Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 02:09 AM BST

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)

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

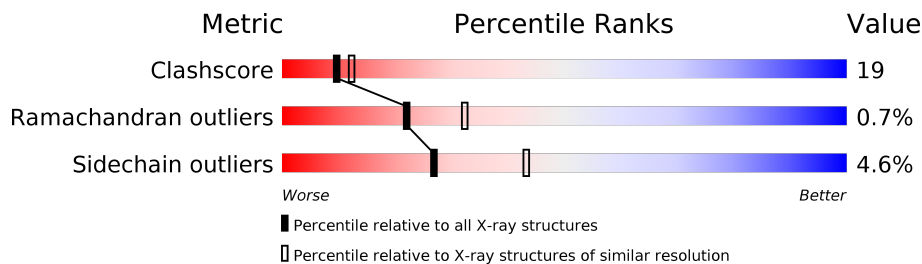|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	Percentile Ranks	Value
Clashscore		19
Ramachandran outliers		0.7%
Sidechain outliers		4.6%

Worse   Better

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

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 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	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%

Continued on next page...

Continued from previous page...

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
1	A	342	Total 2800	C 1807	N 461	O 516	S 16	0	0	0
1	B	343	Total 2807	C 1811	N 462	O 518	S 16	0	0	0
1	C	342	Total 2800	C 1807	N 461	O 516	S 16	0	0	0
1	D	342	Total 2800	C 1807	N 461	O 516	S 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.
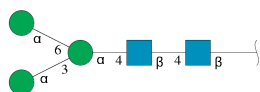

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total 54	C 28	N 2	O 24	0	0	0

- 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
3	F	2	Total 30	C 16	N 2	O 12	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(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-mannopyran ose-(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).

PO4

O3

O⁻

O2 O⁻ — P = O O1

P

O⁻

O4

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

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

1PE

OH7
OH

C26

C16

C15

O

OH5
OH6

C24
C25

O

C13
C14

OH3
OH4

C12
O

C23

HO
C22

OH2
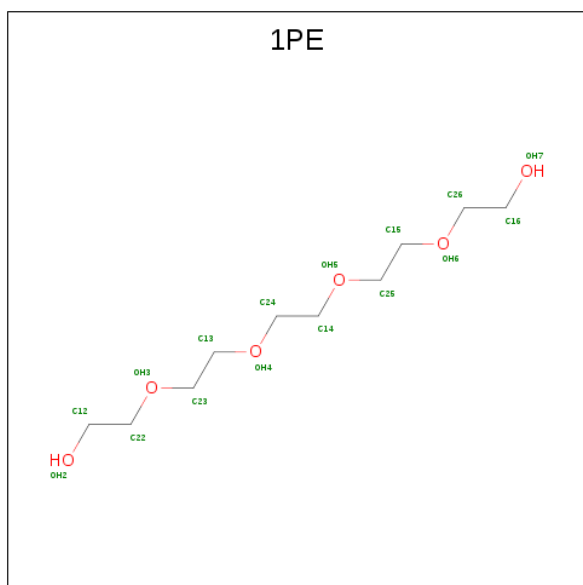
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 16	C 10	O 6	0	0
8	B	1	Total 16	C 10	O 6	0	0
8	C	1	Total 16	C 10	O 6	0	0
8	D	1	Total 16	C 10	O 6	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
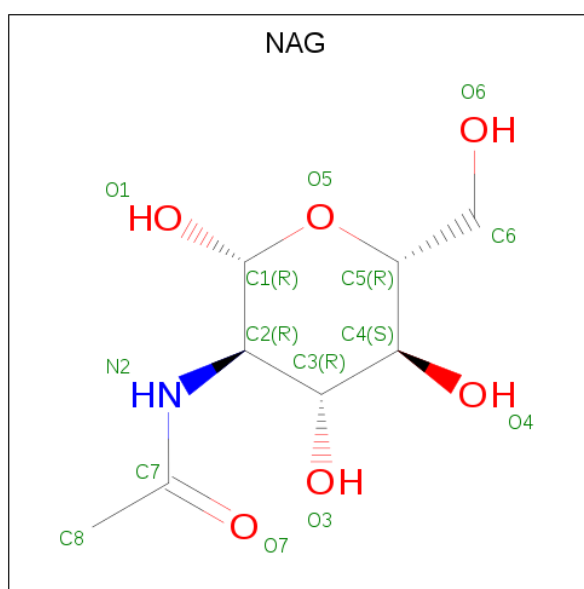
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total 15	C 8	N 1	O 6	0	0
9	D	1	Total 15	C 8	N 1	O 6	0	0

