Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 08:37 AM EDT

PDB ID	:	1ND6
Title	:	Crystal Structures of Human Prostatic Acid Phosphatase in Complex with a Phosphate Ion and alpha-Benzylaminobenzylphosphonic Acid Update the Mechanistic Picture and Offer New Insights into Inhibitor Design
Authors	:	Ortlund, E.; LaCount, M.W.; Lebioda, L.
Deposited on	:	2002-12-07
Resolution	:	2.40 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:

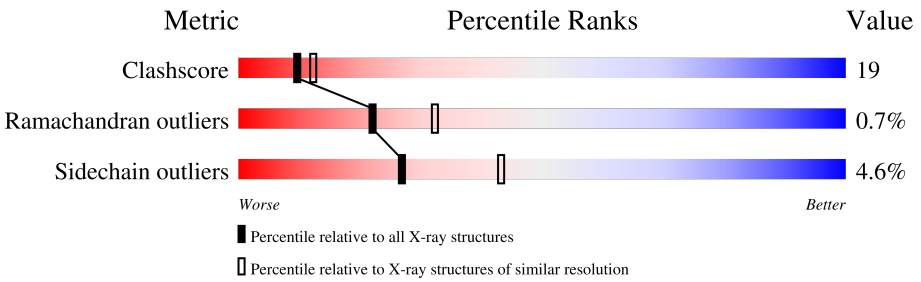
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	354	60% 34% • •
1	B	354	64% 30% • •
1	C	354	64% 31% • •
1	D	354	62% 31% • •
2	E	4	75% 25%
3	F	2	50% 50%
4	G	5	60% 20% 20%
5	H	3	33% 67%

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Mol	Chain	Length	Quality of chain
6	I	5	60% 40%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	E	2	X	-	-	-
2	MAN	E	4	X	-	-	-
3	NAG	F	2	X	-	-	-
4	NAG	G	1	X	-	-	-
4	MAN	G	4	X	-	-	-
4	MAN	G	5	X	-	-	-
5	NAG	H	1	X	-	-	-
5	NAG	H	2	X	-	-	-
5	MAN	H	3	X	-	-	-
6	NAG	I	1	X	-	-	-
9	NAG	B	5006	X	-	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 12048 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
			Total	C	N	O	S			
1	A	342	2800	1807	461	516	16	0	0	0
1	B	343	2807	1811	462	518	16	0	0	0
1	C	342	2800	1807	461	516	16	0	0	0
1	D	342	2800	1807	461	516	16	0	0	0

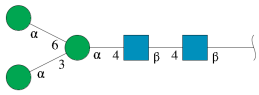
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	4	54	28	2	24	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

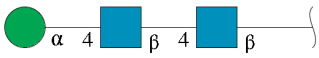
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	2	30	16	2	12	0	0	0

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



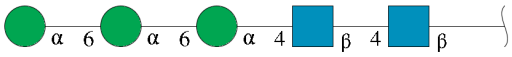
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	5	66	34	2	30	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



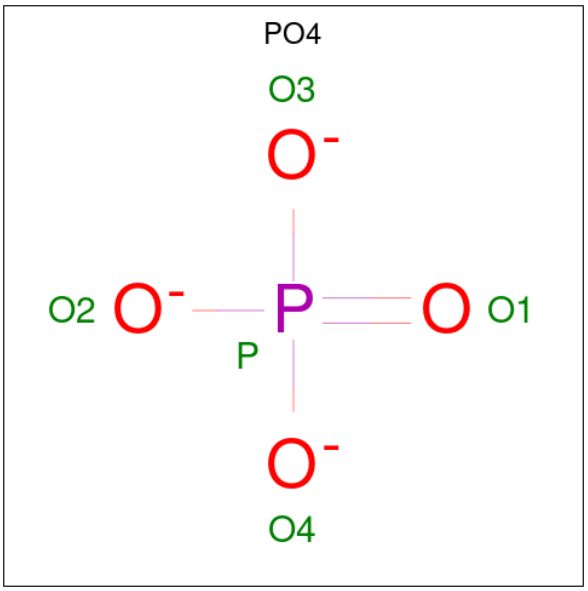
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	H	3	42	22	2	18	0	0	0

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



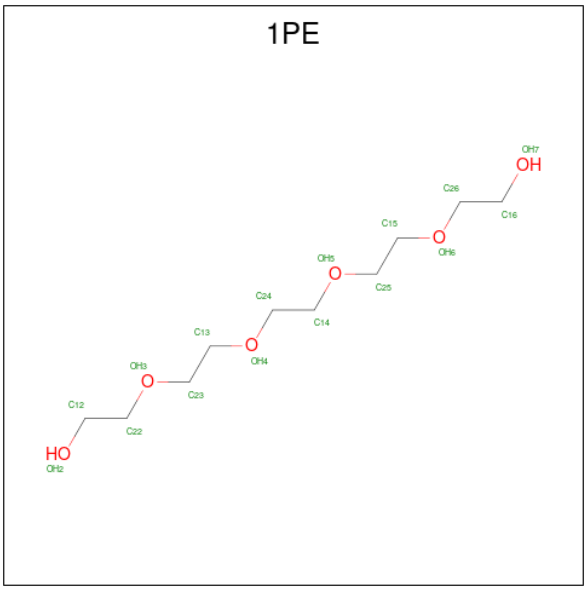
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	I	5	66	34	2	30	0	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



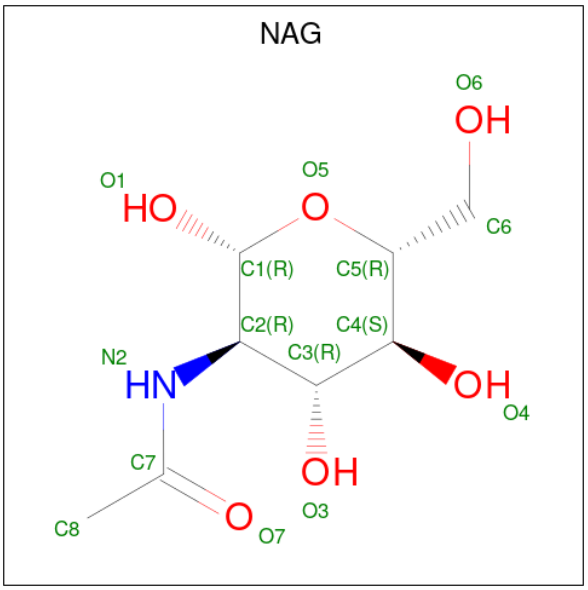
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O P 5 4 1	0	0
7	B	1	Total O P 5 4 1	0	0
7	C	1	Total O P 5 4 1	0	0
7	D	1	Total O P 5 4 1	0	0

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



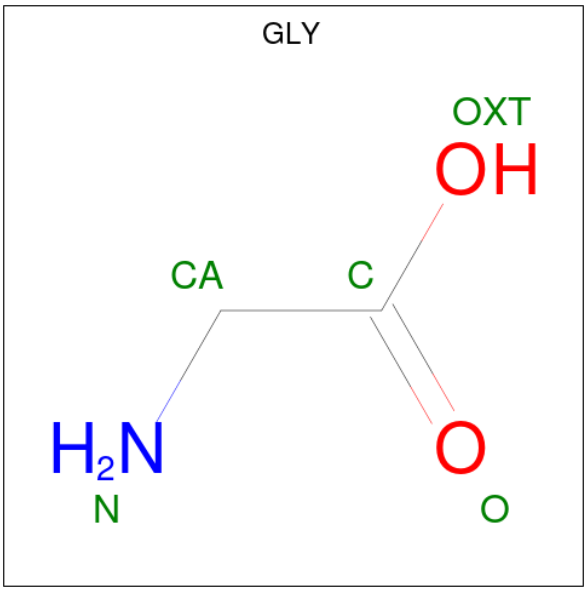
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
8	A	1	16	10	6		0	0
			Total	C	O			
8	B	1	16	10	6		0	0
			Total	C	O			
8	C	1	16	10	6		0	0
			Total	C	O			
8	D	1	16	10	6		0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	B	1	15	8	1	6	0	0
			Total	C	N	O		
9	D	1	15	8	1	6	0	0

- Molecule 10 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	B	1	5	2	1	2	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	147	147	147	0	0
			Total	O		
11	B	134	134	134	0	0
			Total	O		
11	C	89	89	89	0	0
			Total	O		
11	D	94	94	94	0	0

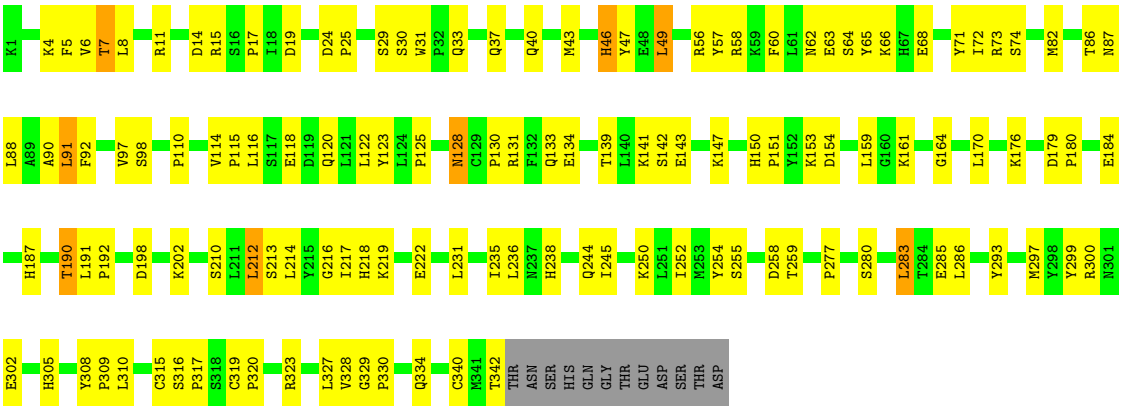
3 Residue-property plots (i)

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.

