B:2179:ASP:HB3	1:B:2180:PRO:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1142:SER:O	1:A:1146:GLN:HG3	2.00	0.61
1:A:1306:GLU:HB3	9:A:5718:HOH:O	1.99	0.61
1:B:2153:LYS:HE3	1:B:2168:GLN:HE22	1.64	0.61
1:A:1270:VAL:CG2	1:A:1310:LEU:HD13	2.30	0.61
1:B:2221:LYS:O	1:B:2225:ARG:HG3	2.01	0.61
1:A:1007:THR:HG21	1:A:1235:ILE:HD12	1.82	0.61
1:B:2121:LEU:HD11	1:B:2231:LEU:HD23	1.82	0.61
1:D:4200:MET:CE	1:D:4200:MET:HA	2.26	0.61
1:A:1048:GLU:HG3	1:A:1049:LEU:N	2.16	0.61
1:A:1150:HIS:HB3	1:A:1151:PRO:HD3	1.81	0.61
1:D:4121:LEU:HD11	1:D:4231:LEU:HD23	1.83	0.61
9:C:5252:HOH:O	4:J:1:NAG:H62	2.00	0.60
1:B:2341:MET:O	1:B:2342:THR:HB	2.01	0.60
1:C:3150:HIS:HB3	1:C:3151:PRO:HD3	1.81	0.60
1:C:3139:THR:O	1:C:3142:SER:HB3	2.02	0.60
1:C:3153:LYS:HE3	1:C:3168:GLN:HE22	1.67	0.60
1:B:2142:SER:O	1:B:2146:GLN:HG3	2.02	0.60
1:D:4245:ILE:HG22	1:D:4247:SER:H	1.67	0.60
1:B:2074:SER:CB	1:B:2255:SER:HB3	2.30	0.59
1:C:3102:PRO:HD2	9:C:5985:HOH:O	2.02	0.59
1:C:3272:ASN:HB3	9:C:5529:HOH:O	2.03	0.59
1:A:1270:VAL:HG21	1:A:1310:LEU:HD13	1.82	0.59
1:A:1153:LYS:HE3	1:A:1168:GLN:HE22	1.68	0.59
1:C:3221:LYS:O	1:C:3225:ARG:HG3	2.03	0.59
1:D:4181:LEU:HD12	1:D:4200:MET:CE	2.33	0.59
1:B:2284:THR:CG2	9:B:5451:HOH:O	2.51	0.59
1:A:1200:MET:HA	1:A:1200:MET:CE	2.32	0.58
1:C:3007:THR:HG21	1:C:3235:ILE:HD12	1.84	0.58
1:B:2181:LEU:HD12	1:B:2200:MET:CE	2.33	0.58
1:A:1245:ILE:HG22	1:A:1247:SER:H	1.68	0.58
1:A:1100:TRP:HH2	1:B:2047:TYR:CD1	2.21	0.58
1:C:3116:LEU:HD22	1:C:3123:TYR:CD2	2.39	0.58
1:C:3015:ARG:HA	1:C:3039:THR:HG23	1.86	0.58
3:F:2:NAG:H3	3:F:3:BMA:H2	1.84	0.58
1:C:3047:TYR:CD1	1:D:4100:TRP:HH2	2.22	0.58
1:D:4162:LEU:HD22	1:D:4194:TRP:CG	2.39	0.58
1:D:4283:LEU:HD23	1:D:4283:LEU:H	1.67	0.58
1:B:2139:THR:O	1:B:2142:SER:HB3	2.04	0.57
1:B:2284:THR:HG22	9:B:5451:HOH:O	2.04	0.57
1:C:3033:GLN:HA	9:D:5962:HOH:O	2.04	0.57
1:A:1341:MET:O	1:A:1342:THR:HB	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2007:THR:HG21	1:B:2235:ILE:HD12	1.86	0.57
1:A:1221:LYS:O	1:A:1225:ARG:HG3	2.04	0.57
1:A:1074:SER:CB	1:A:1255:SER:HB3	2.34	0.57
1:B:2283:LEU:HD23	1:B:2283:LEU:H	1.70	0.57
1:C:3142:SER:O	1:C:3146:GLN:HG3	2.04	0.57
1:D:4048:GLU:HG3	1:D:4049:LEU:N	2.18	0.57
1:D:4142:SER:O	1:D:4146:GLN:HG3	2.05	0.57
1:C:3269:ASP:HB3	1:C:3313:PRO:HG3	1.86	0.57
1:B:2060:PHE:HA	4:G:1:NAG:O6	2.04	0.57
1:B:2245:ILE:HG22	1:B:2247:SER:H	1.70	0.57
1:C:3085:MET:HE1	9:D:5519:HOH:O	2.04	0.57
1:C:3243:THR:HG21	9:C:5114:HOH:O	2.05	0.57
1:B:2245:ILE:HG12	1:D:4026:ILE:HD12	1.87	0.57
1:C:3181:LEU:HD12	1:C:3200:MET:CE	2.34	0.56
1:C:3283:LEU:HD23	1:C:3283:LEU:H	1.69	0.56
1:B:2298:TYR:HB3	1:B:2307:PRO:HB2	1.86	0.56
1:D:4116:LEU:HD22	1:D:4123:TYR:CD2	2.39	0.56
2:E:1:NAG:H61	2:E:2:NAG:N2	2.20	0.56
1:A:1139:THR:O	1:A:1142:SER:HB3	2.06	0.56
1:C:3298:TYR:HB3	1:C:3307:PRO:HB2	1.88	0.56
1:D:4007:THR:HG21	1:D:4235:ILE:HD12	1.88	0.55
1:C:3085:MET:CE	9:D:5519:HOH:O	2.53	0.55
1:D:4074:SER:CB	1:D:4255:SER:HB3	2.35	0.55
1:A:1015:ARG:HA	1:A:1039:THR:HG23	1.88	0.55
1:A:1236:LEU:HA	1:A:1239:MET:HE2	1.88	0.55
1:D:4008:LEU:CD2	1:D:4283:LEU:HB3	2.37	0.55
1:D:4153:LYS:HE3	1:D:4168:GLN:HE22	1.70	0.55
1:D:4341:MET:O	1:D:4342:THR:HB	2.06	0.55
1:D:4139:THR:O	1:D:4142:SER:HB3	2.06	0.55
1:D:4221:LYS:O	1:D:4225:ARG:HG3	2.07	0.55
1:C:3115:PRO:HD3	1:D:4114:VAL:HG22	1.89	0.55
1:D:4200:MET:CE	1:D:4203:LEU:HD12	2.37	0.54
1:A:1222:GLU:HB2	9:A:5063:HOH:O	2.07	0.54
1:A:1298:TYR:HB3	1:A:1307:PRO:HB2	1.89	0.54
1:B:2116:LEU:HD22	1:B:2123:TYR:CD2	2.43	0.54
1:B:2204:ARG:HD3	9:B:6230:HOH:O	2.06	0.54
1:D:4101:ASN:OD1	1:D:4103:ILE:HG13	2.08	0.54
1:A:1283:LEU:HD23	1:A:1283:LEU:H	1.72	0.54
1:C:3224:SER:HB3	1:C:3331:VAL:CG1	2.38	0.54
1:B:2041:LEU:HG	1:B:2045:GLN:NE2	2.24	0.53
1:B:2056:ARG:HH12	1:B:2285:GLU:CD	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4298:TYR:HB3	1:D:4307:PRO:HB2	1.90	0.53
1:A:1269:ASP:HB3	1:A:1313:PRO:HG3	1.89	0.53
1:B:2162:LEU:HD22	1:B:2194:TRP:CG	2.43	0.53
1:D:4269:ASP:HB3	1:D:4313:PRO:HG3	1.90	0.53
1:D:4315:CYS:HB2	1:D:4327:LEU:HD11	1.91	0.53
1:B:2269:ASP:HB3	1:B:2313:PRO:HG3	1.90	0.53
1:B:2101:ASN:OD1	1:B:2103:ILE:HG13	2.09	0.53
1:C:3074:SER:CB	1:C:3255:SER:HB3	2.39	0.53
1:C:3162:LEU:HD22	1:C:3194:TRP:CG	2.44	0.53
1:D:4056:ARG:HH12	1:D:4285:GLU:CD	2.13	0.53
1:D:4015:ARG:HA	1:D:4039:THR:HG23	1.90	0.53
1:A:1315:CYS:HB2	1:A:1327:LEU:CD1	2.38	0.52
1:C:3008:LEU:CD2	1:C:3283:LEU:HB3	2.39	0.52
1:D:4135:LEU:CD1	1:D:4222:GLU:HG2	2.38	0.52
1:C:3016:SER:HB2	1:C:3017:PRO:HD2	1.92	0.52
1:C:3056:ARG:HH12	1:C:3285:GLU:CD	2.12	0.52
1:C:3004:LYS:NZ	9:C:5950:HOH:O	2.43	0.52
1:C:3315:CYS:HB2	1:C:3327:LEU:HD11	1.92	0.52
1:B:2091:LEU:O	1:B:2091:LEU:HD23	2.09	0.52
1:D:4315:CYS:HB2	1:D:4327:LEU:CD1	2.40	0.52
1:D:4323:ARG:HA	1:D:4326:GLU:HG2	1.91	0.52
1:C:3315:CYS:HB2	1:C:3327:LEU:CD1	2.40	0.51
1:A:1113:THR:HG22	1:B:2113:THR:HG22	1.91	0.51
1:C:3323:ARG:HA	1:C:3326:GLU:HG2	1.93	0.51
1:C:3091:LEU:HD13	1:C:3092:PHE:CE2	2.45	0.51
1:C:3288:PHE:CE1	1:C:3291:GLY:HA2	2.46	0.51
1:D:4072:ILE:HD13	1:D:4088:LEU:HD11	1.91	0.51
1:D:4224:SER:HB3	1:D:4331:VAL:CG1	2.40	0.51
1:B:2124:LEU:HD22	1:B:2260:THR:HA	1.92	0.51
1:D:4010:PHE:CE1	1:D:4255:SER:HA	2.45	0.51
1:B:2288:PHE:HB2	1:B:2293:TYR:CE1	2.45	0.51
1:B:2004:LYS:HG2	4:G:2:NAG:H83	1.92	0.51
9:B:5245:HOH:O	5:H:2:NAG:H4	2.10	0.51
1:C:3114:VAL:HG22	1:D:4115:PRO:HD3	1.93	0.51
1:A:1007:THR:HG21	1:A:1235:ILE:CD1	2.41	0.51
1:C:3220:GLN:O	1:C:3223:LYS:HB2	2.11	0.51
1:D:4315:CYS:SG	1:D:4316:SER:N	2.84	0.51
1:A:1315:CYS:HB2	1:A:1327:LEU:HD11	1.93	0.50
1:A:1079:ARG:NH1	8:A:1350:GLY:OXT	2.45	0.50
1:C:3236:LEU:HA	1:C:3239:MET:HE2	1.93	0.50
1:A:1030:SER:CB	1:C:3245:ILE:CG2	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3007:THR:HG21	1:C:3235:ILE:CD1	2.42	0.50
1:D:4124:LEU:HB3	1:D:4215:TYR:OH	2.11	0.50
1:A:1101:ASN:OD1	1:A:1103:ILE:HG13	2.12	0.50
1:A:1091:LEU:HD23	1:A:1091:LEU:O	2.11	0.50
1:D:4288:PHE:HB2	1:D:4293:TYR:CE1	2.46	0.50
1:D:4148:ARG:HA	9:D:5559:HOH:O	2.12	0.50
1:A:1033:GLN:HB2	1:A:1037:GLN:HG2	1.94	0.50
1:C:3091:LEU:HD22	1:C:3092:PHE:CE2	2.47	0.50
1:A:1065:TYR:H	1:A:1092:PHE:HD1	1.59	0.50
1:A:1258:ASP:OD1	1:A:1259:THR:N	2.45	0.50
1:B:2016:SER:HB2	1:B:2017:PRO:HD2	1.92	0.50
1:B:2315:CYS:HB2	1:B:2327:LEU:CD1	2.42	0.50
1:B:2003:LEU:O	4:G:2:NAG:H82	2.11	0.49
1:D:4041:LEU:HG	1:D:4045:GLN:NE2	2.27	0.49
1:C:3115:PRO:HG3	1:D:4114:VAL:HG22	1.94	0.49
1:A:1004:LYS:HB3	9:A:5401:HOH:O	2.11	0.49
1:B:2015:ARG:HA	1:B:2039:THR:HG23	1.93	0.49
1:C:3258:ASP:OD1	1:C:3259:THR:N	2.45	0.49
1:C:3335:ASP:O	1:C:3336:TRP:C	2.51	0.49
1:D:4033:GLN:HB2	1:D:4037:GLN:HG2	1.93	0.49
1:A:1058:ARG:NH1	9:A:5015:HOH:O	2.44	0.49
1:C:3033:GLN:HB2	1:C:3037:GLN:HG2	1.93	0.49
1:A:1030:SER:CB	1:C:3245:ILE:HG21	2.42	0.49
1:D:4014:ASP:H	1:D:4042:GLY:HA2	1.77	0.49
1:D:4173:ILE:O	1:D:4177:VAL:HG22	2.13	0.49
1:A:1037:GLN:NE2	9:A:5402:HOH:O	2.45	0.49
1:B:2135:LEU:CD1	1:B:2222:GLU:HG2	2.39	0.49
1:D:4236:LEU:HA	1:D:4239:MET:HE2	1.94	0.49
1:A:1133:GLN:NE2	9:A:5426:HOH:O	2.33	0.49
1:A:1010:PHE:CE1	1:A:1255:SER:HA	2.48	0.49
1:A:1131:ARG:HD3	1:A:1342:THR:HG21	1.95	0.49