- Molecule 10 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).
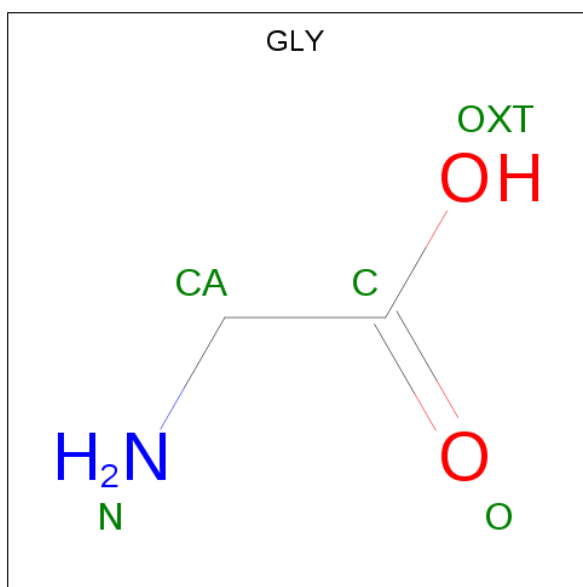
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 11 is water.

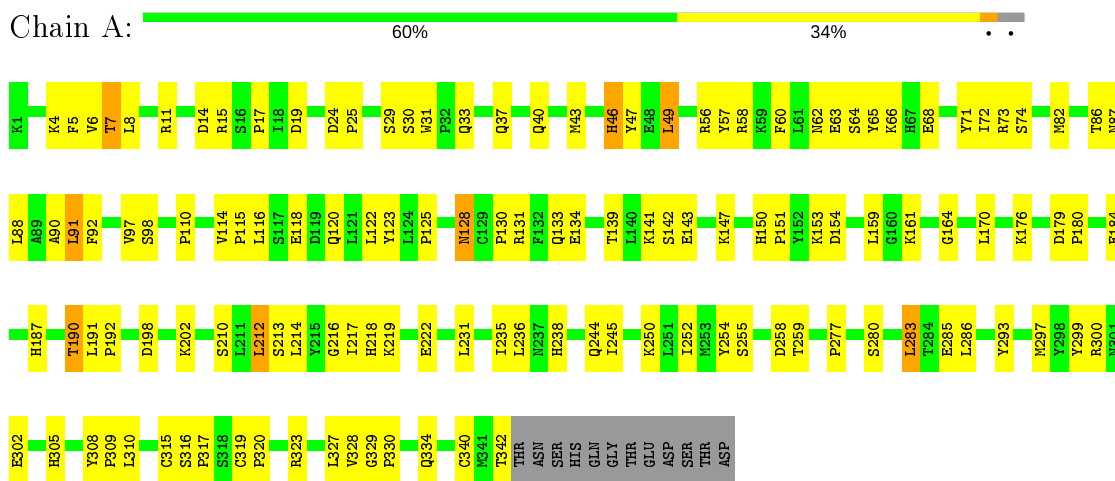| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	147	Total	O	0	0
			147	147		
11	B	134	Total	O	0	0
			134	134		
11	C	89	Total	O	0	0
			89	89		
11	D	94	Total	O	0	0
			94	94		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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:

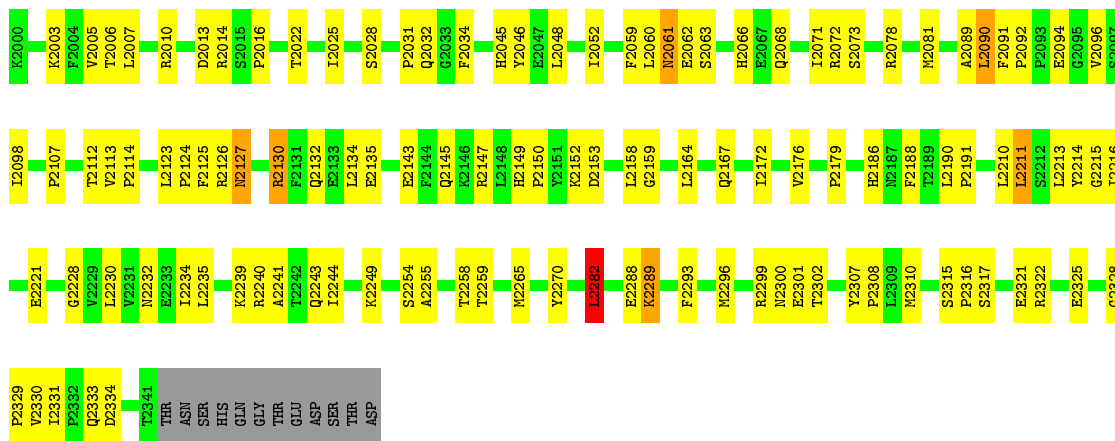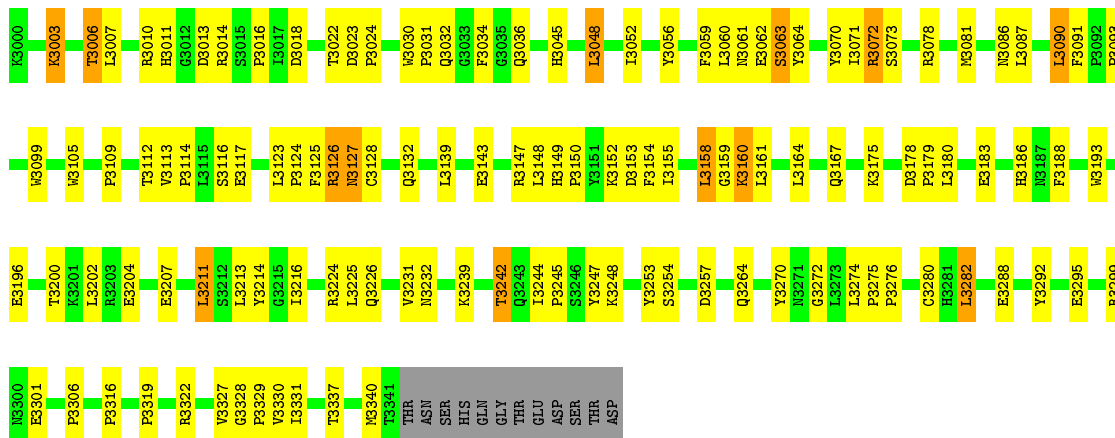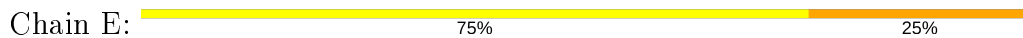K2000 K2003 F2004 V2005 T2006 L2007 R2010 D2013 R2014 S2015 P2016 T2022 I2025 S2028 P2031 Q2032 G2033 F2034 H2045 Y2046 E2047 L2048 I2052 F2059 L2060 N2061 E2062 S2063 H2066 E2067 Q2068 I2071 R2072 S2073 R2078 M2081 A2089 L2090 F2091 P2092 P2093 E2094 G2095 V2096 S2097

I2098 P2107 T2112 V2113 P2114 L2123 P2124 F2125 R2126 N2127 R2130 F2131 Q2132 E2133 L2134 E2135 E2143 F2144 Q2145 K2146 R2147 L2148 H2149 P2150 Y2151 K2152 D2153 L2158 G2159 L2164 Q2167 I2172 V2176 P2179 H2186 N2187 F2188 T2189 L2190 P2191 L2210 L2211 S2212 L2213 Y2214 G2215 I2216

E2221 G2228 V2229 L2230 V2231 N2232 E2233 I2234 L2235 K2239 R2240 A2241 T2242 Q2243 I2244 K2249 S2254 A2255 T2258 T2259 M2265 Y2270 L2282 E2288 K2289 F2293 M2296 R2299 N2300 E2301 T2302 Y2307 P2308 L2309 M2310 S2315 P2316 S2317 E2321 R2322 E2325 G2328

P2329 V2330 I2331 P2332 Q2333 D2334 T2341 THR ASN SER HIS GLN GLY THR GLU ASP SER THR ASP

• Molecule 1: prostatic acid phosphatase

Chain D:

62%   31%

K3000 K3003 T3006 L3007 R3010 H3011 G3012 D3013 R3014 S3015 P3016 I3017 D3018 T3022 D3023 P3024 W3030 P3031 Q3032 G3033 F3034 G3035 Q3036 H3045 L3048 I3052 Y3056 F3059 L3060 N3061 E3062 S3063 Y3064 Y3070 I3071 R3072 S3073 R3078 M3081 N3086 L3087 I3090 F3091 P3092 P3093

W3099 W3105 P3109 T3112 V3113 P3114 L3115 S3116 E3117 L3123 P3124 F3125 R3126 N3127 C3128 Q3132 L3139 E3143 R3147 L3148 H3149 P3150 Y3151 K3152 D3153 F3154 I3155 L3158 G3159 K3160 L3161 L3164 Q3167 K3175 D3178 L3179 L3180 E3183 H3186 N3187 F3188 W3193