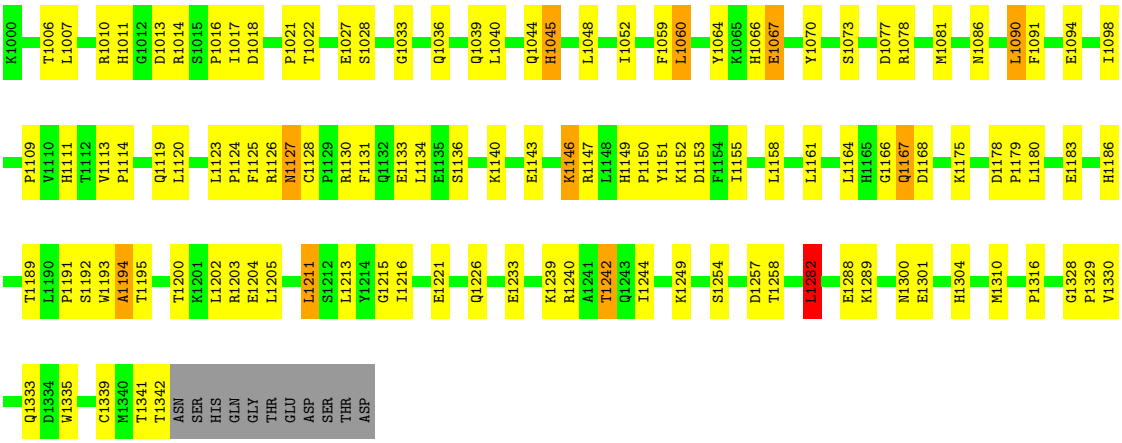
• Molecule 1: prostatic acid phosphatase

Chain A: 60% 34%



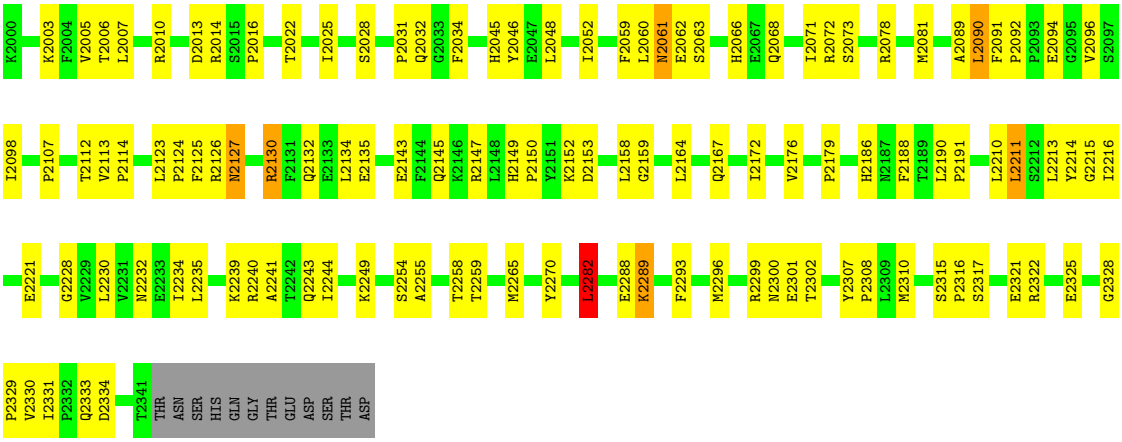
• Molecule 1: prostatic acid phosphatase

Chain B: 64% 30%



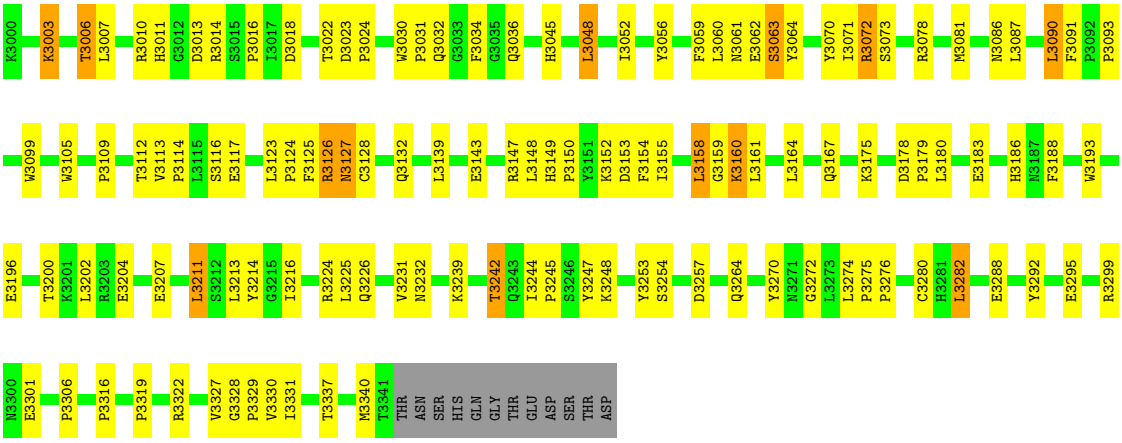
• Molecule 1: prostatic acid phosphatase

Chain C: 64% 31%



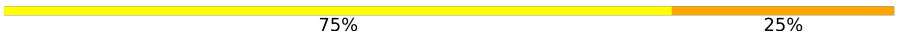
• Molecule 1: prostatic acid phosphatase

Chain D:



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

Chain E:



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

Chain F:

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

Chain G:

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

Chain H:

• Molecule 6: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-alpha-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	119.89Å 203.32Å 70.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.27 – 2.40	Depositor
% Data completeness (in resolution range)	90.6 (35.27-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12048	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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: PO4, NAG, MAN, 1PE

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	0.35	0/2882	0.59	0/3914
1	B	0.34	0/2889	0.60	1/3924 (0.0%)
1	C	0.34	0/2882	0.59	1/3914 (0.0%)
1	D	0.34	0/2882	0.59	0/3914
All	All	0.34	0/11535	0.59	2/15666 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2282	LEU	CA-CB-CG	5.93	128.95	115.30
1	B	1282	LEU	CA-CB-CG	5.68	128.36	115.30

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	2800	0	2749	110	0
1	B	2807	0	2753	122	0
1	C	2800	0	2747	115	0
1	D	2800	0	2746	118	0
2	E	54	0	47	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	30	0	27	1	0
4	G	66	0	57	2	0
5	H	42	0	37	4	0
6	I	66	0	59	1	0
7	A	5	0	0	1	0
7	B	5	0	0	1	0
7	C	5	0	0	1	0
7	D	5	0	0	1	0
8	A	16	0	22	1	0
8	B	16	0	22	3	0
8	C	16	0	22	2	0
8	D	16	0	22	2	0
9	B	15	0	14	1	0
9	D	15	0	14	0	0
10	B	5	0	2	3	0
11	A	147	0	0	7	0
11	B	134	0	0	9	0
11	C	89	0	0	3	0
11	D	94	0	0	4	0
All	All	12048	0	11340	445	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 19.