1:B:2220:GLN:O	1:B:2223:LYS:HB2	2.13	0.49
1:C:3101:ASN:OD1	1:C:3103:ILE:HG13	2.11	0.49
1:A:1300:ARG:NH1	9:A:5057:HOH:O	2.46	0.49
1:C:3124:LEU:HB3	1:C:3215:TYR:OH	2.13	0.49
1:A:1162:LEU:HD22	1:A:1194:TRP:CG	2.48	0.49
1:A:1224:SER:HB3	1:A:1331:VAL:CG1	2.42	0.49
1:D:4012:HIS:CE1	1:D:4015:ARG:HG2	2.48	0.48
1:D:4065:TYR:H	1:D:4092:PHE:HD1	1.60	0.48
1:B:2136:GLU:O	1:B:2140:LEU:HD23	2.13	0.48
1:B:2170:LEU:HA	1:B:2173:ILE:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3200:MET:CE	1:C:3203:LEU:HD12	2.43	0.48
1:D:4091:LEU:HD23	1:D:4091:LEU:O	2.12	0.48
1:A:1288:PHE:HB2	1:A:1293:TYR:CE1	2.48	0.48
1:B:2131:ARG:HD3	1:B:2342:THR:HG21	1.95	0.48
1:C:3065:TYR:H	1:C:3092:PHE:HD1	1.61	0.48
1:C:3288:PHE:HB2	1:C:3293:TYR:CE1	2.48	0.48
1:A:1008:LEU:CD2	1:A:1283:LEU:HB3	2.43	0.48
1:D:4136:GLU:O	1:D:4140:LEU:HD23	2.12	0.48
1:A:1056:ARG:HH12	1:A:1285:GLU:CD	2.15	0.48
1:C:3177:VAL:C	1:C:3180:PRO:HD2	2.34	0.48
1:D:4327:LEU:HD22	9:D:5098:HOH:O	2.13	0.48
1:A:1226:LEU:C	1:A:1227:GLN:HG2	2.34	0.48
1:C:3033:GLN:HG2	9:D:6366:HOH:O	2.14	0.48
1:C:3014:ASP:H	1:C:3042:GLY:HA2	1.77	0.48
1:A:1073:ARG:HA	1:A:1112:HIS:O	2.14	0.48
1:B:2007:THR:HG21	1:B:2235:ILE:CD1	2.43	0.48
1:C:3010:PHE:CE1	1:C:3255:SER:HA	2.48	0.48
1:A:1135:LEU:CD1	1:A:1222:GLU:HG2	2.42	0.48
1:B:2033:GLN:HB2	1:B:2037:GLN:HG2	1.95	0.48
1:D:4258:ASP:OD1	1:D:4259:THR:N	2.47	0.48
5:L:1:NAG:H62	5:L:2:NAG:O5	2.13	0.48
1:B:2010:PHE:CE1	1:B:2255:SER:HA	2.49	0.47
1:B:2226:LEU:C	1:B:2227:GLN:HG2	2.34	0.47
1:D:4140:LEU:HD13	1:D:4145:PHE:CE2	2.49	0.47
1:A:1054:ARG:NH1	1:A:1054:ARG:HG2	2.29	0.47
1:A:1127:ARG:HD2	9:A:5426:HOH:O	2.14	0.47
1:C:3140:LEU:HD13	1:C:3145:PHE:CE2	2.49	0.47
1:C:3135:LEU:CD1	1:C:3222:GLU:HG2	2.43	0.47
1:D:4131:ARG:HD3	1:D:4342:THR:HG21	1.96	0.47
1:A:1277:PRO:HG2	1:A:1280:SER:HB3	1.95	0.47
1:B:2015:ARG:HD2	1:B:2016:SER:O	2.14	0.47
1:A:1032:PRO:HB2	1:A:1033:GLN:CD	2.35	0.47
1:A:1170:LEU:HD21	1:A:1206:LEU:HD22	1.96	0.47
1:B:2323:ARG:HA	1:B:2326:GLU:HG2	1.97	0.47
1:A:1329:GLY:N	1:A:1330:PRO:HD2	2.29	0.47
1:B:2065:TYR:H	1:B:2092:PHE:HD1	1.63	0.47
1:D:4335:ASP:O	1:D:4336:TRP:C	2.52	0.47
1:A:1054:ARG:HH11	1:A:1054:ARG:HG2	1.79	0.47
1:A:1136:GLU:O	1:A:1140:LEU:HD23	2.14	0.47
1:C:3041:LEU:HG	1:C:3045:GLN:NE2	2.30	0.47
1:C:3277:PRO:HG2	1:C:3280:SER:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:SER:HA	1:C:3245:ILE:CG2	2.44	0.47
1:A:1124:LEU:HB3	1:A:1215:TYR:OH	2.15	0.47
1:A:1173:ILE:O	1:A:1177:VAL:HG22	2.14	0.47
1:A:1335:ASP:O	1:A:1336:TRP:C	2.52	0.47
1:C:3114:VAL:HG22	1:D:4115:PRO:HG3	1.97	0.47
1:D:4134:GLU:OE1	1:D:4342:THR:HG23	2.13	0.47
2:E:1:NAG:H3	2:E:1:NAG:O7	2.14	0.47
1:B:2200:MET:CE	1:B:2203:LEU:HD12	2.45	0.47
1:C:3100:TRP:HH2	1:D:4047:TYR:CD1	2.32	0.47
1:C:3226:LEU:C	1:C:3227:GLN:HG2	2.35	0.47
1:D:4007:THR:HG21	1:D:4235:ILE:CD1	2.44	0.47
1:D:4124:LEU:HD22	1:D:4260:THR:HA	1.97	0.47
1:B:2014:ASP:H	1:B:2042:GLY:HA2	1.80	0.47
1:B:2224:SER:HB3	1:B:2331:VAL:CG1	2.43	0.47
1:B:2328:VAL:O	1:B:2332:ILE:HD12	2.15	0.47
1:B:2329:GLY:N	1:B:2330:PRO:HD2	2.30	0.47
1:C:3131:ARG:HD3	1:C:3342:THR:HG21	1.97	0.47
1:A:1014:ASP:H	1:A:1042:GLY:HA2	1.80	0.47
1:A:1140:LEU:HD13	1:A:1145:PHE:CE2	2.50	0.47
1:B:2014:ASP:O	1:B:2038:LEU:HD12	2.15	0.47
1:D:4288:PHE:CE1	1:D:4291:GLY:HA2	2.50	0.47
1:B:2315:CYS:HB2	1:B:2327:LEU:HD11	1.96	0.46
1:B:2177:VAL:C	1:B:2180:PRO:HD2	2.36	0.46
1:B:2124:LEU:HB3	1:B:2215:TYR:OH	2.15	0.46
1:B:2258:ASP:OD1	1:B:2259:THR:N	2.48	0.46
1:D:4103:ILE:H	1:D:4103:ILE:HG13	1.38	0.46
1:B:2008:LEU:CD2	1:B:2283:LEU:HB3	2.45	0.46
1:C:3103:ILE:HG13	1:C:3103:ILE:H	1.41	0.46
1:D:4032:PRO:HB2	1:D:4033:GLN:CD	2.36	0.46
1:A:1200:MET:CE	1:A:1203:LEU:HD12	2.46	0.46
1:C:3091:LEU:O	1:C:3091:LEU:HD23	2.16	0.46
1:C:3173:ILE:O	1:C:3177:VAL:HG22	2.15	0.46
1:C:3060:PHE:CE2	1:C:3250:LYS:HB3	2.51	0.46
1:D:4173:ILE:H	1:D:4173:ILE:HG12	1.40	0.46
1:C:3009:VAL:HG11	1:C:3264:LEU:HD22	1.98	0.46
1:C:3219:LYS:O	1:C:3220:GLN:C	2.54	0.46
1:C:3232:VAL:HG12	1:C:3233:ASN:N	2.31	0.46
1:D:4009:VAL:HG11	1:D:4264:LEU:HD22	1.97	0.46
1:A:1056:ARG:HG2	1:A:1057:TYR:CD1	2.51	0.46
1:D:4077:VAL:HA	9:D:5366:HOH:O	2.16	0.46
1:A:1014:ASP:O	1:A:1038:LEU:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1041:LEU:HG	1:A:1045:GLN:NE2	2.30	0.46
1:A:1323:ARG:HA	1:A:1326:GLU:HG2	1.98	0.46
1:B:2323:ARG:HD3	9:B:5938:HOH:O	2.15	0.46
1:B:2143:GLU:O	1:B:2147:LYS:HB2	2.15	0.45
1:A:1012:HIS:CE1	1:A:1015:ARG:HG2	2.51	0.45
1:A:1010:PHE:HE2	1:A:1253:MET:HE3	1.80	0.45
1:B:2170:LEU:HD21	1:B:2206:LEU:HD22	1.97	0.45
1:B:2288:PHE:CE1	1:B:2291:GLY:HA2	2.51	0.45
1:B:2335:ASP:O	1:B:2336:TRP:C	2.54	0.45
1:D:4054:ARG:HH11	1:D:4054:ARG:HG2	1.80	0.45
1:B:2139:THR:HG23	1:B:2218:HIS:HB2	1.98	0.45
1:B:2338:THR:HA	1:B:2341:MET:SD	2.56	0.45
1:B:2123:TYR:HB3	9:B:6336:HOH:O	2.16	0.45
1:B:2032:PRO:HB2	1:B:2033:GLN:CD	2.37	0.45
1:D:4226:LEU:C	1:D:4227:GLN:HG2	2.36	0.45
1:A:1044:GLU:HB3	2:E:7:NAG:C8	2.46	0.45
1:C:3124:LEU:HD22	1:C:3260:THR:HA	1.98	0.45
1:C:3188:ASN:HB2	9:C:5999:HOH:O	2.17	0.45
1:A:1019:ASP:O	1:A:1180:PRO:HG3	2.17	0.45
1:A:1288:PHE:CE1	1:A:1291:GLY:HA2	2.51	0.45
1:B:2091:LEU:HD13	1:B:2092:PHE:CE2	2.52	0.45
1:B:2010:PHE:HE2	1:B:2253:MET:HE3	1.81	0.45
1:B:2327:LEU:O	1:B:2330:PRO:HD2	2.17	0.45
1:C:3315:CYS:SG	1:C:3316:SER:N	2.90	0.45
1:B:2002:GLU:OE2	4:G:2:NAG:N2	2.49	0.45
1:B:2144:GLU:O	1:B:2148:ARG:HG3	2.17	0.45
1:C:3115:PRO:CG	1:D:4114:VAL:HG22	2.47	0.45
1:C:3136:GLU:O	1:C:3140:LEU:HD23	2.17	0.45
1:D:4054:ARG:NH1	1:D:4054:ARG:HG2	2.32	0.45
1:D:4060:PHE:CE2	1:D:4250:LYS:HB3	2.52	0.45
1:D:4302:GLU:HA	9:D:6094:HOH:O	2.16	0.45
1:D:4328:VAL:O	1:D:4332:ILE:HD12	2.17	0.45
1:B:2054:ARG:HG2	1:B:2054:ARG:NH1	2.31	0.45
1:B:2219:LYS:O	1:B:2220:GLN:C	2.55	0.45
1:A:1319:CYS:HA	1:A:1320:PRO:HD3	1.86	0.44
1:B:2054:ARG:HG2	1:B:2054:ARG:HH11	1.81	0.44
1:C:3091:LEU:HD22	1:C:3092:PHE:CZ	2.52	0.44
1:C:3143:GLU:O	1:C:3147:LYS:HB2	2.17	0.44
1:A:1231:LEU:O	1:A:1235:ILE:HG12	2.17	0.44
1:C:3170:LEU:HA	1:C:3173:ILE:HG13	2.00	0.44
2:E:2:NAG:C1	2:E:8:FUC:HO2	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:GLU:O	1:A:1147:LYS:HB2	2.18	0.44
1:B:2315:CYS:SG	1:B:2316:SER:N	2.90	0.44
1:B:2326:GLU:HG3	1:B:2327:LEU:N	2.33	0.44
1:C:3144:GLU:O	1:C:3148:ARG:HG3	2.17	0.44
1:D:4056:ARG:HG2	1:D:4057:TYR:CD1	2.52	0.44
5:L:1:NAG:C6	5:L:2:NAG:C1	2.95	0.44
1:A:1220:GLN:O	1:A:1223:LYS:HB2	2.18	0.44
1:A:1009:VAL:HG11	1:A:1264:LEU:HD22	1.99	0.44
1:C:3116:LEU:HD13	1:C:3123:TYR:CE2	2.53	0.44
1:A:1012:HIS:CD2	1:A:1079:ARG:HD2	2.52	0.44
1:C:3066:LYS:HB3	1:C:3069:GLN:HG3	1.99	0.44
1:C:3170:LEU:HG	9:C:5038:HOH:O	2.17	0.44
1:C:3329:GLY:N	1:C:3330:PRO:HD2	2.32	0.44
1:D:4019:ASP:O	1:D:4180:PRO:HG3	2.17	0.44
1:D:4219:LYS:O	1:D:4220:GLN:C	2.55	0.44
1:D:4270:VAL:HG23	1:D:4310:LEU:HD13	1.99	0.44
1:C:3169:ASP:O	1:C:3173:ILE:HG12	2.18	0.44
1:C:3319:CYS:HA	1:C:3320:PRO:HD3	1.86	0.44
1:A:1159:LEU:HD23	1:A:1159:LEU:HA	1.81	0.44
1:C:3032:PRO:HB2	1:C:3033:GLN:CD	2.38	0.44
1:C:3054:ARG:HG2	1:C:3054:ARG:HH11	1.83	0.44
1:D:4079:ARG:NH1	8:D:4350:GLY:OXT	2.51	0.44
1:D:4167:GLY:O	1:D:4169:ASP:N	2.51	0.44
1:B:2140:LEU:HD13	1:B:2145:PHE:CE2	2.53	0.44