E3196 T3200 K3201 L3202 R3203 E3204 E3207 L3211 S3212 Y3214 G3215 I3216 R3224 L3225 Q3226 V3231 N3232 K3239 T3242 Q3243 I3244 P3245 S3246 Y3247 K3248 Y3253 S3254 D3257 Q3264 Y3270 N3271 G3272 L3273 L3274 P3275 P3276 C3280 H3281 L3282 E3288 Y3292 E3295 R3299

N3300 E3301 P3306 P3316 P3319 R3322 V3327 G3328 V3330 I3331 T3337 M3340 T3341 THR ASN SER HIS GLN GLY THR GLU ASP SER THR ASP

• 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:

75%   25%

NAG1 NAG2 MAN3 MAN4

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

Chain F:

50%   50%

NAG1 NAG2

• 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:

60% 20% 20%

NAG1 NAG2 MAN3 MAN4 MAN5

• 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:

33% 67%

NAG1 NAG2 MAN3

• 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:

60% 40%

NAG1 NAG2 MAN3 MAN4 MAN5

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, 1PE, 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	0.35	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

Continued from previous page...

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:H	1:C:2127:ASN:HD22	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

Continued from previous page...

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:ND2	1:C:2127:ASN:H	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:N	1:B:1127:ASN:HD22	1.81	0.68
1:A:128:ASN:N	1:A:128:ASN:HD22	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

Continued on next page...

Continued from previous page...

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:HG2	1:D:3322:ARG:HH11	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:N	1:A:141:LYS:HD2	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

Continued on next page...

Continued from previous page...

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:D:3007:LEU:CD2	1:D:3282:LEU:HD22	2.35	0.56
1:B:1010:ARG:HD3	1:B:1257:ASP:HB3	1.87	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:O	1:C:2167:GLN:HG3	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

Continued on next page...

Continued from previous page...

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:N	1:D:3071:ILE:HD12	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:HH11	1:D:3014:ARG:HG3	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

Continued on next page...

Continued from previous page...

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:HA	1:C:2145:GLN:NE2	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:HD23	1:D:3282:LEU:N	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

Continued on next page...

Continued from previous page...

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:ND2	1:D:3127:ASN:H	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
1:B:1149:HIS:HA	1:B:1152:LYS:CD	2.42	0.48
11:A:4285:HOH:O	8:C:7001:1PE:H152	2.14	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:O	1:A:245:ILE:HG23	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:2081:MET:CE	1:D:3109:PRO:HD3	2.45	0.47
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2013:ASP:OD1	1:C:2186:HIS:HE1	1.97	0.47
1:C:2288:GLU:O	1:C:2289:LYS:CB	2.62	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:2126:ARG:NH1	1:C:2126:ARG:HG2	2.30	0.46
1:C:2113:VAL:HG22	1:D:3114:PRO:HD3	1.95	0.46
1:D:3148:LEU:HD21	1:D:3167:GLN:HE21	1.80	0.46
1:A:131:ARG:HD3	1:A:222:GLU:OE2	2.15	0.46
1:A:118:GLU:CG	1:D:3160:LYS:HE3	2.45	0.46
1:A:190:THR:HG21	1:C:2239:LYS:HB3	1.97	0.46
1:A:58:ARG:NH1	1:A:58:ARG:HG2	2.30	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:1151:TYR:CG	1:B:1205:LEU:HD21	2.51	0.46
1:B:1123:LEU:O	1:B:1258:THR:CG2	2.64	0.46
1:C:2215:GLY:O	1:C:2216:ILE:HB	2.16	0.46
1:B:1126:ARG:HH11	1:B:1126:ARG:HG2	1.81	0.46
1:A:139:THR:O	1:A:142:SER:HB3	2.15	0.46
1:A:74:SER:HB2	1:A:255:SER:HB3	1.98	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

Continued on next page...

Continued from previous page...

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:B:1010:ARG:HD3	1:B:1257:ASP:CA	2.47	0.45
1:A:82:MET:HE2	1:B:1109:PRO:HD3	1.99	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:N	1:C:2061:ASN:HD22	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:C:2014:ARG:HG3	1:C:2014:ARG:HH11	1.83	0.44
1:A:30:SER:HB3	1:C:2244:ILE:HG21	1.99	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:122:LEU:HD11	1:A:254:TYR:HD2	1.83	0.44
1:A:11:ARG:HD3	1:A:258:ASP:CB	2.47	0.44

Continued on next page...

Continued from previous page...