All (445) 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:B:1304:HIS:HB3	10:B:9000:GLY:OXT	1.47	1.12
1:B:1146:LYS:HE3	1:B:1146:LYS:HA	1.38	1.03
1:C:2310:MET:HE2	1:C:2315:SER:HA	1.45	0.98
1:B:1127:ASN:HD22	1:B:1127:ASN:H	1.02	0.97
1:C:2127:ASN:HD22	1:C:2127:ASN:H	1.07	0.97
1:A:128:ASN:H	1:A:128:ASN:HD22	1.04	0.97
1:A:125:PRO:HD3	1:A:259:THR:HG21	1.49	0.94
1:B:1125:PHE:H	1:B:1226:GLN:HE22	1.16	0.94
1:B:1158:LEU:HD21	1:B:1202:LEU:HD21	1.49	0.93
1:C:2307:TYR:CE1	5:H:1:NAG:O1	2.22	0.93
1:B:1304:HIS:CB	10:B:9000:GLY:OXT	2.18	0.92
1:D:3155:ILE:HG21	1:D:3167:GLN:HG3	1.52	0.91
1:D:3125:PHE:H	1:D:3226:GLN:HE22	1.21	0.84
1:B:1124:PRO:HD3	1:B:1258:THR:HG21	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2112:THR:HG22	1:D:3112:THR:HG22	1.61	0.82
1:D:3126:ARG:NH1	1:D:3132:GLN:HE22	1.78	0.81
1:B:1155:ILE:HG21	1:B:1167:GLN:HG3	1.62	0.80
1:D:3127:ASN:HD22	1:D:3127:ASN:H	1.31	0.79
1:C:2006:THR:HG22	11:C:4253:HOH:O	1.83	0.78
1:D:3032:GLN:HB3	1:D:3036:GLN:HG2	1.64	0.78
1:A:125:PRO:CD	1:A:259:THR:HG21	2.16	0.75
1:B:1127:ASN:H	1:B:1127:ASN:ND2	1.83	0.75
1:B:1134:LEU:HD11	1:B:1221:GLU:HG2	1.67	0.75
1:B:1186:HIS:HA	9:B:5006:NAG:H82	1.67	0.74
1:C:2310:MET:CE	1:C:2316:PRO:HD3	2.18	0.74
1:B:1149:HIS:HA	1:B:1152:LYS:HD3	1.70	0.74
1:B:1090:LEU:HD13	1:B:1091:PHE:CE1	2.23	0.74
1:C:2149:HIS:HB3	1:C:2150:PRO:HD3	1.70	0.73
2:E:1:NAG:H61	2:E:2:NAG:H82	1.71	0.73
1:B:1288:GLU:HG2	1:B:1289:LYS:HG3	1.70	0.73
1:C:2124:PRO:HD3	1:C:2258:THR:HG21	1.71	0.73
1:A:66:LYS:HE3	1:A:68:GLU:OE1	1.88	0.73
1:D:3056:TYR:HB3	1:D:3060:LEU:HD13	1.70	0.73
1:A:8:LEU:CD2	1:A:283:LEU:HD13	2.20	0.72
1:D:3160:LYS:HB2	1:D:3160:LYS:NZ	2.05	0.72
1:C:2310:MET:HE2	1:C:2316:PRO:HD3	1.70	0.72
1:D:3006:THR:HG22	11:D:4316:HOH:O	1.88	0.71
1:D:3018:ASP:OD2	1:D:3175:LYS:HE2	1.90	0.71
1:A:110:PRO:HD3	1:B:1081:MET:HE2	1.73	0.71
1:D:3007:LEU:HD22	1:D:3282:LEU:HD22	1.73	0.71
1:B:1124:PRO:CD	1:B:1258:THR:HG21	2.22	0.70
1:B:1077:ASP:HB3	1:B:1081:MET:HE3	1.72	0.70
1:C:2107:PRO:HG2	1:D:3081:MET:HE2	1.72	0.70
1:C:2127:ASN:H	1:C:2127:ASN:ND2	1.85	0.69
1:A:150:HIS:HB3	1:A:151:PRO:HD3	1.74	0.69
1:D:3149:HIS:HA	1:D:3152:LYS:HD3	1.75	0.68
1:C:2310:MET:CE	1:C:2315:SER:HA	2.20	0.68
1:A:342:THR:HG22	11:A:4199:HOH:O	1.93	0.68
1:B:1127:ASN:HD22	1:B:1127:ASN:N	1.81	0.68
1:A:128:ASN:HD22	1:A:128:ASN:N	1.80	0.68
1:A:180:PRO:O	1:A:184:GLU:HG2	1.93	0.68
1:C:2127:ASN:HD22	1:C:2127:ASN:N	1.79	0.68
1:B:1239:LYS:O	1:B:1242:THR:HG22	1.95	0.67
1:C:2159:GLY:HA2	1:C:2164:LEU:O	1.94	0.67
1:A:72:ILE:HD13	1:A:88:LEU:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1010:ARG:HD2	7:B:8001:PO4:O2	1.95	0.67
1:B:1164:LEU:CD1	1:B:1175:LYS:HD3	2.25	0.66
1:A:120:GLN:HB3	8:A:6000:1PE:H152	1.77	0.66
1:B:1192:SER:HA	11:B:4243:HOH:O	1.95	0.66
1:C:2066:HIS:HE1	1:D:3032:GLN:O	1.79	0.66
1:C:2300:ASN:OD1	1:C:2301:GLU:HG2	1.94	0.66
1:C:2124:PRO:CD	1:C:2258:THR:HG21	2.26	0.66
1:D:3301:GLU:OE2	6:I:1:NAG:O1	2.14	0.65
1:B:1178:ASP:HB3	1:B:1179:PRO:HD3	1.77	0.65
1:A:56:ARG:HG2	1:A:57:TYR:CE2	2.32	0.65
1:C:2007:LEU:CD2	1:C:2282:LEU:HD13	2.27	0.65
1:B:1007:LEU:CD2	1:B:1282:LEU:HD13	2.26	0.64
1:C:2123:LEU:O	1:C:2258:THR:HG21	1.97	0.64
1:A:164:GLY:HA2	1:D:3116:SER:HB3	1.78	0.64
1:D:3322:ARG:HH11	1:D:3322:ARG:HG2	1.63	0.64
1:A:8:LEU:HD22	1:A:283:LEU:HD13	1.78	0.64
1:C:2321:GLU:O	1:C:2325:GLU:HG3	1.97	0.64
1:A:190:THR:HG22	1:C:2243:GLN:HE22	1.62	0.64
1:B:1006:THR:HG22	11:B:4188:HOH:O	1.98	0.63
1:D:3179:PRO:O	1:D:3183:GLU:HG2	1.97	0.63
1:A:19:ASP:O	1:A:180:PRO:HG3	1.97	0.63
1:B:1119:GLN:HB3	8:B:7000:1PE:H251	1.80	0.63
1:B:1200:THR:HG23	1:B:1203:ARG:NH2	2.14	0.63
1:A:7:THR:HG22	11:A:4080:HOH:O	1.98	0.63
1:A:141:LYS:HD2	1:A:141:LYS:N	2.14	0.62
1:B:1329:PRO:HG2	11:B:4166:HOH:O	1.98	0.62
1:A:187:HIS:HA	2:E:1:NAG:H82	1.82	0.62
1:B:1304:HIS:CG	10:B:9000:GLY:OXT	2.51	0.62
1:A:98:SER:HA	1:B:1039:GLN:HE22	1.65	0.62
1:C:2010:ARG:HD2	7:C:8002:PO4:O3	1.99	0.62
1:D:3160:LYS:HB2	1:D:3160:LYS:HZ2	1.64	0.62
1:B:1007:LEU:HD13	1:B:1052:ILE:HD13	1.82	0.62
1:A:56:ARG:HG2	1:A:57:TYR:CD2	2.35	0.61
1:A:190:THR:HG23	1:C:2240:ARG:HG3	1.83	0.61
1:A:184:GLU:HG3	1:A:191:LEU:CD2	2.31	0.60
1:A:46:HIS:HD2	1:A:87:ASN:HD22	1.49	0.60
1:B:1021:PRO:CD	1:B:1164:LEU:HG	2.32	0.60
1:D:3337:THR:HA	1:D:3340:MET:HE2	1.83	0.60
1:A:191:LEU:HB3	1:A:192:PRO:HD2	1.84	0.60
1:A:323:ARG:HH11	1:A:323:ARG:HG2	1.65	0.60
1:C:2061:ASN:ND2	1:C:2062:GLU:HG3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:NAG:C6	2:E:2:NAG:H82	2.32	0.59
1:B:1077:ASP:HB3	1:B:1081:MET:CE	2.32	0.59
1:C:2003:LYS:HE3	1:C:2241:ALA:O	2.03	0.59
1:B:1022:THR:HG21	1:B:1161:LEU:O	2.02	0.59
1:C:2059:PHE:CZ	1:C:2249:LYS:HB3	2.38	0.59
1:D:3018:ASP:O	1:D:3179:PRO:HG3	2.02	0.59
1:A:128:ASN:H	1:A:128:ASN:ND2	1.86	0.58
1:D:3183:GLU:HB2	1:D:3188:PHE:HB2	1.86	0.58
1:D:3337:THR:HA	1:D:3340:MET:CE	2.33	0.58
1:A:11:ARG:HD2	7:A:8000:PO4:O3	2.03	0.58
1:D:3178:ASP:HB3	1:D:3179:PRO:HD3	1.83	0.58
1:A:161:LYS:HA	1:D:3116:SER:HB2	1.86	0.58
1:D:3299:ARG:HG3	1:D:3306:PRO:HG3	1.86	0.58
1:B:1127:ASN:HD21	8:B:7000:1PE:H131	1.69	0.58
1:B:1149:HIS:HB3	1:B:1150:PRO:HD3	1.86	0.57
1:B:1007:LEU:CD1	1:B:1052:ILE:HD13	2.34	0.57
1:A:179:ASP:HB3	1:A:180:PRO:HD3	1.87	0.57
1:B:1164:LEU:HD13	1:B:1175:LYS:HD3	1.87	0.57
1:D:3231:VAL:CG1	1:D:3327:VAL:HG11	2.34	0.57
1:B:1067:GLU:HB2	11:B:4134:HOH:O	2.04	0.57
1:C:2114:PRO:HD3	1:D:3113:VAL:HG22	1.87	0.57
1:A:11:ARG:HD3	1:A:258:ASP:HB3	1.87	0.57
1:C:2107:PRO:O	1:D:3081:MET:HE2	2.05	0.56
1:D:3006:THR:HB	11:D:4350:HOH:O	2.04	0.56
1:B:1010:ARG:HD3	1:B:1257:ASP:HB3	1.87	0.56
1:D:3007:LEU:CD2	1:D:3282:LEU:HD22	2.35	0.56
1:D:3207:GLU:HG3	1:D:3274:LEU:HG	1.87	0.56
1:A:114:VAL:HG13	1:A:115:PRO:HD2	1.88	0.56
1:B:1010:ARG:CD	1:B:1257:ASP:HB3	2.36	0.56
1:C:2006:THR:HB	11:C:4213:HOH:O	2.06	0.56
1:B:1125:PHE:N	1:B:1226:GLN:HE22	1.96	0.56
1:C:2006:THR:HG21	1:C:2234:ILE:HD13	1.88	0.56
1:C:2167:GLN:HG3	1:C:2167:GLN:O	2.06	0.56
1:B:1073:SER:HB2	1:B:1254:SER:HB3	1.87	0.55
1:A:143:GLU:O	1:A:147:LYS:HD3	2.06	0.55
1:C:2072:ARG:HG2	1:C:2073:SER:N	2.21	0.55
1:D:3060:LEU:N	1:D:3060:LEU:HD12	2.22	0.55
1:B:1180:LEU:HD23	1:B:1183:GLU:OE1	2.06	0.55
1:A:62:ASN:O	1:A:63:GLU:HG3	2.06	0.55
1:D:3010:ARG:HD2	7:D:8003:PO4:O2	2.07	0.55
1:A:49:LEU:HD13	1:A:87:ASN:ND2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PHE:CZ	1:A:250:LYS:HB3	2.41	0.55
1:D:3239:LYS:O	1:D:3242:THR:HB	2.07	0.55
1:B:1341:THR:HG23	1:B:1342:THR:H	1.72	0.54
1:D:3071:ILE:HD12	1:D:3071:ILE:N	2.22	0.54
1:B:1143:GLU:O	1:B:1147:ARG:HG3	2.08	0.54
1:D:3231:VAL:HG11	1:D:3327:VAL:CG1	2.38	0.54
1:A:11:ARG:HD3	1:A:258:ASP:CA	2.37	0.54
1:A:49:LEU:HD13	1:A:87:ASN:HD21	1.72	0.54
1:D:3224:ARG:HA	1:D:3330:VAL:O	2.07	0.54
1:C:2107:PRO:HG2	1:D:3081:MET:CE	2.38	0.54
1:D:3244:ILE:HG22	1:D:3245:PRO:O	2.08	0.54
1:A:115:PRO:HD3	1:B:1113:VAL:HG22	1.90	0.54
1:B:1153:ASP:HB3	11:B:4236:HOH:O	2.06	0.54