1:C:3054:ARG:NH1	9:C:5042:HOH:O	2.51	0.44
1:B:2012:HIS:CE1	1:B:2015:ARG:HG2	2.53	0.44
1:C:3012:HIS:CE1	1:C:3015:ARG:HG2	2.52	0.44
1:D:4016:SER:HB2	1:D:4017:PRO:HD2	2.00	0.44
1:A:1064:SER:O	1:A:1065:TYR:C	2.56	0.43
1:A:1170:LEU:HA	1:A:1173:ILE:HG13	1.98	0.43
1:B:2033:GLN:N	9:B:5004:HOH:O	2.49	0.43
1:B:2121:LEU:HD12	1:B:2121:LEU:O	2.18	0.43
1:C:3014:ASP:O	1:C:3038:LEU:HD12	2.17	0.43
2:E:2:NAG:C1	2:E:8:FUC:O2	2.66	0.43
1:A:1030:SER:HA	1:C:3245:ILE:HG23	2.00	0.43
1:C:3298:TYR:CE1	1:C:3309:PRO:HB3	2.53	0.43
1:D:4009:VAL:HG11	1:D:4264:LEU:CD2	2.48	0.43
1:A:1010:PHE:CE2	1:A:1253:MET:HE3	2.54	0.43
1:B:2206:LEU:HA	1:B:2206:LEU:HD23	1.90	0.43
1:C:3079:ARG:NH1	8:C:3350:GLY:OXT	2.52	0.43
1:C:3231:LEU:HA	1:C:3231:LEU:HD23	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:PRO:HD3	1:A:1259:THR:HG21	2.01	0.43
1:A:1232:VAL:HG12	1:A:1233:ASN:N	2.33	0.43
1:B:2169:ASP:O	1:B:2173:ILE:HG12	2.18	0.43
1:B:2257:HIS:N	1:B:2257:HIS:CD2	2.87	0.43
1:C:3218:HIS:CE1	1:C:3219:LYS:HD2	2.54	0.43
1:D:4220:GLN:O	1:D:4223:LYS:HB2	2.19	0.43
1:D:4329:GLY:N	1:D:4330:PRO:HD2	2.33	0.43
1:C:3095:GLU:H	1:C:3098:SER:HB2	1.84	0.43
1:C:3159:LEU:HA	1:C:3159:LEU:HD23	1.84	0.43
1:B:2072:ILE:HD13	1:B:2088:LEU:HD11	2.00	0.43
1:B:2167:GLY:O	1:B:2169:ASP:N	2.52	0.43
1:B:2231:LEU:O	1:B:2235:ILE:HG12	2.19	0.43
1:C:3054:ARG:HG2	1:C:3054:ARG:NH1	2.33	0.43
1:D:4012:HIS:CD2	1:D:4079:ARG:HD2	2.54	0.43
1:D:4073:ARG:HA	1:D:4112:HIS:O	2.19	0.43
1:A:1014:ASP:HA	1:A:1278:TYR:CD1	2.53	0.43
1:A:1177:VAL:CG2	1:A:1178:TYR:N	2.82	0.43
1:B:2073:ARG:HA	1:B:2112:HIS:O	2.18	0.43
1:C:3014:ASP:HB2	1:C:3045:GLN:HE22	1.84	0.43
1:C:3047:TYR:CD1	1:D:4100:TRP:CH2	3.04	0.43
1:D:4091:LEU:HD22	1:D:4092:PHE:CZ	2.54	0.43
1:D:4231:LEU:O	1:D:4235:ILE:HG12	2.18	0.43
1:A:1065:TYR:HB2	1:A:1092:PHE:CG	2.54	0.43
1:B:2022:PRO:HG2	1:B:2164:GLY:HA3	2.01	0.43
1:C:3019:ASP:O	1:C:3180:PRO:HG3	2.19	0.43
1:C:3172:GLY:O	1:C:3173:ILE:C	2.57	0.43
1:D:4065:TYR:HB2	1:D:4092:PHE:CG	2.53	0.43
1:B:2066:LYS:HB3	1:B:2069:GLN:HG3	2.00	0.42
1:C:3167:GLY:O	1:C:3169:ASP:N	2.51	0.42
1:B:2091:LEU:HD22	1:B:2092:PHE:CZ	2.54	0.42
1:B:2159:LEU:HA	1:B:2159:LEU:HD23	1.81	0.42
1:C:3170:LEU:HD21	1:C:3206:LEU:HD22	2.01	0.42
1:C:3134:GLU:OE1	1:C:3342:THR:HG23	2.19	0.42
1:D:4144:GLU:O	1:D:4148:ARG:HG3	2.19	0.42
1:A:1060:PHE:CE2	1:A:1250:LYS:HB3	2.54	0.42
1:B:2060:PHE:CE2	1:B:2250:LYS:HB3	2.54	0.42
1:D:4125:PRO:HD3	1:D:4259:THR:HG21	2.01	0.42
1:A:1134:GLU:OE1	1:A:1342:THR:HG23	2.18	0.42
1:A:1167:GLY:O	1:A:1169:ASP:N	2.52	0.42
1:C:3114:VAL:HG22	1:D:4115:PRO:CG	2.49	0.42
1:C:3283:LEU:CD2	1:C:3283:LEU:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1326:GLU:HG3	1:A:1327:LEU:N	2.33	0.42
1:C:3301:ASN:OD1	1:C:3302:GLU:HG2	2.20	0.42
1:A:1144:GLU:O	1:A:1148:ARG:HG3	2.20	0.42
1:A:1172:GLY:O	1:A:1173:ILE:C	2.58	0.42
1:A:1298:TYR:CE1	1:A:1309:PRO:HB3	2.55	0.42
1:C:3072:ILE:HD13	1:C:3088:LEU:HD11	2.01	0.42
1:D:4094:PRO:HB2	1:D:4099:ILE:HG12	2.02	0.42
1:D:4177:VAL:C	1:D:4180:PRO:HD2	2.39	0.42
1:A:1084:ALA:HB2	1:A:1255:SER:HB2	2.00	0.42
1:B:2125:PRO:HD3	1:B:2259:THR:HG21	2.01	0.42
1:C:3328:VAL:O	1:C:3332:ILE:HD12	2.19	0.42
1:B:2232:VAL:HG12	1:B:2233:ASN:N	2.35	0.42
1:D:4091:LEU:HD22	1:D:4092:PHE:CE2	2.55	0.42
2:E:1:NAG:H62	2:E:2:NAG:H82	2.01	0.42
1:A:1066:LYS:HB3	1:A:1069:GLN:HG3	2.02	0.42
1:A:1124:LEU:HD22	1:A:1260:THR:HA	2.02	0.42
1:A:1219:LYS:O	1:A:1220:GLN:C	2.58	0.42
1:C:3323:ARG:O	1:C:3324:PHE:C	2.56	0.42
1:D:4277:PRO:HG2	1:D:4280:SER:HB3	2.01	0.42
1:D:4323:ARG:O	1:D:4324:PHE:C	2.57	0.42
1:B:2014:ASP:HA	1:B:2278:TYR:CD1	2.55	0.41
1:A:1257:HIS:N	1:A:1257:HIS:CD2	2.87	0.41
1:C:3320:PRO:O	1:C:3321:LEU:C	2.58	0.41
1:D:4133:GLN:HA	1:D:4133:GLN:OE1	2.20	0.41
9:D:6108:HOH:O	4:M:2:NAG:H82	2.20	0.41
1:B:2010:PHE:CE2	1:B:2253:MET:HE3	2.55	0.41
1:C:3173:ILE:H	1:C:3173:ILE:HG12	1.43	0.41
1:D:4014:ASP:HA	1:D:4278:TYR:CD1	2.55	0.41
1:A:1016:SER:HB2	1:A:1017:PRO:HD2	2.02	0.41
1:A:1016:SER:HB3	9:A:5711:HOH:O	2.19	0.41
1:A:1143:GLU:HG3	1:A:1144:GLU:N	2.36	0.41
1:A:1169:ASP:O	1:A:1173:ILE:HG12	2.19	0.41
1:D:4143:GLU:O	1:D:4147:LYS:HB2	2.20	0.41
1:D:4298:TYR:CE1	1:D:4309:PRO:HB3	2.55	0.41
1:A:1009:VAL:HG11	1:A:1264:LEU:CD2	2.50	0.41
1:A:1100:TRP:CE3	1:B:2043:MET:HB3	2.56	0.41
1:B:2073:ARG:CZ	9:B:5463:HOH:O	2.66	0.41
1:B:2120:GLN:HG3	9:B:5024:HOH:O	2.20	0.41
1:C:3165:LEU:HB3	9:C:5955:HOH:O	2.20	0.41
1:D:4064:SER:O	1:D:4065:TYR:C	2.58	0.41
1:D:4091:LEU:HD13	1:D:4092:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4125:PRO:HG3	1:D:4214:LEU:HD11	2.02	0.41
1:D:4231:LEU:HA	1:D:4231:LEU:HD23	1.84	0.41
2:E:1:NAG:H61	2:E:8:FUC:O2	2.20	0.41
1:B:2037:GLN:HE22	1:B:2078:ASP:HB3	1.85	0.41
1:B:2009:VAL:HG11	1:B:2264:LEU:HD22	2.02	0.41
1:B:2011:ARG:HD3	1:B:2277:PRO:C	2.40	0.41
1:A:1029:SER:HB2	1:C:3247:SER:CB	2.50	0.41
1:D:4170:LEU:HD21	1:D:4206:LEU:HD22	2.01	0.41
1:D:4218:HIS:CG	1:D:4219:LYS:N	2.88	0.41
1:B:2241:ARG:HD2	1:B:2248:TYR:OH	2.21	0.41
1:B:2270:VAL:O	1:B:2270:VAL:HG23	2.20	0.41
1:C:3064:SER:O	1:C:3065:TYR:C	2.58	0.41
1:C:3073:ARG:HA	1:C:3112:HIS:O	2.21	0.41
1:C:3143:GLU:HG3	1:C:3144:GLU:N	2.35	0.41
1:C:3196:THR:HG23	1:C:3199:THR:OG1	2.21	0.41
1:C:3212:LEU:HA	1:C:3212:LEU:HD23	1.90	0.41
1:D:4155:PHE:HE1	1:D:4199:THR:HG23	1.85	0.41
1:D:4170:LEU:HA	1:D:4173:ILE:HG13	2.01	0.41
1:C:3216:GLY:O	1:C:3217:ILE:HG12	2.21	0.41
1:D:4212:LEU:HA	1:D:4212:LEU:HD23	1.86	0.41
1:A:1116:LEU:HD22	1:A:1123:TYR:CE2	2.56	0.41
1:A:1327:LEU:O	1:A:1330:PRO:HD2	2.21	0.41
1:B:2019:ASP:O	1:B:2180:PRO:HG3	2.21	0.41
1:C:3139:THR:HG23	1:C:3218:HIS:HB2	2.03	0.41
1:A:1030:SER:CB	1:C:3245:ILE:HG23	2.51	0.41
1:B:2022:PRO:CD	1:B:2165:LEU:HD23	2.41	0.40
1:B:2172:GLY:O	1:B:2173:ILE:C	2.59	0.40
1:D:4082:MET:O	1:D:4086:THR:OG1	2.38	0.40
1:D:4169:ASP:O	1:D:4173:ILE:HG12	2.21	0.40
1:C:3218:HIS:NE2	1:C:3219:LYS:HD2	2.36	0.40
1:A:1100:TRP:CH2	1:B:2086:THR:HG22	2.57	0.40
1:B:2014:ASP:N	1:B:2042:GLY:HA2	2.35	0.40
1:B:2064:SER:O	1:B:2065:TYR:C	2.60	0.40
1:B:2277:PRO:HG2	1:B:2280:SER:HB3	2.04	0.40
1:A:1125:PRO:HG3	1:A:1214:LEU:HD11	2.02	0.40
1:B:2320:PRO:O	1:B:2321:LEU:C	2.60	0.40
1:C:3125:PRO:HD3	1:C:3259:THR:HG21	2.03	0.40
1:D:4055:LYS:O	1:D:4058:ARG:HB2	2.22	0.40
1:D:4172:GLY:O	1:D:4173:ILE:C	2.60	0.40
1:A:1177:VAL:C	1:A:1180:PRO:HD2	2.41	0.40
1:A:1181:LEU:CD1	1:A:1200:MET:HE1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1315:CYS:SG	1:A:1316:SER:N	2.94	0.40
1:A:1131:ARG:HA	1:A:1342:THR:CG2	2.52	0.40
1:B:2014:ASP:HB2	1:B:2045:GLN:HE22	1.87	0.40
1:B:2270:VAL:HG23	1:B:2310:LEU:HD13	2.00	0.40
1:B:2048:GLU:OE2	1:B:2303:THR:HG23	2.21	0.40
1:C:3177:VAL:CG2	1:C:3178:TYR:N	2.84	0.40
1:C:3218:HIS:CG	1:C:3219:LYS:N	2.89	0.40
1:D:4056:ARG:NH2	9:D:6052:HOH:O	2.55	0.40
1:D:4326:GLU:HG3	1:D:4327:LEU:N	2.36	0.40
6:I:1:NAG:H61	6:I:2:NAG:C8	2.51	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	340/342 (99%)	298 (88%)	33 (10%)	9 (3%)	5	31
1	B	340/342 (99%)	298 (88%)	34 (10%)	8 (2%)	6	34
1	C	340/342 (99%)	298 (88%)	34 (10%)	8 (2%)	6	34
1	D	340/342 (99%)	301 (88%)	30 (9%)	9 (3%)	5	31
All	All	1360/1368 (99%)	1195 (88%)	131 (10%)	34 (2%)	5	32