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:CG2	1:C:2022:THR:O	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:O	1:D:3211:LEU:HD13	2.18	0.43
1:A:334:GLN:HA	1:A:334:GLN:NE2	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:B:1328:GLY:N	1:B:1329:PRO:HD2	2.35	0.42
1:A:308:TYR:CE1	3:F:1:NAG:H1	2.55	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:O	1:C:2096:VAL:HG22	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

Continued on next page...

Continued from previous page...

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:HA	1:C:2322:ARG:HD2	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:O	1:B:1189:THR:HG23	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:D:3125:PHE:N	1:D:3226:GLN:HE22	2.02	0.41
1:C:2307:TYR:CD1	5:H:1:NAG:O1	2.68	0.41
1:B:1146:LYS:CE	1:B:1146:LYS:HA	2.24	0.41
1:B:1134:LEU:CD1	1:B:1221:GLU:HG2	2.42	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:D:3295:GLU:HG2	1:D:3316:PRO:O	2.21	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:A:170:LEU:HB3	1:A:210:SER:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:VAL:HG22	1:A:285:GLU:HG2	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:NE2	1:B:1333:GLN:HA	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:HG22	1:C:2022:THR:O	2.20	0.40
1:C:2126:ARG:HH11	1:C:2126:ARG:HG2	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:HH11	1:A:11:ARG:HD2	1.78	0.40
1:A:159:LEU:HD13	1:A:159:LEU:C	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Some 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

Continued on next page...

Continued from previous page...