1:B:1200:THR:O	1:B:1204:GLU:HG3	2.08	0.54
1:D:3322:ARG:HG2	1:D:3322:ARG:NH1	2.23	0.54
1:D:3045:HIS:HD2	1:D:3086:ASN:HD22	1.56	0.53
1:B:1028:SER:HB2	11:B:4112:HOH:O	2.08	0.53
1:A:46:HIS:CD2	1:A:87:ASN:HD22	2.27	0.53
1:B:1123:LEU:O	1:B:1258:THR:HG21	2.08	0.53
1:C:2130:ARG:O	1:C:2134:LEU:HG	2.08	0.53
1:A:14:ASP:OD1	1:A:187:HIS:HE1	1.91	0.53
1:A:11:ARG:CD	1:A:258:ASP:HB3	2.39	0.53
1:C:2016:PRO:HG2	1:C:2034:PHE:CE2	2.43	0.53
1:D:3022:THR:HG21	11:D:4438:HOH:O	2.09	0.53
1:B:1136:SER:O	1:B:1140:LYS:HD3	2.08	0.53
1:B:1193:TRP:O	1:B:1195:THR:N	2.41	0.53
1:D:3010:ARG:HD3	1:D:3257:ASP:N	2.24	0.53
1:B:1040:LEU:O	1:B:1044:GLN:HG3	2.10	0.52
1:C:2210:LEU:HD23	1:C:2270:TYR:OH	2.09	0.52
1:C:2255:ALA:HB1	1:C:2259:THR:OG1	2.09	0.52
1:A:7:THR:HG21	1:A:235:ILE:HG12	1.91	0.52
1:B:1164:LEU:HD11	1:B:1175:LYS:HD3	1.90	0.52
1:D:3014:ARG:HG3	1:D:3014:ARG:HH11	1.75	0.52
1:C:2031:PRO:HB2	1:C:2032:GLN:NE2	2.25	0.52
1:D:3016:PRO:HG2	1:D:3034:PHE:CE2	2.43	0.52
4:G:2:NAG:O3	4:G:3:MAN:H2	2.09	0.52
1:A:11:ARG:HD3	1:A:258:ASP:N	2.24	0.52
1:B:1014:ARG:HD3	1:B:1078:ARG:CD	2.40	0.52
1:C:2124:PRO:HD3	1:C:2258:THR:CG2	2.39	0.52
1:C:2211:LEU:HD12	1:C:2216:ILE:HG12	1.91	0.52
1:D:3011:HIS:CE1	1:D:3078:ARG:HD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PRO:O	1:A:134:GLU:HG3	2.10	0.52
1:C:2014:ARG:HD3	1:C:2078:ARG:CD	2.40	0.52
1:C:2176:VAL:C	1:C:2179:PRO:HD2	2.31	0.52
1:D:3159:GLY:HA2	1:D:3164:LEU:O	2.09	0.52
1:B:1081:MET:HE3	11:B:4100:HOH:O	2.10	0.51
1:B:1126:ARG:NH1	1:B:1126:ARG:HG2	2.25	0.51
1:C:2006:THR:HG21	1:C:2234:ILE:CD1	2.40	0.51
1:A:216:GLY:O	1:A:217:ILE:HB	2.10	0.51
1:C:2211:LEU:HD12	1:C:2216:ILE:CD1	2.40	0.51
1:B:1045:HIS:HD2	1:B:1086:ASN:HD22	1.57	0.51
1:A:213:SER:HA	1:A:217:ILE:HD12	1.92	0.51
1:D:3073:SER:HB2	1:D:3254:SER:HB3	1.93	0.51
1:B:1211:LEU:HD12	1:B:1216:ILE:CD1	2.41	0.51
1:C:2158:LEU:CD1	1:C:2172:ILE:HD12	2.40	0.51
1:C:2061:ASN:HD22	1:C:2062:GLU:N	2.08	0.51
1:A:114:VAL:HG22	1:B:1114:PRO:HD3	1.93	0.50
1:A:329:GLY:N	1:A:330:PRO:HD2	2.27	0.50
1:B:1007:LEU:HD22	1:B:1282:LEU:HD13	1.92	0.50
1:B:1018:ASP:O	1:B:1179:PRO:HG3	2.11	0.50
1:C:2123:LEU:O	1:C:2258:THR:CG2	2.60	0.50
1:C:2073:SER:HB2	1:C:2254:SER:HB3	1.92	0.50
1:D:3127:ASN:HD21	8:D:7002:1PE:H131	1.75	0.50
1:C:2007:LEU:HD22	1:C:2282:LEU:HD13	1.93	0.50
1:C:2211:LEU:HD12	1:C:2216:ILE:HD11	1.94	0.50
1:D:3200:THR:O	1:D:3204:GLU:HG3	2.12	0.50
1:B:1288:GLU:OE2	1:B:1289:LYS:HE2	2.12	0.50
1:C:2145:GLN:NE2	1:C:2145:GLN:HA	2.26	0.50
1:D:3003:LYS:HG3	1:D:3292:TYR:HE2	1.76	0.50
1:B:1191:PRO:HG2	1:B:1194:ALA:HB2	1.94	0.49
1:C:2232:ASN:HD22	1:C:2331:ILE:HD13	1.77	0.49
1:D:3139:LEU:HD11	11:D:4332:HOH:O	2.11	0.49
1:D:3158:LEU:HD11	1:D:3202:LEU:HD21	1.94	0.49
1:B:1333:GLN:HE21	1:B:1333:GLN:HA	1.77	0.49
1:D:3282:LEU:N	1:D:3282:LEU:HD23	2.26	0.49
1:D:3319:PRO:HG2	1:D:3322:ARG:HB3	1.93	0.49
1:B:1133:GLU:OE1	1:B:1341:THR:OG1	2.30	0.49
1:C:2149:HIS:HA	1:C:2152:LYS:CD	2.43	0.49
1:B:1022:THR:CG2	1:B:1022:THR:O	2.60	0.49
1:D:3327:VAL:O	1:D:3330:VAL:HG22	2.12	0.49
1:B:1341:THR:OG1	1:B:1342:THR:N	2.46	0.49
1:D:3264:GLN:HE21	1:D:3270:TYR:HD1	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2063:SER:HB3	11:C:4428:HOH:O	2.13	0.49
1:D:3270:TYR:CE2	1:D:3272:GLY:HA2	2.47	0.49
1:B:1211:LEU:HD12	1:B:1216:ILE:HD11	1.95	0.49
1:C:2130:ARG:HD3	1:C:2221:GLU:OE2	2.13	0.49
1:C:2158:LEU:HD12	1:C:2172:ILE:HD12	1.93	0.49
1:D:3127:ASN:H	1:D:3127:ASN:ND2	2.05	0.49
1:A:190:THR:HG22	1:C:2243:GLN:NE2	2.26	0.49
1:D:3231:VAL:HG11	1:D:3327:VAL:HG11	1.94	0.49
1:B:1240:ARG:HB3	1:B:1244:ILE:HD12	1.95	0.48
1:A:125:PRO:HD3	1:A:259:THR:CG2	2.34	0.48
1:B:1200:THR:HG23	1:B:1203:ARG:HH22	1.76	0.48
1:B:1130:ARG:HB3	1:B:1339:CYS:HA	1.95	0.48
1:D:3016:PRO:HB3	1:D:3179:PRO:HA	1.95	0.48
1:D:3124:PRO:HB3	1:D:3213:LEU:HD21	1.95	0.48
1:A:202:LYS:HE3	11:A:4040:HOH:O	2.12	0.48
11:A:4130:HOH:O	1:B:1066:HIS:HB3	2.13	0.48
1:B:1127:ASN:ND2	8:B:7000:1PE:H131	2.28	0.48
1:C:2125:PHE:CD1	8:C:7001:1PE:H241	2.48	0.48
1:D:3161:LEU:HD13	1:D:3193:TRP:CB	2.43	0.48
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.78	0.48
1:A:212:LEU:HD13	1:A:212:LEU:O	2.14	0.48
1:A:283:LEU:O	1:A:297:MET:HA	2.13	0.48
1:C:2132:GLN:HA	1:C:2132:GLN:NE2	2.28	0.48
1:C:2228:GLY:HA3	1:C:2330:VAL:O	2.13	0.48
11:A:4285:HOH:O	8:C:7001:1PE:H152	2.14	0.48
1:B:1149:HIS:HA	1:B:1152:LYS:CD	2.42	0.48
1:D:3149:HIS:HB3	1:D:3150:PRO:HD3	1.94	0.48
1:B:1021:PRO:HD2	1:B:1164:LEU:HG	1.96	0.48
1:C:2081:MET:HE2	1:D:3109:PRO:HD3	1.95	0.47
1:D:3070:TYR:HB2	1:D:3248:LYS:HE2	1.96	0.47
1:A:245:ILE:HG23	1:A:245:ILE:O	2.14	0.47
1:C:2149:HIS:HA	1:C:2152:LYS:HE3	1.97	0.47
1:D:3328:GLY:N	1:D:3329:PRO:HD2	2.29	0.47
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.79	0.47
1:A:302:GLU:OE2	1:A:305:HIS:HD2	1.98	0.47
1:B:1341:THR:HG23	1:B:1342:THR:N	2.30	0.47
1:D:3114:PRO:HG2	1:D:3117:GLU:HB2	1.96	0.47
1:A:47:TYR:CD1	1:A:90:ALA:HB2	2.48	0.47
1:C:2013:ASP:OD1	1:C:2186:HIS:HE1	1.97	0.47
1:C:2081:MET:CE	1:D:3109:PRO:HD3	2.45	0.47
1:C:2288:GLU:O	1:C:2289:LYS:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2310:MET:HE3	1:C:2316:PRO:HD3	1.92	0.47
1:D:3090:LEU:HD13	1:D:3091:PHE:CE1	2.49	0.47
1:A:277:PRO:HD2	1:A:280:SER:HB3	1.97	0.47
1:C:2123:LEU:C	1:C:2258:THR:HG21	2.35	0.47
1:C:2127:ASN:ND2	1:C:2127:ASN:N	2.52	0.47
1:C:2299:ARG:NH2	1:C:2302:THR:HG22	2.29	0.47
1:A:97:VAL:O	1:B:1039:GLN:NE2	2.48	0.46
1:C:2176:VAL:O	1:C:2179:PRO:HD2	2.15	0.46
4:G:2:NAG:H4	4:G:3:MAN:O2	2.15	0.46
1:C:2113:VAL:HG22	1:D:3114:PRO:HD3	1.95	0.46
1:C:2126:ARG:NH1	1:C:2126:ARG:HG2	2.30	0.46
1:D:3148:LEU:HD21	1:D:3167:GLN:HE21	1.80	0.46
1:A:118:GLU:CG	1:D:3160:LYS:HE3	2.45	0.46
1:A:131:ARG:HD3	1:A:222:GLU:OE2	2.15	0.46
1:A:58:ARG:HG2	1:A:58:ARG:NH1	2.30	0.46
1:A:190:THR:HG21	1:C:2239:LYS:HB3	1.97	0.46
1:B:1113:VAL:HG13	1:B:1114:PRO:HD2	1.97	0.46
1:B:1128:CYS:HB2	1:B:1335:TRP:CZ2	2.51	0.46
1:C:2090:LEU:HD13	1:C:2091:PHE:CE1	2.50	0.46
1:C:2149:HIS:HA	1:C:2152:LYS:CE	2.46	0.46
1:B:1123:LEU:O	1:B:1258:THR:CG2	2.64	0.46
1:B:1151:TYR:CG	1:B:1205:LEU:HD21	2.51	0.46
1:C:2215:GLY:O	1:C:2216:ILE:HB	2.16	0.46
1:B:1126:ARG:HG2	1:B:1126:ARG:HH11	1.81	0.46
1:A:74:SER:HB2	1:A:255:SER:HB3	1.98	0.46
1:A:139:THR:O	1:A:142:SER:HB3	2.15	0.46
1:C:2333:GLN:HA	1:C:2333:GLN:NE2	2.30	0.46
1:D:3014:ARG:HD3	1:D:3078:ARG:CD	2.46	0.46
1:A:43:MET:O	1:A:86:THR:HG21	2.15	0.46
1:C:2016:PRO:HG2	1:C:2034:PHE:CD2	2.50	0.46
1:C:2068:GLN:OE1	1:C:2249:LYS:HE2	2.16	0.46
1:D:3232:ASN:HB2	1:D:3331:ILE:HG23	1.96	0.46
1:A:116:LEU:HD22	1:A:123:TYR:CE1	2.51	0.46
1:A:299:TYR:HB2	1:A:310:LEU:HD11	1.98	0.46
1:B:1147:ARG:CZ	1:B:1216:ILE:HD12	2.45	0.46
1:C:2190:LEU:HB3	1:C:2191:PRO:HD2	1.98	0.46
1:A:190:THR:HG21	1:C:2239:LYS:CB	2.47	0.45
1:B:1016:PRO:HB3	1:B:1179:PRO:HA	1.98	0.45
1:B:1215:GLY:O	1:B:1216:ILE:HB	2.16	0.45
1:C:2061:ASN:HD22	1:C:2062:GLU:H	1.64	0.45