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1065	TYR
1	A	1217	ILE
1	A	1220	GLN
1	B	2065	TYR
1	B	2217	ILE

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Mol	Chain	Res	Type
1	B	2220	GLN
1	C	3065	TYR
1	C	3217	ILE
1	C	3220	GLN
1	D	4065	TYR
1	D	4217	ILE
1	D	4220	GLN
1	A	1067	HIS
1	A	1168	GLN
1	A	1305	HIS
1	B	2305	HIS
1	C	3305	HIS
1	D	4029	SER
1	D	4168	GLN
1	D	4305	HIS
1	A	1029	SER
1	B	2029	SER
1	B	2168	GLN
1	C	3029	SER
1	C	3099	ILE
1	C	3168	GLN
1	D	4099	ILE
1	A	1099	ILE
1	B	2099	ILE
1	B	2336	TRP
1	C	3336	TRP
1	D	4336	TRP
1	A	1336	TRP
1	D	4067	HIS

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	314/314 (100%)	252 (80%)	62 (20%)	1 7
1	B	314/314 (100%)	251 (80%)	63 (20%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	314/314 (100%)	255 (81%)	59 (19%)	1 8
1	D	314/314 (100%)	252 (80%)	62 (20%)	1 7
All	All	1256/1256 (100%)	1010 (80%)	246 (20%)	1 7

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1006	VAL
1	A	1009	VAL
1	A	1010	PHE
1	A	1011	ARG
1	A	1015	ARG
1	A	1018	ILE
1	A	1027	LYS
1	A	1029	SER
1	A	1037	GLN
1	A	1040	GLN
1	A	1048	GLU
1	A	1049	LEU
1	A	1051	GLU
1	A	1055	LYS
1	A	1056	ARG
1	A	1059	LYS
1	A	1061	LEU
1	A	1066	LYS
1	A	1067	HIS
1	A	1068	GLU
1	A	1069	GLN
1	A	1080	THR
1	A	1081	LEU
1	A	1086	THR
1	A	1091	LEU
1	A	1103	ILE
1	A	1117	SER
1	A	1118	GLU
1	A	1123	TYR
1	A	1142	SER
1	A	1147	LYS
1	A	1154	ASP
1	A	1159	LEU
1	A	1161	LYS

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Mol	Chain	Res	Type
1	A	1173	ILE
1	A	1177	VAL
1	A	1191	LEU
1	A	1193	SER
1	A	1196	THR
1	A	1202	LYS
1	A	1211	LEU
1	A	1214	LEU
1	A	1217	ILE
1	A	1219	LYS
1	A	1230	VAL
1	A	1231	LEU
1	A	1241	ARG
1	A	1243	THR
1	A	1244	GLN
1	A	1247	SER
1	A	1249	LYS
1	A	1257	HIS
1	A	1259	THR
1	A	1283	LEU
1	A	1284	THR
1	A	1285	GLU
1	A	1303	THR
1	A	1306	GLU
1	A	1316	SER
1	A	1323	ARG
1	A	1334	GLN
1	A	1337	SER
1	B	2006	VAL
1	B	2009	VAL
1	B	2010	PHE
1	B	2011	ARG
1	B	2015	ARG
1	B	2018	ILE
1	B	2027	LYS
1	B	2029	SER
1	B	2037	GLN
1	B	2040	GLN
1	B	2048	GLU
1	B	2049	LEU
1	B	2051	GLU
1	B	2055	LYS

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Mol	Chain	Res	Type
1	B	2056	ARG
1	B	2059	LYS
1	B	2061	LEU
1	B	2066	LYS
1	B	2067	HIS
1	B	2068	GLU
1	B	2069	GLN
1	B	2080	THR
1	B	2081	LEU
1	B	2086	THR
1	B	2091	LEU
1	B	2103	ILE
1	B	2117	SER
1	B	2123	TYR
1	B	2142	SER
1	B	2147	LYS
1	B	2153	LYS
1	B	2154	ASP
1	B	2159	LEU
1	B	2161	LYS
1	B	2173	ILE
1	B	2177	VAL
1	B	2191	LEU
1	B	2193	SER
1	B	2196	THR
1	B	2202	LYS
1	B	2211	LEU
1	B	2214	LEU
1	B	2217	ILE
1	B	2219	LYS
1	B	2230	VAL
1	B	2231	LEU
1	B	2241	ARG
1	B	2243	THR
1	B	2244	GLN
1	B	2247	SER
1	B	2249	LYS
1	B	2257	HIS
1	B	2259	THR
1	B	2283	LEU
1	B	2284	THR
1	B	2285	GLU

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Mol	Chain	Res	Type
1	B	2299	TYR
1	B	2303	THR
1	B	2306	GLU
1	B	2316	SER
1	B	2323	ARG
1	B	2334	GLN
1	B	2337	SER
1	C	3006	VAL
1	C	3009	VAL
1	C	3010	PHE
1	C	3011	ARG
1	C	3015	ARG
1	C	3018	ILE
1	C	3027	LYS
1	C	3029	SER
1	C	3037	GLN
1	C	3040	GLN
1	C	3048	GLU
1	C	3049	LEU
1	C	3051	GLU
1	C	3055	LYS
1	C	3056	ARG
1	C	3061	LEU
1	C	3066	LYS
1	C	3067	HIS
1	C	3068	GLU
1	C	3069	GLN
1	C	3080	THR
1	C	3081	LEU
1	C	3086	THR
1	C	3091	LEU
1	C	3103	ILE
1	C	3117	SER
1	C	3123	TYR
1	C	3142	SER
1	C	3147	LYS
1	C	3154	ASP
1	C	3161	LYS
1	C	3173	ILE
1	C	3177	VAL
1	C	3191	LEU
1	C	3193	SER

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Mol	Chain	Res	Type
1	C	3196	THR
1	C	3202	LYS
1	C	3211	LEU
1	C	3214	LEU
1	C	3217	ILE
1	C	3219	LYS
1	C	3230	VAL
1	C	3231	LEU
1	C	3241	ARG
1	C	3243	THR
1	C	3244	GLN
1	C	3247	SER
1	C	3249	LYS
1	C	3257	HIS
1	C	3259	THR
1	C	3283	LEU
1	C	3284	THR
1	C	3285	GLU
1	C	3303	THR
1	C	3306	GLU
1	C	3316	SER
1	C	3323	ARG
1	C	3334	GLN
1	C	3337	SER
1	D	4006	VAL
1	D	4009	VAL
1	D	4010	PHE
1	D	4011	ARG
1	D	4015	ARG
1	D	4018	ILE
1	D	4027	LYS
1	D	4029	SER
1	D	4037	GLN
1	D	4040	GLN
1	D	4048	GLU
1	D	4049	LEU
1	D	4051	GLU
1	D	4055	LYS
1	D	4056	ARG
1	D	4059	LYS
1	D	4061	LEU
1	D	4062	ASN

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Mol	Chain	Res	Type
1	D	4066	LYS
1	D	4067	HIS
1	D	4068	GLU
1	D	4069	GLN
1	D	4080	THR
1	D	4081	LEU
1	D	4086	THR
1	D	4091	LEU
1	D	4103	ILE
1	D	4117	SER
1	D	4123	TYR
1	D	4142	SER
1	D	4147	LYS
1	D	4154	ASP
1	D	4159	LEU
1	D	4161	LYS
1	D	4173	ILE
1	D	4177	VAL
1	D	4191	LEU
1	D	4193	SER
1	D	4196	THR
1	D	4202	LYS
1	D	4211	LEU
1	D	4214	LEU
1	D	4217	ILE
1	D	4219	LYS
1	D	4230	VAL
1	D	4231	LEU
1	D	4241	ARG
1	D	4243	THR
1	D	4244	GLN
1	D	4247	SER
1	D	4249	LYS
1	D	4257	HIS
1	D	4259	THR
1	D	4283	LEU
1	D	4284	THR
1	D	4285	GLU
1	D	4303	THR
1	D	4306	GLU
1	D	4316	SER
1	D	4323	ARG

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Mol	Chain	Res	Type
1	D	4334	GLN
1	D	4337	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1037	GLN
1	A	1168	GLN
1	A	1265	GLN
1	A	1334	GLN
1	B	2037	GLN
1	B	2168	GLN
1	B	2237	ASN
1	B	2244	GLN
1	B	2265	GLN
1	B	2334	GLN
1	C	3037	GLN
1	C	3168	GLN
1	C	3265	GLN
1	C	3334	GLN
1	D	4037	GLN
1	D	4168	GLN
1	D	4265	GLN
1	D	4334	GLN

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)

38 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	E	1	1,2	14,14,15	0.51	0	17,19,21	1.01	1 (5%)
2	NAG	E	2	2	14,14,15	0.61	0	17,19,21	0.80	1 (5%)
2	BMA	E	3	2	11,11,12	0.57	0	15,15,17	0.58	0
2	MAN	E	4	2	11,11,12	0.79	0	15,15,17	0.82	0
2	NAG	E	5	2	14,14,15	0.50	0	17,19,21	0.75	1 (5%)
2	MAN	E	6	2	11,11,12	0.72	0	15,15,17	0.63	1 (6%)
2	NAG	E	7	2	14,14,15	0.47	0	17,19,21	0.76	1 (5%)
2	FUC	E	8	2	10,10,11	0.60	0	14,14,16	0.45	0
3	NAG	F	1	1,3	14,14,15	0.57	0	17,19,21	0.64	0
3	NAG	F	2	3	14,14,15	0.79	0	17,19,21	1.32	2 (11%)
3	BMA	F	3	3	11,11,12	0.58	0	15,15,17	0.98	1 (6%)
3	MAN	F	4	3	11,11,12	0.73	0	15,15,17	0.59	0
4	NAG	G	1	1,4	14,14,15	0.49	0	17,19,21	0.99	1 (5%)
4	NAG	G	2	4	14,14,15	0.59	0	17,19,21	0.59	0
4	BMA	G	3	4	11,11,12	0.54	0	15,15,17	0.21	0
5	NAG	H	1	1,5	14,14,15	0.64	0	17,19,21	0.62	0
5	NAG	H	2	5	14,14,15	0.64	0	17,19,21	0.77	0
5	BMA	H	3	5	11,11,12	0.66	0	15,15,17	0.34	0
5	MAN	H	4	5	11,11,12	0.66	0	15,15,17	0.65	1 (6%)
6	NAG	I	1	1,6	14,14,15	0.46	0	17,19,21	0.64	0
6	NAG	I	2	6	14,14,15	0.64	0	17,19,21	0.93	2 (11%)
6	BMA	I	3	6	11,11,12	0.73	0	15,15,17	0.44	0
6	MAN	I	4	6	11,11,12	0.74	0	15,15,17	0.77	1 (6%)
6	MAN	I	5	6	11,11,12	0.69	0	15,15,17	0.69	0
6	MAN	I	6	6	11,11,12	0.61	0	15,15,17	0.90	1 (6%)
4	NAG	J	1	1,4	14,14,15	0.65	0	17,19,21	0.82	1 (5%)
4	NAG	J	2	4	14,14,15	0.66	0	17,19,21	0.83	0
4	BMA	J	3	4	11,11,12	0.53	0	15,15,17	0.33	0
4	NAG	K	1	1,4	14,14,15	0.67	0	17,19,21	1.24	3 (17%)
4	NAG	K	2	4	14,14,15	0.89	0	17,19,21	1.01	2 (11%)
4	BMA	K	3	4	11,11,12	0.58	0	15,15,17	0.59	0
5	NAG	L	1	1,5	14,14,15	0.87	0	17,19,21	0.94	0
5	NAG	L	2	5	14,14,15	0.67	0	17,19,21	0.90	0
5	BMA	L	3	5	11,11,12	0.79	0	15,15,17	0.52	0
5	MAN	L	4	5	11,11,12	0.60	0	15,15,17	0.81	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	M	1	1,4	14,14,15	0.63	0	17,19,21	0.99	1 (5%)
4	NAG	M	2	4	14,14,15	0.69	0	17,19,21	0.71	0
4	BMA	M	3	4	11,11,12	0.57	0	15,15,17	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
2	NAG	E	5	2	-	2/6/23/26	0/1/1/1
2	MAN	E	6	2	-	1/2/19/22	0/1/1/1
2	NAG	E	7	2	-	2/6/23/26	0/1/1/1
2	FUC	E	8	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	2/2/19/22	0/1/1/1
6	MAN	I	4	6	-	2/2/19/22	0/1/1/1
6	MAN	I	5	6	-	0/2/19/22	0/1/1/1
6	MAN	I	6	6	-	2/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	BMA	J	3	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	3/6/23/26	0/1/1/1
4	BMA	K	3	4	-	0/2/19/22	0/1/1/1
5	NAG	L	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	MAN	L	4	5	-	0/2/19/22	0/1/1/1
4	NAG	M	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	6	MAN	C1-O5-C5	2.98	116.23	112.19
3	F	2	NAG	C2-N2-C7	-2.97	118.68	122.90
4	G	1	NAG	C4-C3-C2	-2.91	106.75	111.02
3	F	2	NAG	C4-C3-C2	-2.80	106.92	111.02
5	L	4	MAN	C1-O5-C5	2.69	115.83	112.19
3	F	3	BMA	C1-C2-C3	-2.66	106.40	109.67
4	M	1	NAG	C2-N2-C7	-2.53	119.31	122.90
4	K	1	NAG	C4-C3-C2	2.45	114.61	111.02
2	E	1	NAG	C4-C3-C2	-2.44	107.45	111.02
6	I	2	NAG	C2-N2-C7	-2.44	119.43	122.90
5	H	4	MAN	C1-O5-C5	2.37	115.40	112.19
6	I	4	MAN	C1-O5-C5	2.29	115.30	112.19
2	E	5	NAG	C2-N2-C7	-2.27	119.67	122.90
6	I	2	NAG	C4-C3-C2	-2.23	107.75	111.02
4	K	1	NAG	C2-N2-C7	-2.23	119.73	122.90
2	E	7	NAG	C2-N2-C7	-2.21	119.75	122.90
4	J	1	NAG	C2-N2-C7	-2.21	119.76	122.90
4	K	1	NAG	O5-C1-C2	-2.21	107.80	111.29
2	E	2	NAG	C2-N2-C7	-2.17	119.81	122.90
4	K	2	NAG	C2-N2-C7	-2.12	119.89	122.90
2	E	6	MAN	C1-O5-C5	2.05	114.97	112.19
4	K	2	NAG	C3-C4-C5	2.03	113.85	110.24