1:C:2071:ILE:HD12	1:C:2071:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PHE:CZ	1:A:238:HIS:HB3	2.51	0.45
1:D:3022:THR:HG21	1:D:3161:LEU:O	2.17	0.45
1:A:82:MET:HE2	1:B:1109:PRO:HD3	1.99	0.45
1:B:1010:ARG:HD3	1:B:1257:ASP:CA	2.47	0.45
1:A:286:LEU:HD11	1:A:293:TYR:HB3	1.98	0.45
1:B:1123:LEU:N	1:B:1123:LEU:HD12	2.32	0.45
1:D:3126:ARG:HH12	1:D:3132:GLN:HE22	1.60	0.45
1:B:1011:HIS:CE1	1:B:1078:ARG:HD2	2.52	0.45
1:B:1017:ILE:HD11	1:B:1078:ARG:NH2	2.32	0.45
1:D:3059:PHE:C	1:D:3060:LEU:HD12	2.37	0.45
1:D:3126:ARG:HH11	1:D:3132:GLN:HE22	1.61	0.45
1:B:1036:GLN:HE22	1:B:1077:ASP:CB	2.30	0.45
1:A:4:LYS:HD3	1:A:293:TYR:HE2	1.82	0.45
1:A:46:HIS:HD2	1:A:87:ASN:HB2	1.82	0.45
1:C:2214:TYR:HB2	1:C:2265:MET:HG3	1.98	0.45
1:A:114:VAL:CG1	1:A:115:PRO:HD2	2.46	0.45
1:C:2010:ARG:O	1:C:2045:HIS:HE1	2.00	0.45
1:C:2288:GLU:O	1:C:2289:LYS:HG3	2.17	0.45
1:A:222:GLU:HB2	11:A:4207:HOH:O	2.16	0.44
1:D:3048:LEU:HD13	1:D:3086:ASN:HD21	1.82	0.44
2:E:3:MAN:H61	2:E:4:MAN:H2	1.76	0.44
1:D:3125:PHE:CD1	8:D:7002:1PE:H132	2.52	0.44
1:A:19:ASP:OD2	1:A:176:LYS:HG2	2.17	0.44
1:D:3010:ARG:O	1:D:3045:HIS:HE1	1.99	0.44
1:D:3093:PRO:HG3	1:D:3105:TRP:N	2.32	0.44
1:A:213:SER:CA	1:A:217:ILE:HD12	2.48	0.44
1:B:1021:PRO:HD3	1:B:1164:LEU:HG	2.00	0.44
1:C:2061:ASN:HD22	1:C:2061:ASN:N	2.16	0.44
1:D:3154:PHE:O	1:D:3158:LEU:HB2	2.18	0.44
1:D:3244:ILE:O	1:D:3247:TYR:HB2	2.18	0.44
1:A:17:PRO:HD2	1:A:31:TRP:CE2	2.52	0.44
1:B:1014:ARG:HG3	1:B:1014:ARG:HH11	1.82	0.44
1:B:1120:LEU:HD11	1:B:1233:GLU:HB2	1.99	0.44
1:D:3207:GLU:CG	1:D:3274:LEU:HG	2.47	0.44
1:D:3213:LEU:HD22	1:D:3214:TYR:CE2	2.52	0.44
1:A:30:SER:HB3	1:C:2244:ILE:HG21	1.99	0.44
1:C:2014:ARG:HG3	1:C:2014:ARG:HH11	1.83	0.44
1:A:66:LYS:HB3	1:A:68:GLU:OE1	2.18	0.44
1:B:1124:PRO:HD3	1:B:1258:THR:CG2	2.38	0.44
1:A:11:ARG:HD3	1:A:258:ASP:CB	2.47	0.44
1:A:122:LEU:HD11	1:A:254:TYR:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:HIS:HA	1:A:153:LYS:HE3	1.99	0.44
1:B:1094:GLU:HA	1:B:1098:ILE:HD11	2.00	0.43
1:C:2282:LEU:O	1:C:2296:MET:HA	2.18	0.43
1:D:3180:LEU:HD23	1:D:3183:GLU:OE1	2.17	0.43
1:B:1211:LEU:HD12	1:B:1216:ILE:HG12	2.00	0.43
1:D:3113:VAL:HG13	1:D:3114:PRO:HD2	2.00	0.43
1:D:3127:ASN:HD22	1:D:3127:ASN:N	1.96	0.43
1:A:19:ASP:OD2	1:A:176:LYS:HE2	2.18	0.43
1:C:2094:GLU:HA	1:C:2098:ILE:HD11	2.00	0.43
1:D:3062:GLU:O	1:D:3063:SER:C	2.57	0.43
1:D:3143:GLU:O	1:D:3147:ARG:HG3	2.18	0.43
1:D:3032:GLN:CB	1:D:3036:GLN:HG2	2.40	0.43
1:D:3280:CYS:SG	1:D:3282:LEU:CD2	3.07	0.43
5:H:2:NAG:H62	5:H:3:MAN:H62	2.00	0.43
1:A:33:GLN:HB3	1:A:37:GLN:HG2	2.01	0.43
1:C:2022:THR:O	1:C:2022:THR:CG2	2.67	0.43
1:D:3007:LEU:CD1	1:D:3052:ILE:HD13	2.48	0.43
1:D:3123:LEU:N	1:D:3123:LEU:HD12	2.33	0.43
1:C:2211:LEU:HD12	1:C:2216:ILE:CG1	2.47	0.43
1:D:3071:ILE:HG12	1:D:3087:LEU:HD11	2.01	0.43
1:D:3211:LEU:HD13	1:D:3211:LEU:O	2.18	0.43
1:A:334:GLN:NE2	1:A:334:GLN:HA	2.34	0.43
1:B:1010:ARG:HD3	1:B:1257:ASP:N	2.34	0.43
1:C:2123:LEU:N	1:C:2123:LEU:HD12	2.33	0.43
1:D:3023:ASP:HA	1:D:3024:PRO:HD3	1.85	0.43
1:D:3059:PHE:CD2	1:D:3060:LEU:CD1	3.02	0.43
1:C:2132:GLN:NE2	1:C:2135:GLU:OE2	2.52	0.43
1:C:2288:GLU:HB3	1:C:2293:PHE:CE1	2.54	0.43
1:A:71:TYR:O	1:A:252:ILE:HA	2.19	0.42
1:C:2149:HIS:HA	1:C:2152:LYS:HD2	2.01	0.42
1:D:3013:ASP:OD1	1:D:3186:HIS:HE1	2.02	0.42
1:A:131:ARG:HB3	1:A:340:CYS:HA	2.01	0.42
1:D:3061:ASN:C	1:D:3062:GLU:HG3	2.39	0.42
1:A:258:ASP:OD2	1:A:259:THR:N	2.53	0.42
1:A:308:TYR:CE1	3:F:1:NAG:H1	2.55	0.42
1:B:1328:GLY:N	1:B:1329:PRO:HD2	2.35	0.42
1:B:1060:LEU:HA	11:B:4125:HOH:O	2.18	0.42
1:C:2005:VAL:HG12	1:C:2059:PHE:HE2	1.83	0.42
1:C:2096:VAL:HG22	1:C:2096:VAL:O	2.18	0.42
1:C:2143:GLU:O	1:C:2147:ARG:HG3	2.19	0.42
1:D:3128:CYS:SG	1:D:3225:LEU:HD13	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:SER:HB2	1:A:317:PRO:HD2	2.00	0.42
1:B:1123:LEU:C	1:B:1258:THR:HG21	2.39	0.42
1:C:2172:ILE:O	1:C:2176:VAL:HB	2.20	0.42
1:C:2322:ARG:HD2	1:C:2322:ARG:HA	1.85	0.42
1:C:2089:ALA:O	1:C:2092:PRO:HD3	2.20	0.42
1:C:2300:ASN:OD1	5:H:1:NAG:O1	2.36	0.42
1:A:218:HIS:CE1	1:A:219:LYS:HZ2	2.37	0.42
1:B:1330:VAL:HG13	11:B:4166:HOH:O	2.19	0.42
1:A:118:GLU:HG3	1:D:3160:LYS:HE3	2.01	0.41
1:A:319:CYS:HA	1:A:320:PRO:HD2	1.97	0.41
1:D:3016:PRO:HD2	1:D:3030:TRP:CE2	2.55	0.41
1:D:3072:ARG:O	1:D:3253:TYR:HA	2.20	0.41
1:D:3164:LEU:HD11	1:D:3175:LYS:HB3	2.01	0.41
1:D:3275:PRO:HA	1:D:3276:PRO:HD3	1.85	0.41
1:A:198:ASP:HB2	11:A:4056:HOH:O	2.19	0.41
1:B:1059:PHE:CZ	1:B:1249:LYS:HD2	2.55	0.41
1:C:2328:GLY:N	1:C:2329:PRO:HD2	2.35	0.41
1:B:1155:ILE:HG21	1:B:1167:GLN:CG	2.41	0.41
1:B:1341:THR:CG2	1:B:1342:THR:H	2.30	0.41
1:A:24:ASP:HA	1:A:25:PRO:HD3	1.94	0.41
1:D:3211:LEU:HD12	1:D:3216:ILE:HG12	2.02	0.41
1:A:308:TYR:HA	1:A:309:PRO:HD3	1.94	0.41
1:A:315:CYS:HB2	1:A:327:LEU:CD1	2.51	0.41
1:B:1027:GLU:HG3	1:B:1033:GLY:HA2	2.02	0.41
1:B:1189:THR:HG23	1:B:1189:THR:O	2.20	0.41
1:C:2046:TYR:CD1	1:D:3099:TRP:HH2	2.38	0.41
1:B:1191:PRO:HG2	1:B:1194:ALA:CB	2.50	0.41
1:B:1013:ASP:OD1	1:B:1186:HIS:HE1	2.03	0.41
1:C:2307:TYR:CD1	5:H:1:NAG:O1	2.68	0.41
1:D:3125:PHE:N	1:D:3226:GLN:HE22	2.02	0.41
1:B:1134:LEU:CD1	1:B:1221:GLU:HG2	2.42	0.41
1:B:1146:LYS:HA	1:B:1146:LYS:CE	2.24	0.41
1:B:1300:ASN:OD1	1:B:1301:GLU:HG2	2.20	0.41
1:C:2061:ASN:HD21	1:C:2062:GLU:HG3	1.84	0.41
1:C:2288:GLU:HB3	1:C:2293:PHE:HE1	1.86	0.41
1:C:2307:TYR:HA	1:C:2308:PRO:HD3	1.94	0.41
1:A:91:LEU:HD22	1:A:92:PHE:CE2	2.56	0.41
1:B:1166:GLY:C	1:B:1168:ASP:H	2.24	0.41
1:D:3245:PRO:C	1:D:3247:TYR:H	2.24	0.41
1:D:3295:GLU:HG2	1:D:3316:PRO:O	2.21	0.41
1:A:6:VAL:HG22	1:A:285:GLU:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HB3	1:A:210:SER:HB2	2.03	0.41
1:B:1070:TYR:CE1	1:B:1111:HIS:CD2	3.09	0.41
1:C:2007:LEU:HD13	1:C:2052:ILE:HD13	2.03	0.41
1:D:3126:ARG:NH1	1:D:3132:GLN:NE2	2.59	0.41
1:B:1301:GLU:OE2	1:B:1304:HIS:HD2	2.04	0.40
1:B:1333:GLN:HA	1:B:1333:GLN:NE2	2.36	0.40
1:D:3127:ASN:ND2	1:D:3127:ASN:N	2.66	0.40
1:A:110:PRO:HD3	1:B:1081:MET:CE	2.48	0.40
1:D:3030:TRP:HA	1:D:3031:PRO:HD3	1.85	0.40
1:C:2022:THR:O	1:C:2022:THR:HG22	2.20	0.40
1:C:2126:ARG:HG2	1:C:2126:ARG:HH11	1.86	0.40
1:A:5:PHE:HZ	1:A:252:ILE:HD12	1.85	0.40
1:A:11:ARG:O	1:A:46:HIS:HE1	2.04	0.40
1:B:1211:LEU:O	1:B:1211:LEU:HD13	2.21	0.40
1:B:1310:MET:HE2	1:B:1316:PRO:HG3	2.04	0.40
1:C:2025:ILE:HD13	1:C:2188:PHE:CD1	2.57	0.40
1:D:3213:LEU:HD22	1:D:3214:TYR:CD2	2.57	0.40
1:A:11:ARG:HD2	1:A:11:ARG:HH11	1.78	0.40
1:A:159:LEU:C	1:A:159:LEU:HD13	2.42	0.40
1:B:1131:PHE:HZ	1:B:1213:LEU:HD23	1.85	0.40
1:C:2061:ASN:ND2	1:C:2062:GLU:N	2.68	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	340/354 (96%)	319 (94%)	19 (6%)	2 (1%)	25 36
1	B	341/354 (96%)	311 (91%)	28 (8%)	2 (1%)	25 36
1	C	340/354 (96%)	310 (91%)	28 (8%)	2 (1%)	25 36
1	D	340/354 (96%)	318 (94%)	19 (6%)	3 (1%)	17 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1361/1416 (96%)	1258 (92%)	94 (7%)	9 (1%)	22	32

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	SER
1	B	1064	TYR
1	C	2289	LYS
1	D	3064	TYR
1	A	65	TYR
1	D	3063	SER
1	C	2334	ASP
1	D	3288	GLU
1	B	1194	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	314/325 (97%)	295 (94%)	19 (6%)	18	30
1	B	315/325 (97%)	304 (96%)	11 (4%)	36	55
1	C	314/325 (97%)	300 (96%)	14 (4%)	27	44
1	D	314/325 (97%)	300 (96%)	14 (4%)	27	44
All	All	1257/1300 (97%)	1199 (95%)	58 (5%)	27	43

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	29	SER
1	A	40	GLN
1	A	46	HIS
1	A	49	LEU
1	A	73	ARG

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Mol	Chain	Res	Type
1	A	91	LEU
1	A	128	ASN
1	A	133	GLN
1	A	154	ASP
1	A	190	THR
1	A	212	LEU
1	A	214	LEU
1	A	231	LEU
1	A	236	LEU
1	A	244	GLN
1	A	283	LEU
1	A	300	ARG
1	A	328	VAL
1	B	1045	HIS
1	B	1048	LEU
1	B	1060	LEU
1	B	1067	GLU
1	B	1090	LEU
1	B	1127	ASN
1	B	1146	LYS
1	B	1167	GLN
1	B	1211	LEU
1	B	1242	THR
1	B	1282	LEU
1	C	2028	SER
1	C	2048	LEU
1	C	2060	LEU
1	C	2061	ASN
1	C	2090	LEU
1	C	2127	ASN
1	C	2130	ARG
1	C	2153	ASP
1	C	2211	LEU
1	C	2213	LEU
1	C	2230	LEU
1	C	2235	LEU
1	C	2282	LEU
1	C	2317	SER
1	D	3003	LYS
1	D	3006	THR
1	D	3048	LEU
1	D	3072	ARG

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Mol	Chain	Res	Type
1	D	3090	LEU
1	D	3126	ARG
1	D	3127	ASN
1	D	3153	ASP
1	D	3158	LEU
1	D	3160	LYS
1	D	3196	GLU
1	D	3211	LEU
1	D	3242	THR
1	D	3282	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	46	HIS
1	A	128	ASN
1	A	146	GLN
1	A	168	GLN
1	A	187	HIS
1	A	233	ASN
1	A	244	GLN
1	A	265	GLN
1	A	305	HIS
1	A	334	GLN
1	B	1036	GLN
1	B	1039	GLN
1	B	1045	HIS
1	B	1127	ASN
1	B	1145	GLN
1	B	1186	HIS
1	B	1226	GLN
1	B	1232	ASN
1	B	1264	GLN
1	B	1303	GLN
1	B	1304	HIS
1	B	1333	GLN
1	C	2032	GLN
1	C	2039	GLN
1	C	2061	ASN
1	C	2066	HIS
1	C	2086	ASN

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Mol	Chain	Res	Type
1	C	2127	ASN
1	C	2145	GLN
1	C	2186	HIS
1	C	2232	ASN
1	C	2264	GLN
1	C	2303	GLN
1	C	2304	HIS
1	C	2333	GLN
1	D	3036	GLN
1	D	3086	ASN
1	D	3127	ASN
1	D	3132	GLN
1	D	3167	GLN
1	D	3186	HIS
1	D	3226	GLN
1	D	3232	ASN
1	D	3264	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)

19 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	2,1	15,15,15	0.48	0	21,21,21	0.98	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	2	2	15,15,15	0.51	0	21,21,21	0.57	0
2	MAN	E	3	2	12,12,12	0.50	0	17,17,17	0.45	0
2	MAN	E	4	2	12,12,12	0.40	0	17,17,17	0.62	0
3	NAG	F	1	3,1	15,15,15	0.41	0	21,21,21	0.91	2 (9%)
3	NAG	F	2	3	15,15,15	0.41	0	21,21,21	0.62	0
4	NAG	G	1	4,1	15,15,15	0.48	0	21,21,21	0.72	0
4	NAG	G	2	4	15,15,15	0.59	0	21,21,21	0.98	1 (4%)
4	MAN	G	3	4	12,12,12	0.51	0	17,17,17	0.61	0
4	MAN	G	4	4	12,12,12	0.39	0	17,17,17	0.43	0
4	MAN	G	5	4	12,12,12	0.40	0	17,17,17	0.39	0
5	NAG	H	1	5,1	15,15,15	0.53	0	21,21,21	1.18	2 (9%)
5	NAG	H	2	5	15,15,15	0.81	0	21,21,21	1.31	2 (9%)
5	MAN	H	3	5	12,12,12	0.50	0	17,17,17	0.39	0
6	NAG	I	1	6,1	15,15,15	0.44	0	21,21,21	0.65	0
6	NAG	I	2	6	15,15,15	0.46	0	21,21,21	0.98	1 (4%)
6	MAN	I	3	6	12,12,12	0.46	0	17,17,17	0.46	0
6	MAN	I	4	6	12,12,12	0.49	0	17,17,17	0.40	0
6	MAN	I	5	6	12,12,12	0.34	0	17,17,17	0.62	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	2,1	-	0/6/26/26	0/1/1/1
2	NAG	E	2	2	1/1/6/7	4/6/26/26	0/1/1/1
2	MAN	E	3	2	-	2/2/22/22	0/1/1/1
2	MAN	E	4	2	1/1/5/5	2/2/22/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/26/26	0/1/1/1
3	NAG	F	2	3	1/1/6/7	2/6/26/26	0/1/1/1
4	NAG	G	1	4,1	1/1/6/7	0/6/26/26	0/1/1/1
4	NAG	G	2	4	-	2/6/26/26	0/1/1/1
4	MAN	G	3	4	-	2/2/22/22	0/1/1/1
4	MAN	G	4	4	1/1/5/5	0/2/22/22	0/1/1/1
4	MAN	G	5	4	1/1/5/5	2/2/22/22	0/1/1/1
5	NAG	H	1	5,1	1/1/6/7	0/6/26/26	0/1/1/1
5	NAG	H	2	5	1/1/6/7	6/6/26/26	0/1/1/1
5	MAN	H	3	5	1/1/5/5	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	I	1	6,1	1/1/6/7	0/6/26/26	0/1/1/1
6	NAG	I	2	6	-	0/6/26/26	0/1/1/1
6	MAN	I	3	6	-	0/2/22/22	0/1/1/1
6	MAN	I	4	6	-	0/2/22/22	0/1/1/1
6	MAN	I	5	6	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	2	NAG	C1-C2-C3	-4.02	105.06	110.54
6	I	2	NAG	O1-C1-C2	-3.46	102.03	109.22
5	H	1	NAG	C4-C3-C2	3.33	115.22	110.34
4	G	2	NAG	O1-C1-C2	-3.31	102.33	109.22
2	E	1	NAG	O1-C1-C2	-2.76	103.48	109.22
3	F	1	NAG	O1-C1-C2	-2.56	103.89	109.22
5	H	2	NAG	C3-C4-C5	2.48	114.66	110.24
3	F	1	NAG	O1-C1-O5	-2.03	104.28	110.38
5	H	1	NAG	O4-C4-C3	-2.01	105.71	110.35

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	2	NAG	C1
2	E	4	MAN	C1
3	F	2	NAG	C1
4	G	1	NAG	C1
4	G	4	MAN	C1
4	G	5	MAN	C1
5	H	1	NAG	C1
5	H	2	NAG	C1
5	H	3	MAN	C1
6	I	1	NAG	C1

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
4	G	3	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
2	E	3	MAN	O5-C5-C6-O6
4	G	3	MAN	C4-C5-C6-O6
4	G	5	MAN	C4-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
2	E	3	MAN	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O5-C5-C6-O6
5	H	2	NAG	O7-C7-N2-C2
5	H	3	MAN	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
5	H	3	MAN	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	H	2	NAG	C3-C2-N2-C7

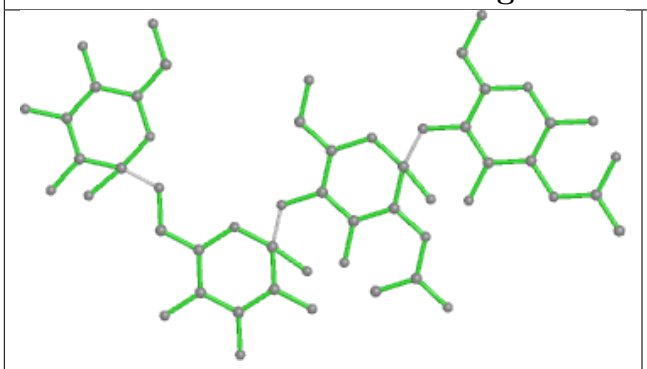
There are no ring outliers.