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C3-C2-N2-C7
4	G	3	BMA	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
5	H	4	MAN	O5-C5-C6-O6
2	E	5	NAG	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
5	H	4	MAN	C4-C5-C6-O6
6	I	6	MAN	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
2	E	5	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
6	I	6	MAN	C4-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
6	I	4	MAN	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
4	M	3	BMA	C4-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
6	I	4	MAN	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
6	I	3	BMA	C4-C5-C6-O6
2	E	6	MAN	O5-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
2	E	7	NAG	C4-C5-C6-O6
2	E	7	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C1-C2-N2-C7

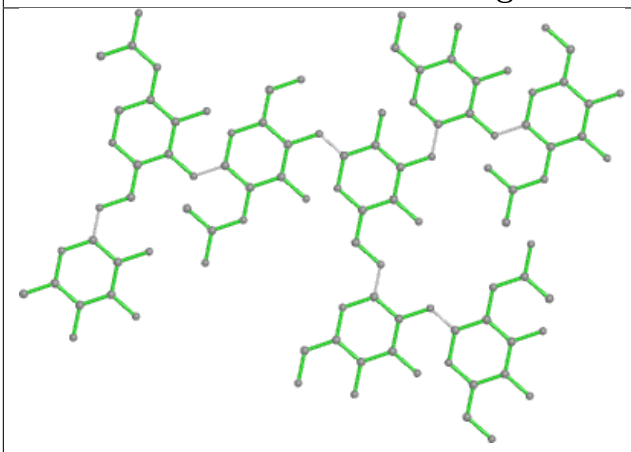
There are no ring outliers.

19 monomers are involved in 25 short contacts:

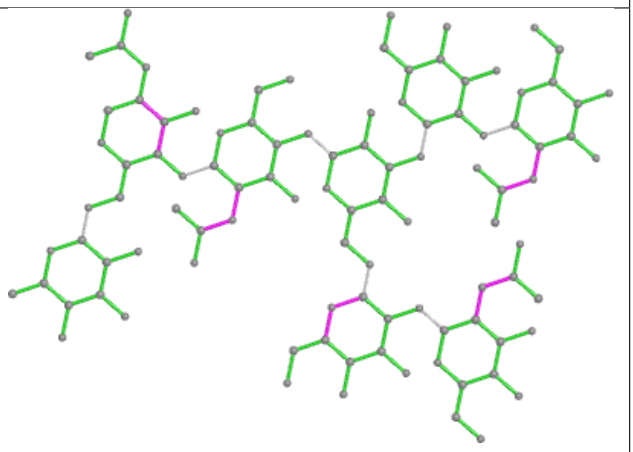
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	8	FUC	3	0
4	G	2	NAG	3	0
4	J	1	NAG	2	0
5	L	2	NAG	2	0
5	L	1	NAG	2	0
2	E	2	NAG	4	0
3	F	2	NAG	1	0
3	F	3	BMA	1	0
6	I	1	NAG	2	0
5	H	2	NAG	3	0
4	G	1	NAG	1	0
6	I	2	NAG	2	0
2	E	7	NAG	3	0
2	E	6	MAN	1	0
2	E	1	NAG	4	0
4	M	2	NAG	1	0
5	H	3	BMA	2	0
4	J	3	BMA	1	0
4	J	2	NAG	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.