11 monomers are involved in 12 short contacts:

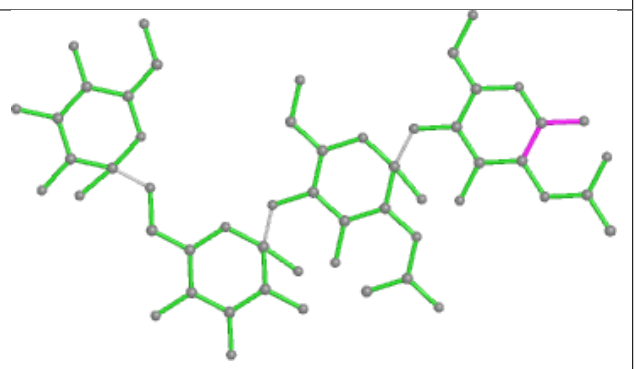
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	2	0
2	E	4	MAN	1	0
2	E	2	NAG	2	0
5	H	3	MAN	1	0
6	I	1	NAG	1	0
2	E	1	NAG	3	0
3	F	1	NAG	1	0
4	G	3	MAN	2	0
5	H	2	NAG	1	0
5	H	1	NAG	3	0
2	E	3	MAN	1	0

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

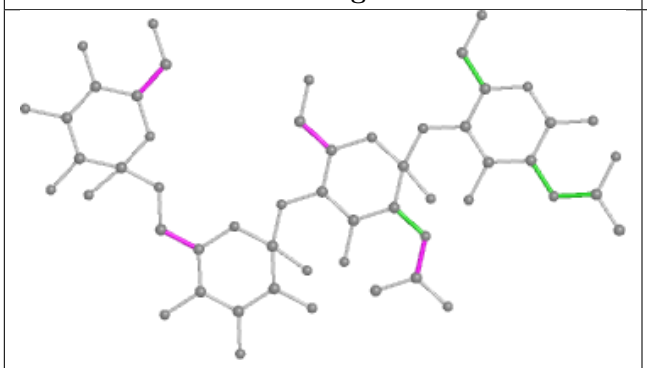
Oligosaccharide Chain E



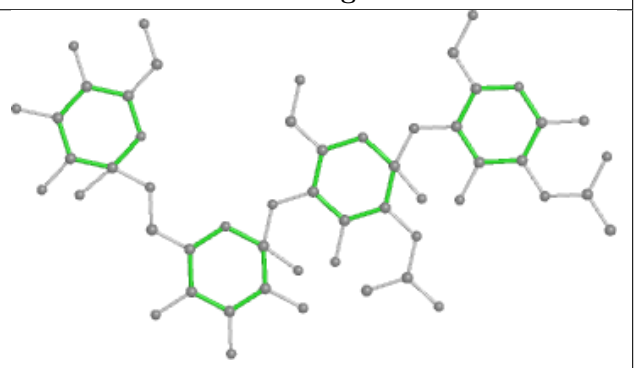
Bond lengths



Bond angles

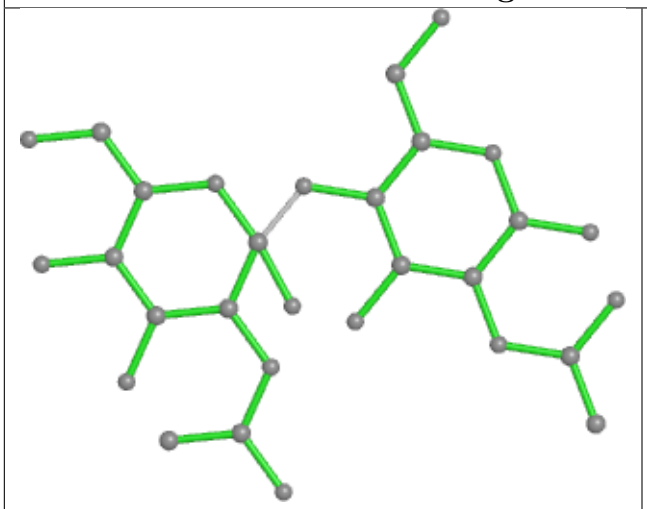


Torsions

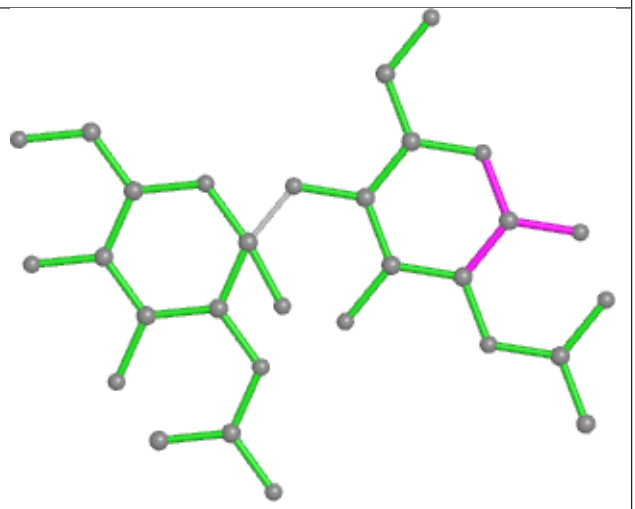


Rings

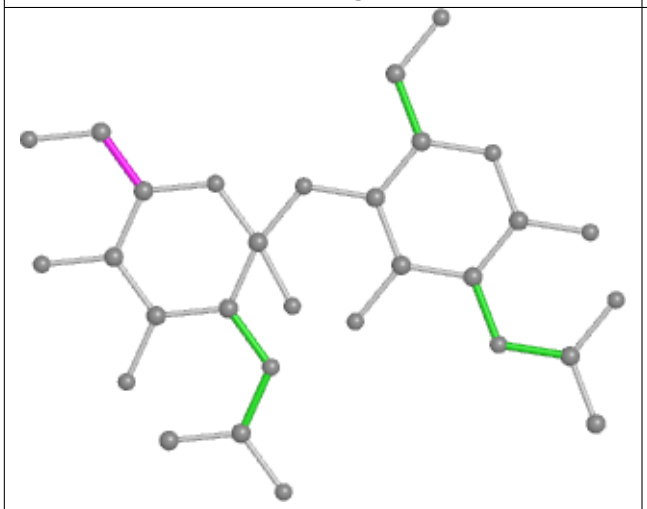
Oligosaccharide Chain F



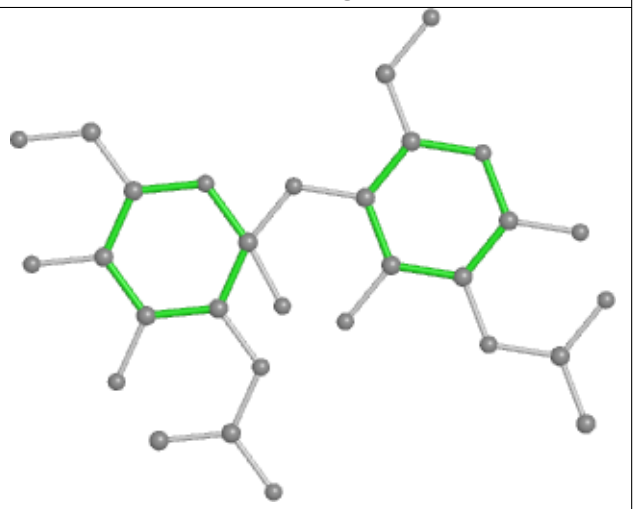
Bond lengths



Bond angles

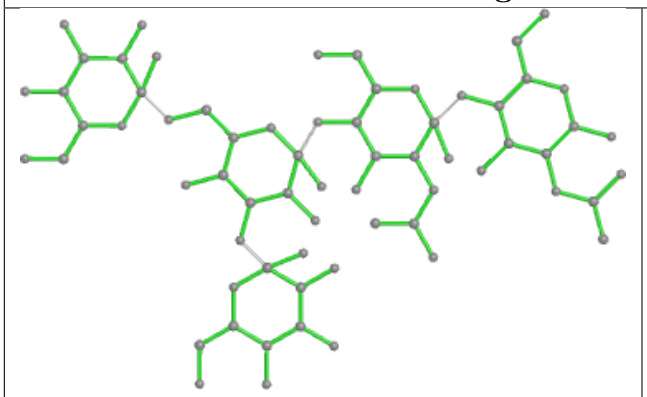


Torsions

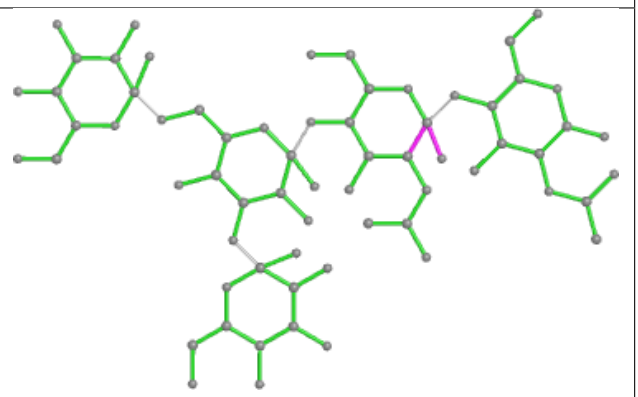


Rings

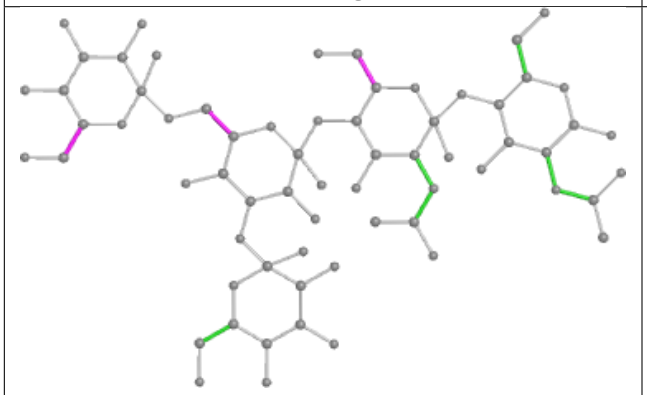
Oligosaccharide Chain G



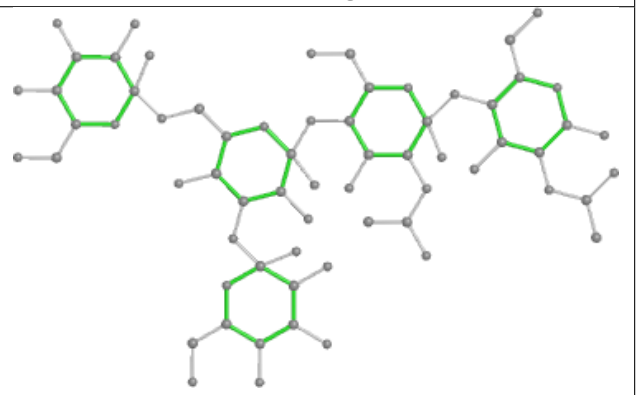
Bond lengths



Bond angles

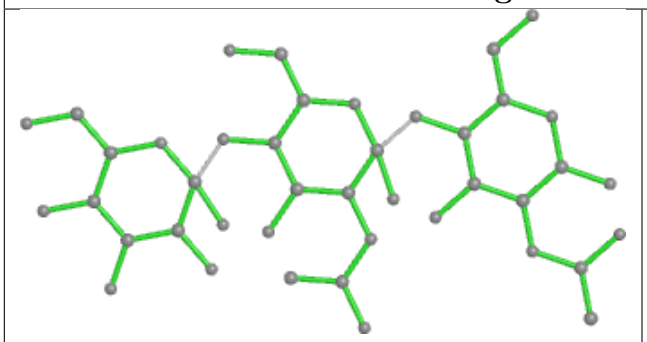


Torsions

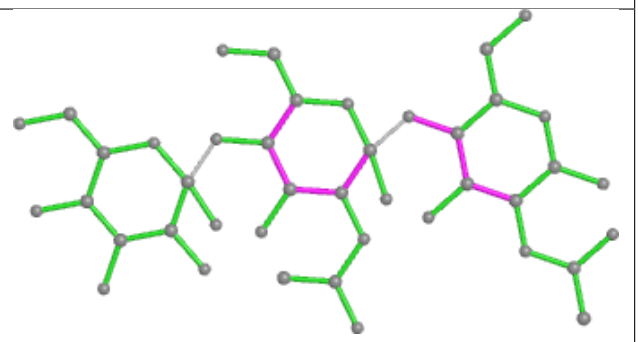


Rings

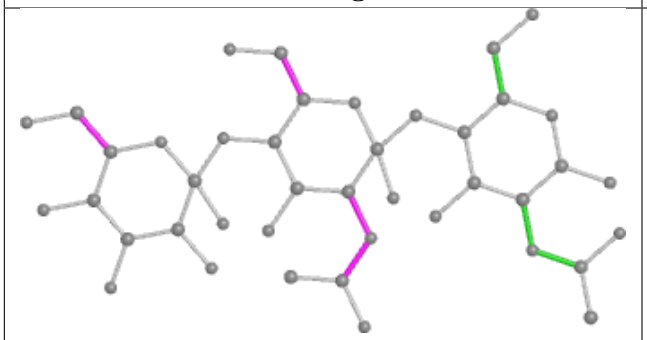
Oligosaccharide Chain H



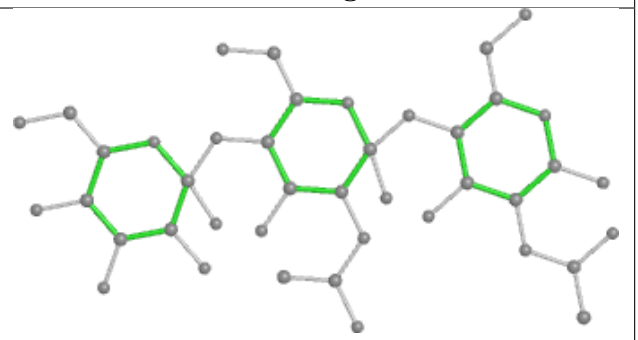
Bond lengths



Bond angles

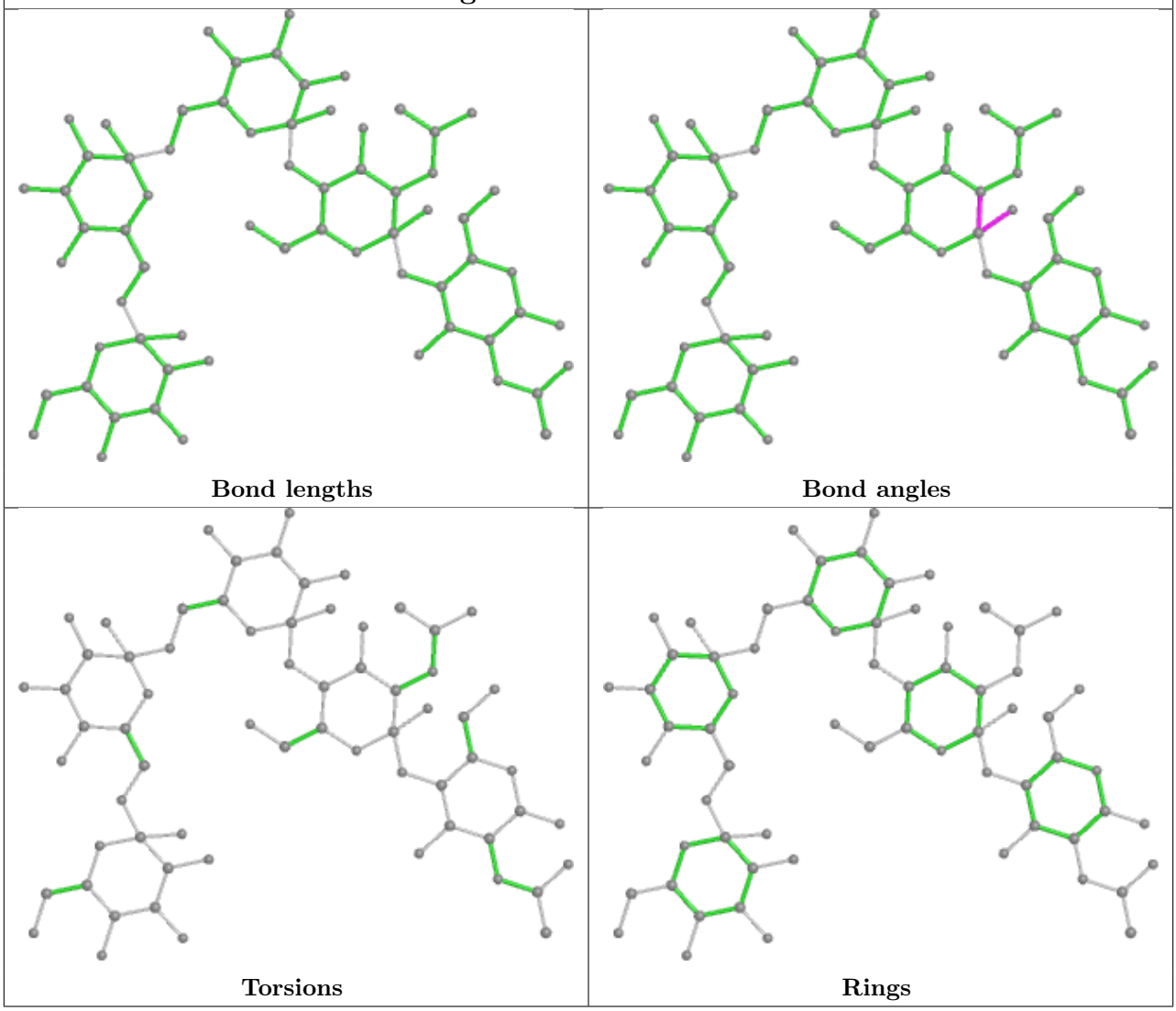


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
10	GLY	B	9000	-	4,4,4	1.29	1 (25%)	3,4,4	0.33	0
7	PO4	B	8001	-	4,4,4	1.66	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	B	5006	1	15,15,15	0.39	0	21,21,21	0.80	0
8	1PE	C	7001	-	15,15,15	0.79	0	14,14,14	1.49	4 (28%)
7	PO4	D	8003	-	4,4,4	1.51	0	6,6,6	0.42	0
9	NAG	D	5015	1	15,15,15	0.46	0	21,21,21	1.00	1 (4%)
7	PO4	C	8002	-	4,4,4	1.60	0	6,6,6	0.44	0
8	1PE	A	6000	-	15,15,15	0.79	0	14,14,14	1.51	4 (28%)
7	PO4	A	8000	-	4,4,4	1.61	0	6,6,6	0.45	0
8	1PE	D	7002	-	15,15,15	0.80	0	14,14,14	1.49	4 (28%)
8	1PE	B	7000	-	15,15,15	0.75	0	14,14,14	1.51	4 (28%)

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
10	GLY	B	9000	-	-	2/2/2/2	-
9	NAG	B	5006	1	1/1/6/7	4/6/26/26	0/1/1/1
8	1PE	C	7001	-	-	1/13/13/13	-
9	NAG	D	5015	1	-	4/6/26/26	0/1/1/1
8	1PE	D	7002	-	-	6/13/13/13	-
8	1PE	A	6000	-	-	6/13/13/13	-