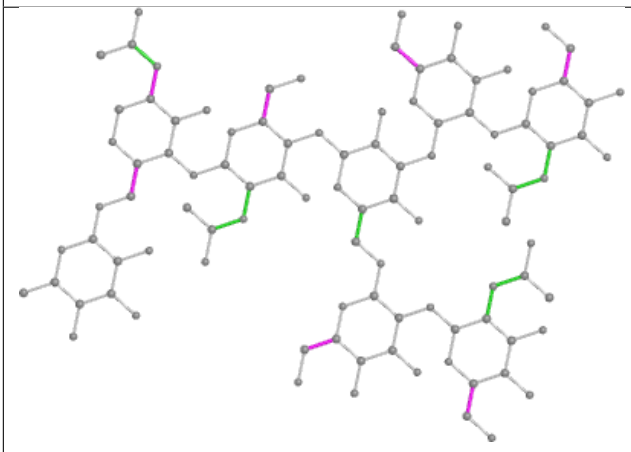
Oligosaccharide Chain E



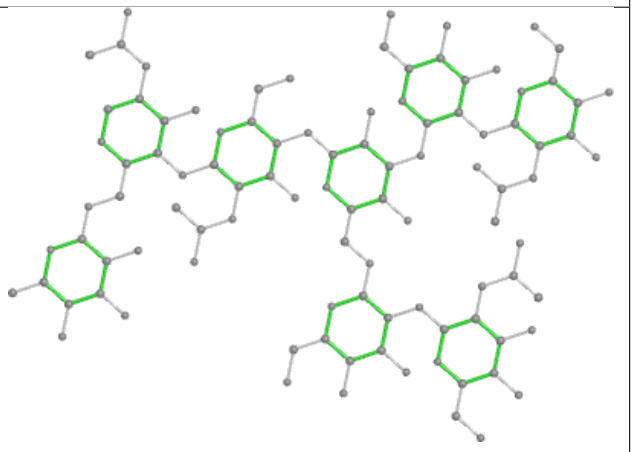
Bond lengths



Bond angles

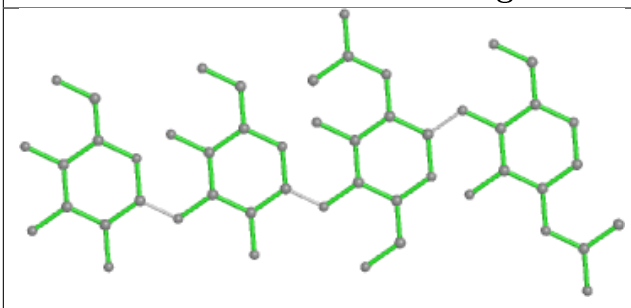


Torsions

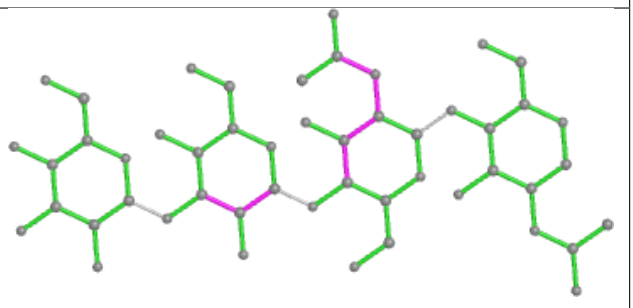


Rings

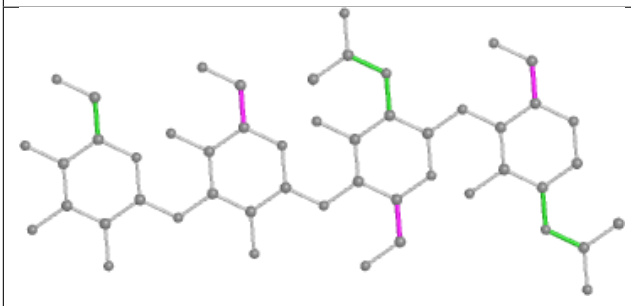
Oligosaccharide Chain F



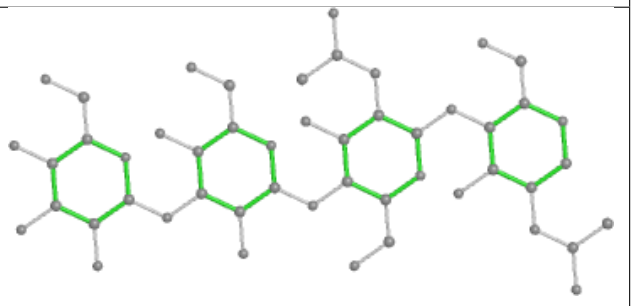
Bond lengths



Bond angles

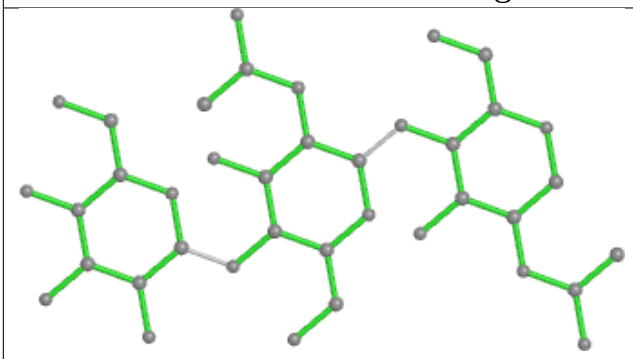


Torsions

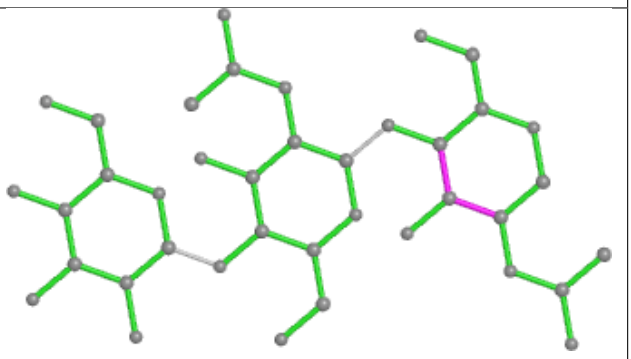


Rings

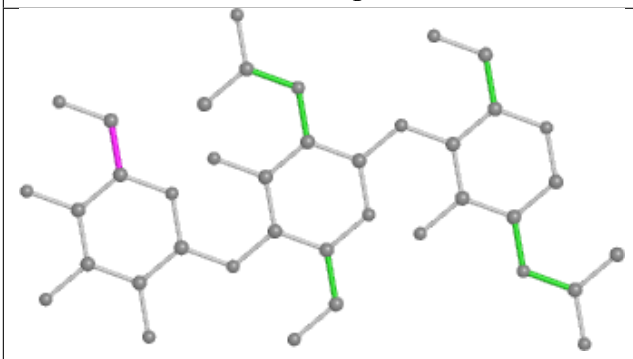
Oligosaccharide Chain G



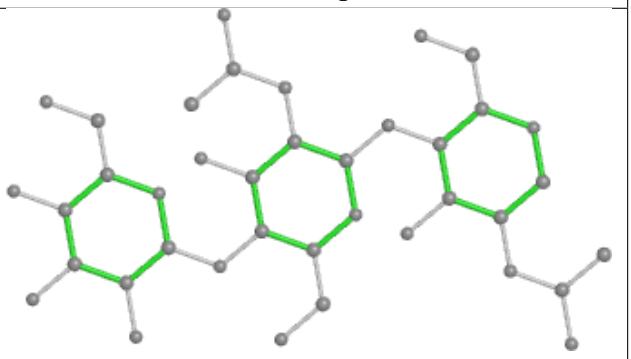
Bond lengths



Bond angles

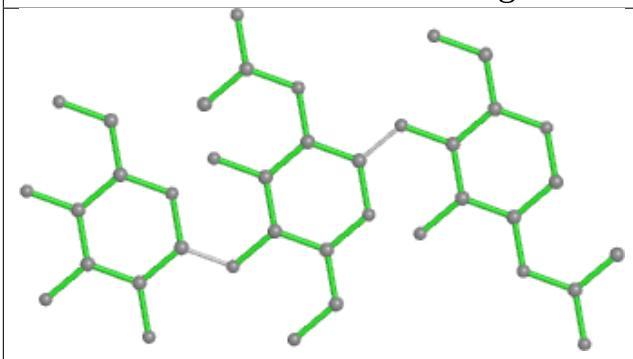


Torsions

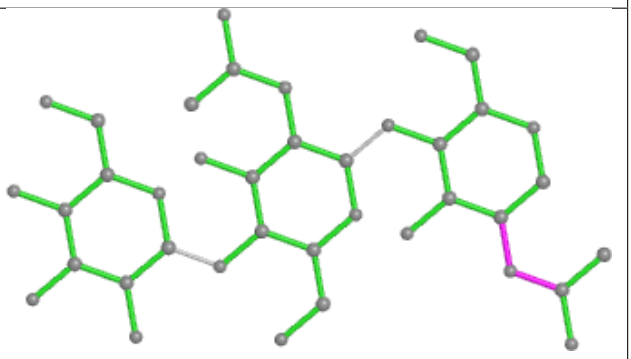


Rings

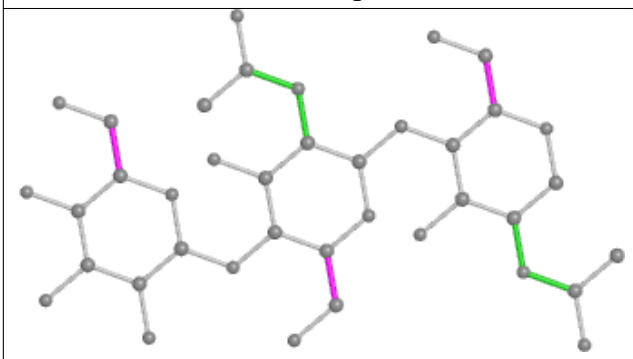
Oligosaccharide Chain J



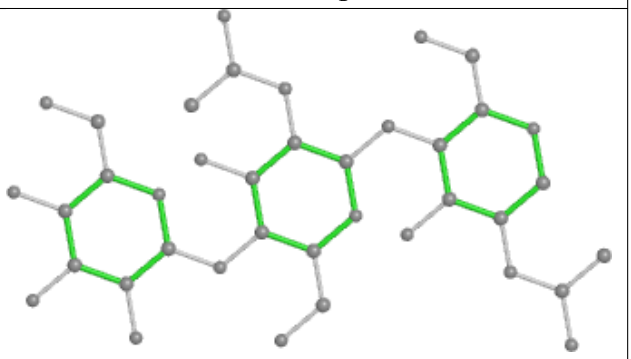
Bond lengths



Bond angles

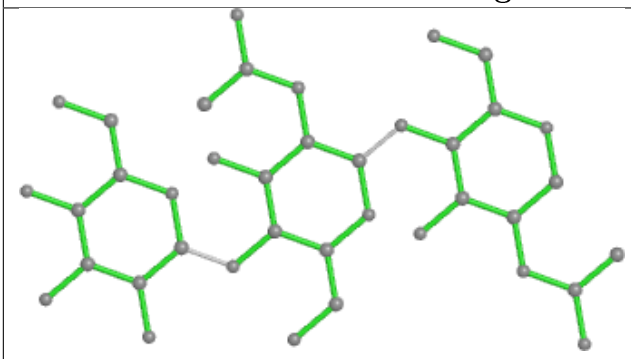


Torsions

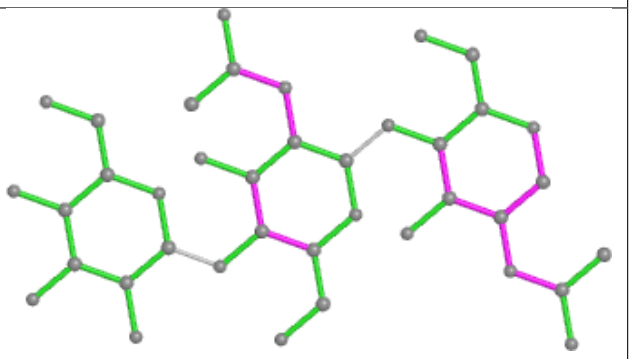


Rings

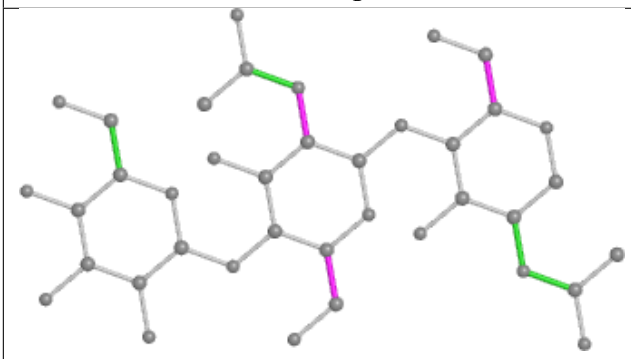
Oligosaccharide Chain K



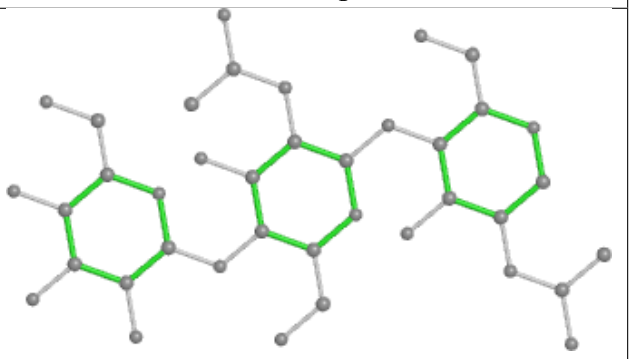
Bond lengths



Bond angles

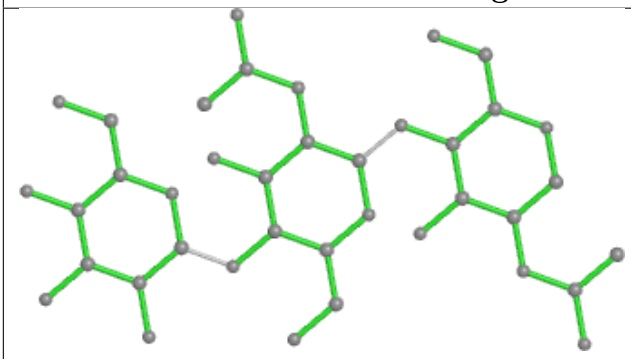


Torsions

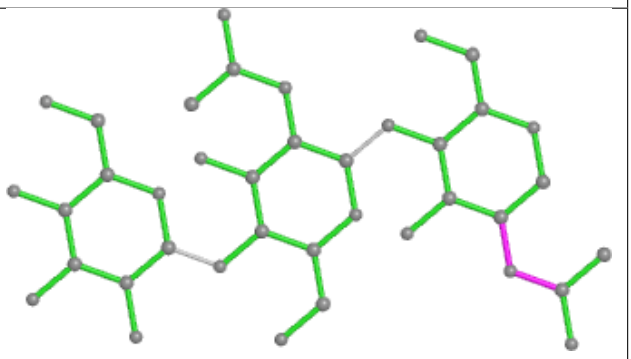


Rings

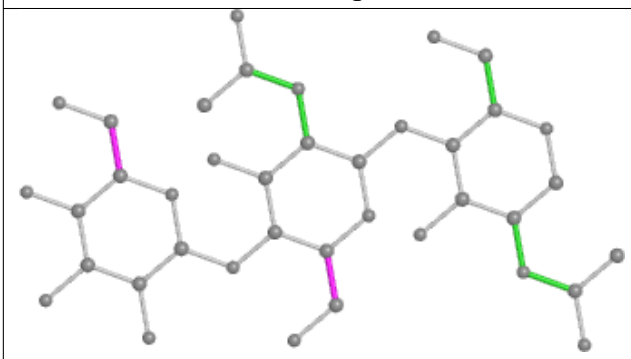
Oligosaccharide Chain M