8	1PE	B	7000	-	-	6/13/13/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	9000	GLY	OXT-C	-2.45	1.22	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	6000	1PE	C25-OH5-C14	2.70	125.01	113.29
8	C	7001	1PE	C25-OH5-C14	2.69	124.95	113.29
8	B	7000	1PE	C25-OH5-C14	2.67	124.85	113.29
8	D	7002	1PE	C25-OH5-C14	2.64	124.72	113.29
8	B	7000	1PE	OH6-C26-C16	2.56	121.31	110.07
9	D	5015	NAG	O1-C1-C2	-2.53	103.97	109.22
8	D	7002	1PE	OH6-C26-C16	2.50	121.04	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	6000	1PE	OH6-C26-C16	2.48	120.96	110.07
8	C	7001	1PE	OH6-C26-C16	2.48	120.95	110.07
8	B	7000	1PE	OH4-C13-C23	2.40	121.23	110.39
8	A	6000	1PE	OH4-C13-C23	2.35	121.00	110.39
8	C	7001	1PE	OH4-C13-C23	2.35	121.00	110.39
8	D	7002	1PE	OH4-C13-C23	2.31	120.83	110.39
8	B	7000	1PE	OH3-C22-C12	2.29	120.14	110.07
8	A	6000	1PE	OH3-C22-C12	2.28	120.08	110.07
8	D	7002	1PE	OH3-C22-C12	2.26	119.99	110.07
8	C	7001	1PE	OH3-C22-C12	2.22	119.81	110.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	B	5006	NAG	C1

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	5015	NAG	C8-C7-N2-C2
9	D	5015	NAG	O7-C7-N2-C2
10	B	9000	GLY	O-C-CA-N
10	B	9000	GLY	OXT-C-CA-N
8	D	7002	1PE	OH2-C12-C22-OH3
8	D	7002	1PE	OH7-C16-C26-OH6
9	D	5015	NAG	O5-C5-C6-O6
8	D	7002	1PE	OH6-C15-C25-OH5
8	B	7000	1PE	OH6-C15-C25-OH5
9	D	5015	NAG	C4-C5-C6-O6
8	B	7000	1PE	OH7-C16-C26-OH6
8	C	7001	1PE	OH4-C13-C23-OH3
8	A	6000	1PE	OH2-C12-C22-OH3
8	A	6000	1PE	OH6-C15-C25-OH5
8	A	6000	1PE	OH4-C13-C23-OH3
9	B	5006	NAG	C4-C5-C6-O6
8	B	7000	1PE	OH4-C13-C23-OH3
8	D	7002	1PE	C24-C14-OH5-C25
8	B	7000	1PE	C15-C25-OH5-C14
9	B	5006	NAG	O5-C5-C6-O6
8	A	6000	1PE	C12-C22-OH3-C23
8	B	7000	1PE	C12-C22-OH3-C23
8	A	6000	1PE	C24-C14-OH5-C25

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Mol	Chain	Res	Type	Atoms
9	B	5006	NAG	C8-C7-N2-C2
8	A	6000	1PE	C14-C24-OH4-C13
9	B	5006	NAG	O7-C7-N2-C2
8	D	7002	1PE	C15-C25-OH5-C14
8	B	7000	1PE	C24-C14-OH5-C25
8	D	7002	1PE	OH5-C14-C24-OH4

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	9000	GLY	3	0
7	B	8001	PO4	1	0
9	B	5006	NAG	1	0
8	C	7001	1PE	2	0
7	D	8003	PO4	1	0
7	C	8002	PO4	1	0
8	A	6000	1PE	1	0
7	A	8000	PO4	1	0
8	D	7002	1PE	2	0
8	B	7000	1PE	3	0

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.