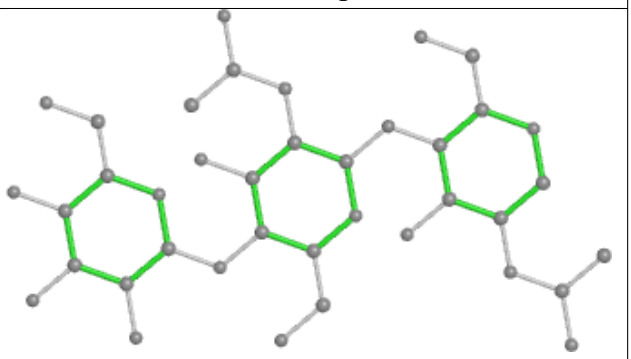
Bond lengths



Bond angles

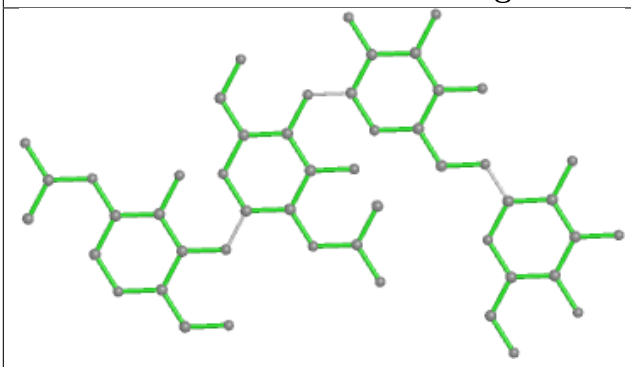


Torsions

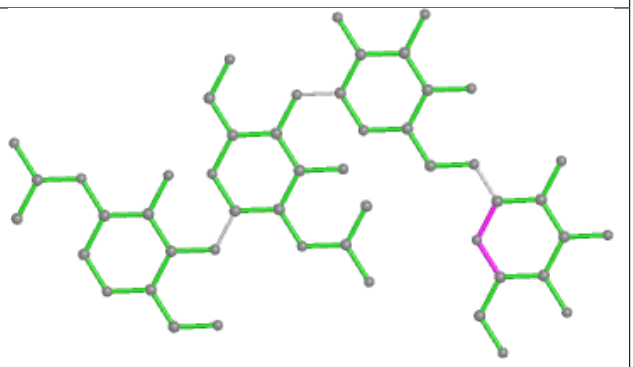


Rings

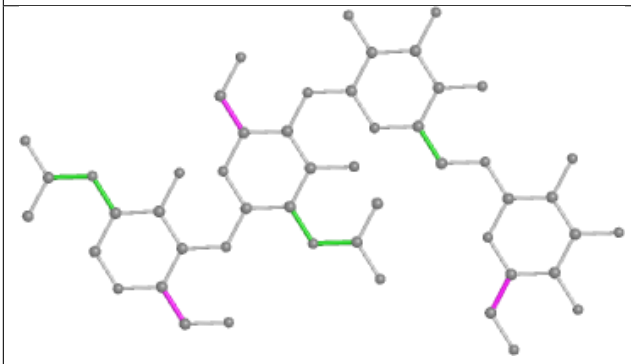
Oligosaccharide Chain H



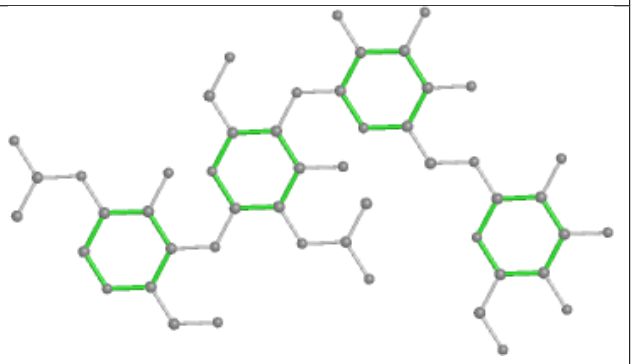
Bond lengths



Bond angles

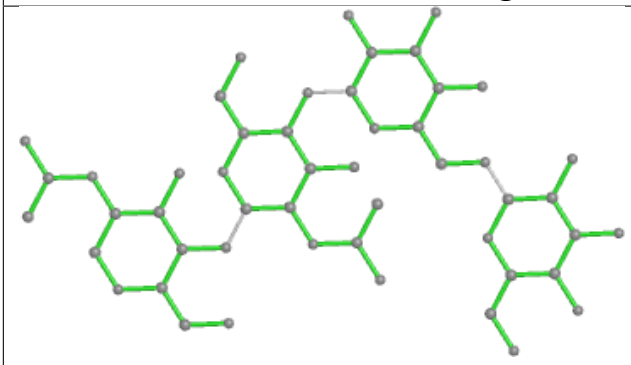


Torsions

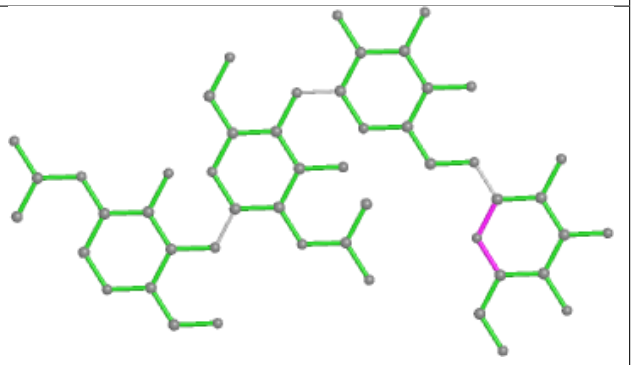


Rings

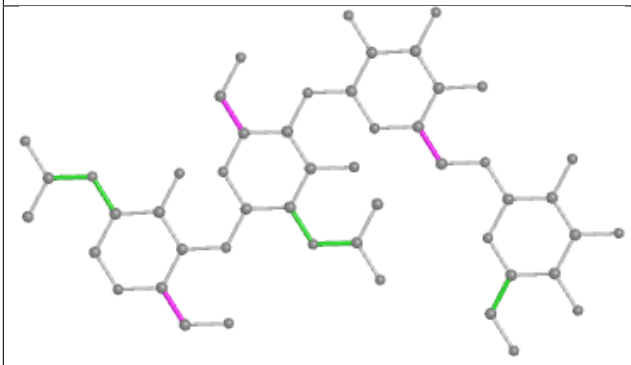
Oligosaccharide Chain L



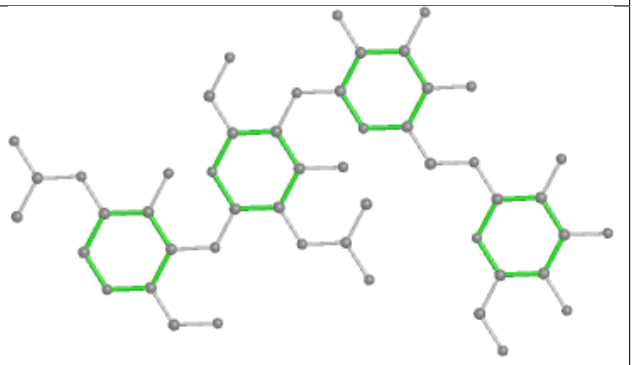
Bond lengths



Bond angles

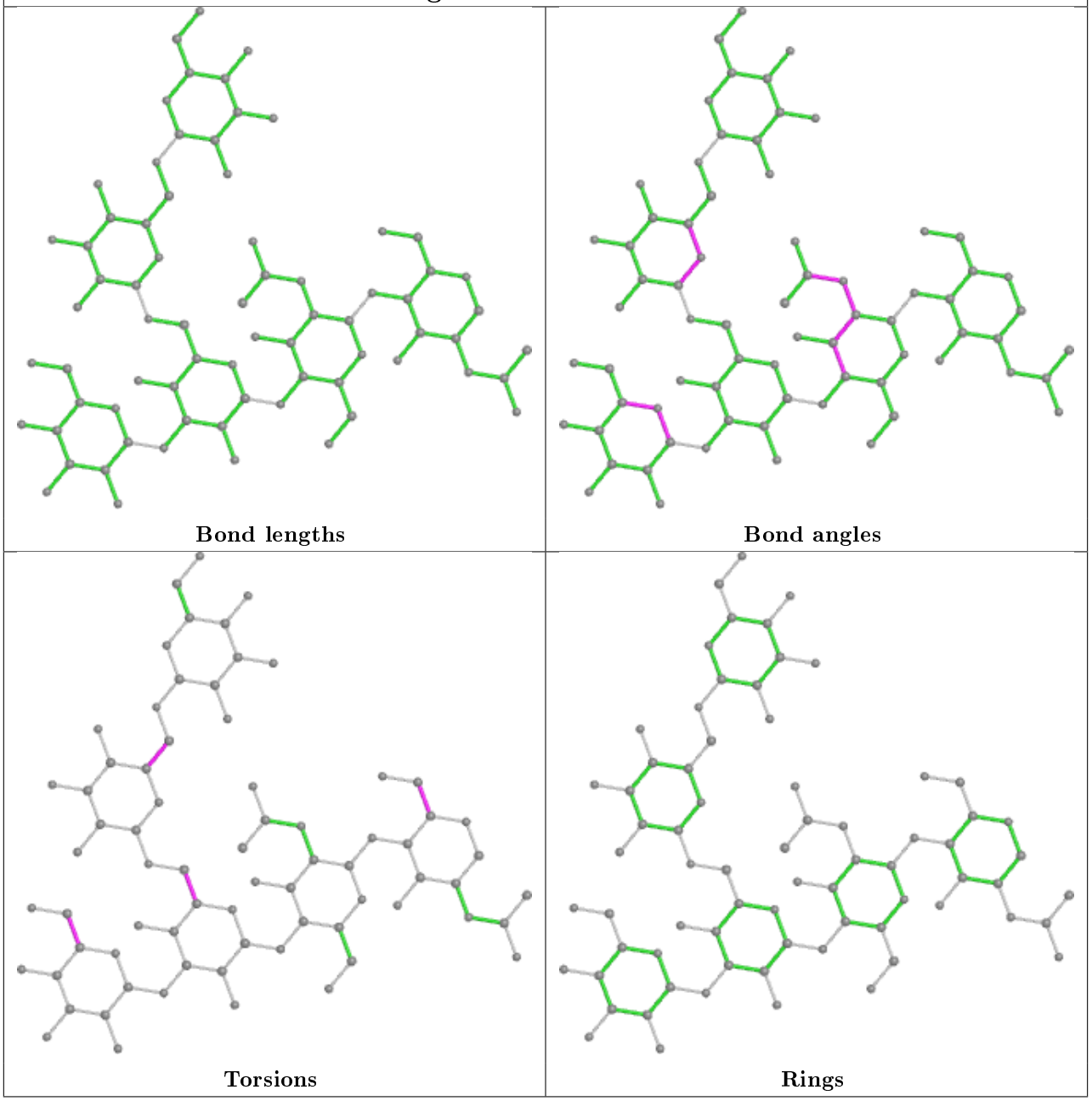


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	A	1361	1	14,14,15	0.57	0	17,19,21	0.72	1 (5%)
7	NAG	D	4371	1	14,14,15	0.53	0	17,19,21	0.64	0
7	NAG	C	3361	1	14,14,15	0.58	0	17,19,21	0.80	1 (5%)

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
7	NAG	A	1361	1	-	2/6/23/26	0/1/1/1
7	NAG	D	4371	1	-	2/6/23/26	0/1/1/1
7	NAG	C	3361	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	3361	NAG	C2-N2-C7	-2.41	119.48	122.90
7	A	1361	NAG	C2-N2-C7	-2.16	119.83	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	4371	NAG	O5-C5-C6-O6
7	D	4371	NAG	C4-C5-C6-O6
7	A	1361	NAG	C4-C5-C6-O6
7	C	3361	NAG	C4-C5-C6-O6
7	A	1361	NAG	O5-C5-C6-O6
7	C	3361	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.