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	1,2	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	1,3	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	1,4	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	1,5	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	1,6	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	1,2	-	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	1,3	-	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	1,4	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	1,5	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	I	1	1,6	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
4	G	1	NAG	C1
5	H	1	NAG	C1
4	G	5	MAN	C1
3	F	2	NAG	C1
2	E	4	MAN	C1
4	G	4	MAN	C1
6	I	1	NAG	C1
5	H	3	MAN	C1
2	E	2	NAG	C1
5	H	2	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	3	MAN	O5-C5-C6-O6
4	G	5	MAN	C4-C5-C6-O6
4	G	3	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	4	MAN	C4-C5-C6-O6
2	E	2	NAG	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
5	H	1	NAG	3	0
2	E	1	NAG	3	0
3	F	1	NAG	1	0
2	E	4	MAN	1	0
4	G	2	NAG	2	0
6	I	1	NAG	1	0
4	G	3	MAN	2	0
5	H	3	MAN	1	0
2	E	3	MAN	1	0
2	E	2	NAG	2	0
5	H	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 H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings
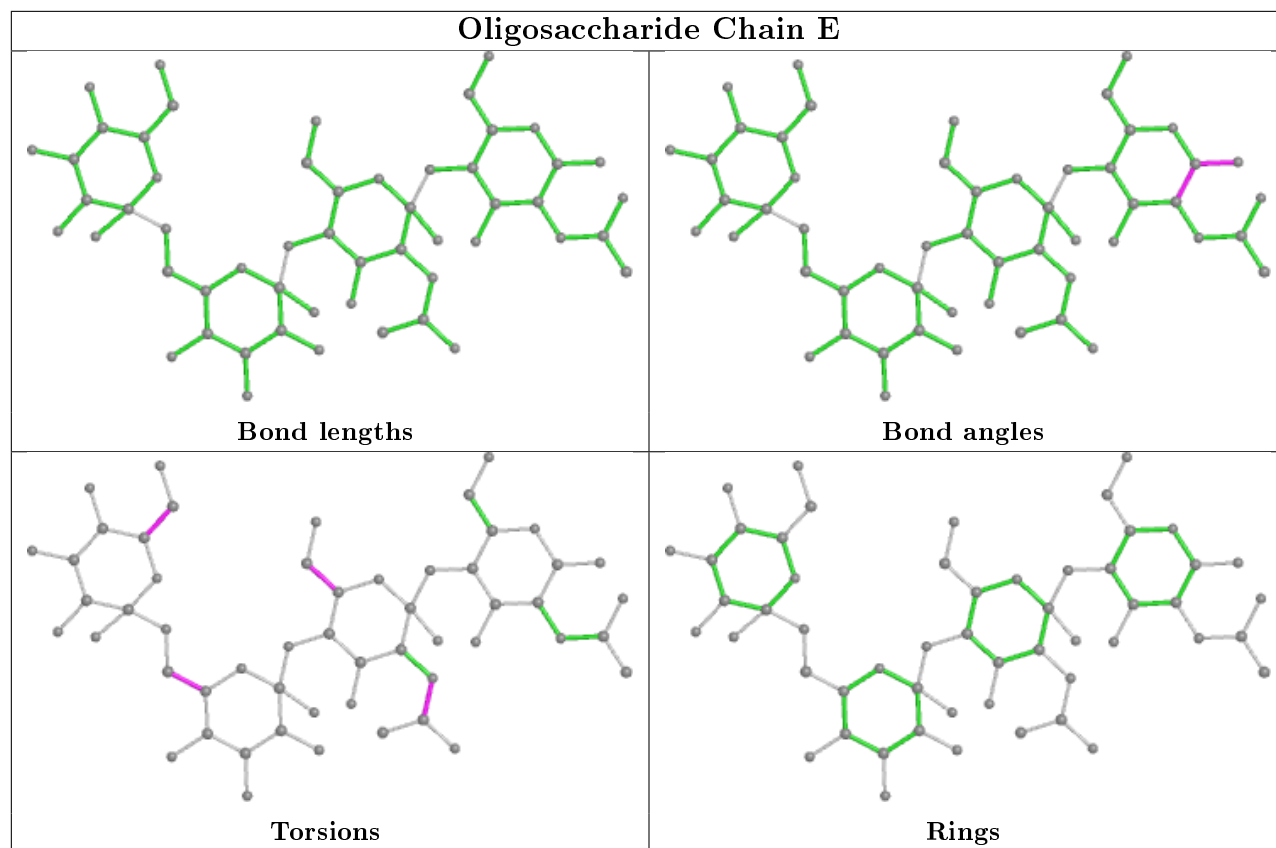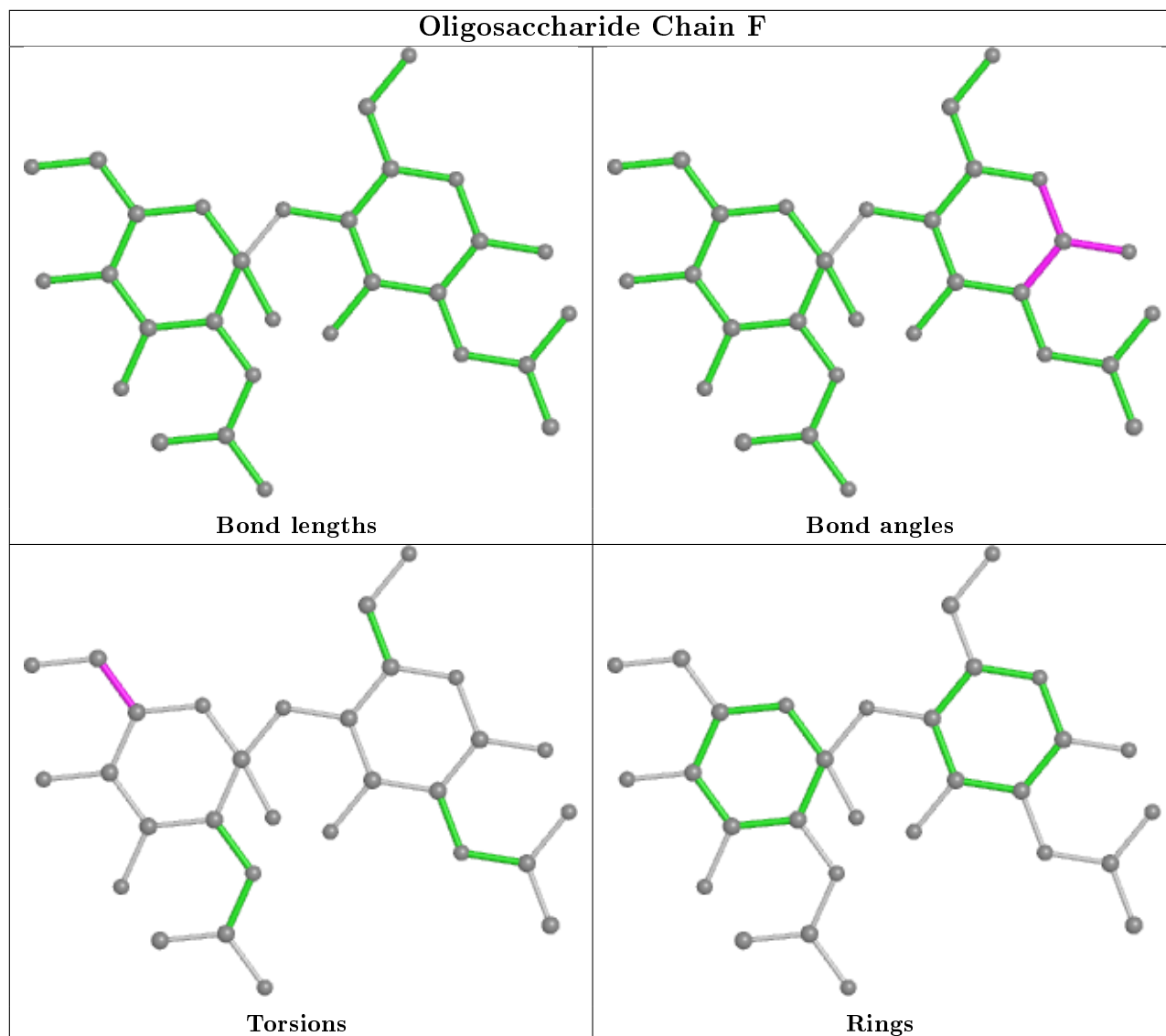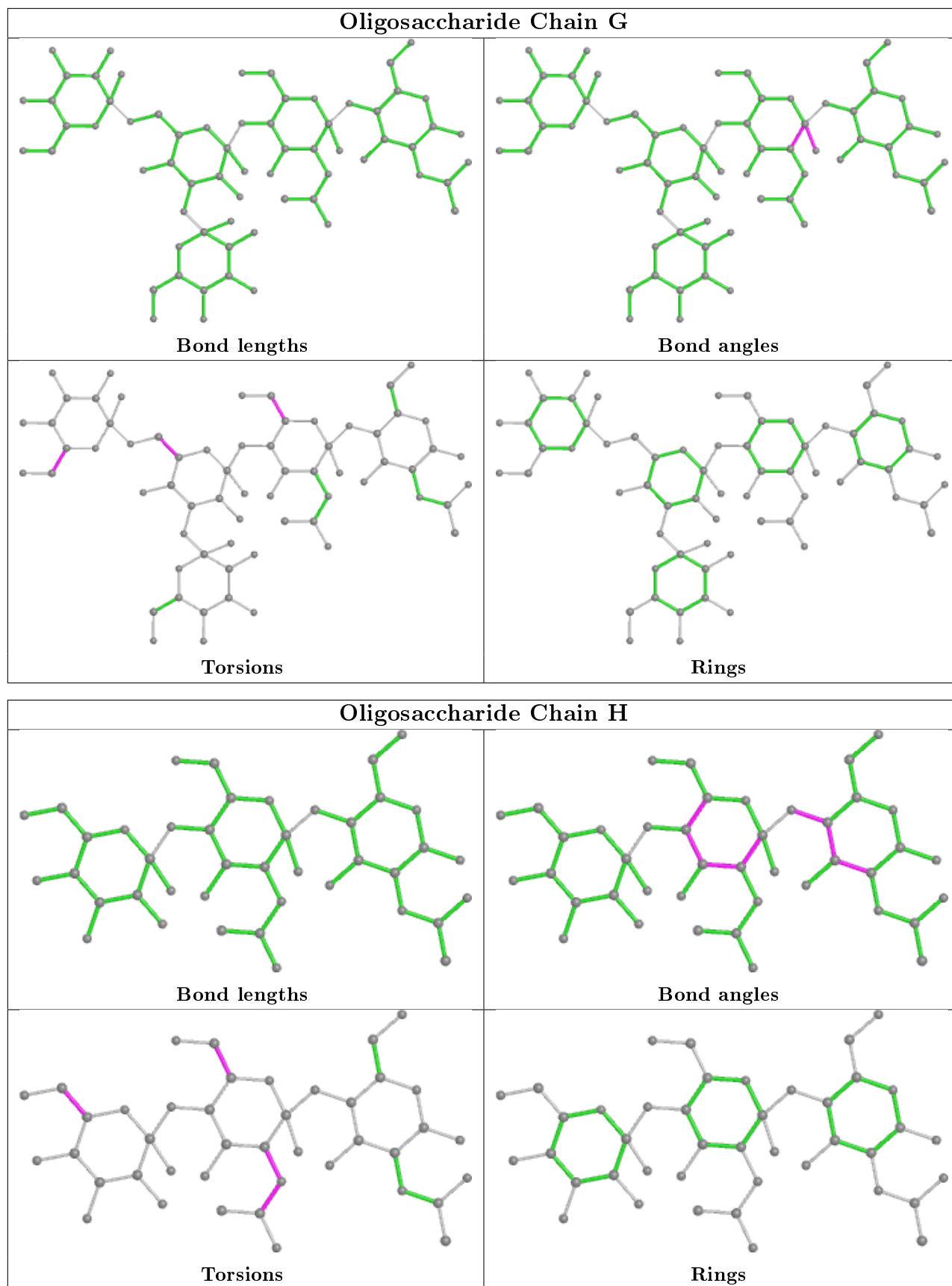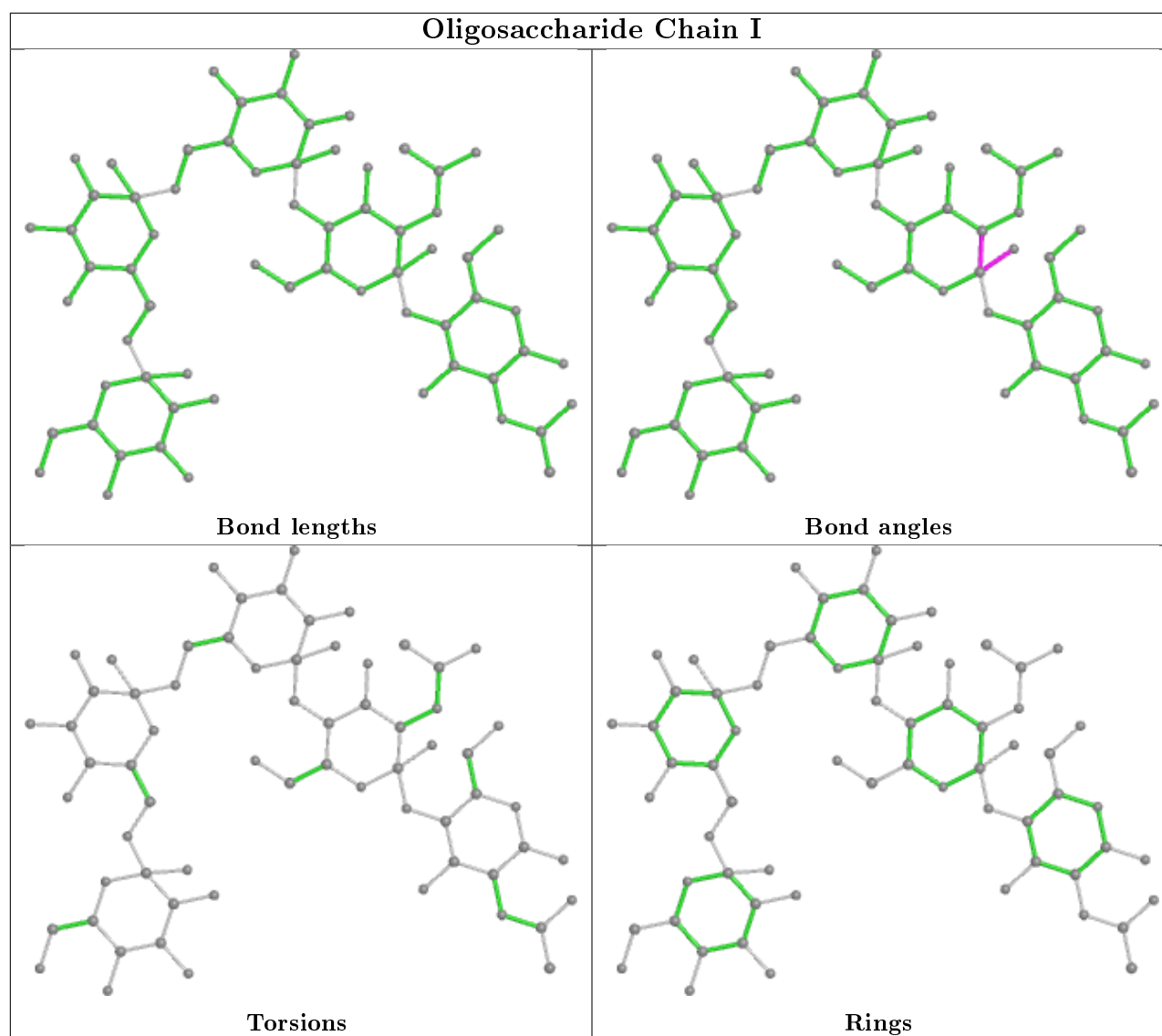
5.6 Ligand geometry ⓘ

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	$\#|Z| > 2$
7	PO4	D	8003	-	4,4,4	1.51	0	6,6,6	0.42	0
7	PO4	C	8002	-	4,4,4	1.60	0	6,6,6	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
8	1PE	B	7000	-	15,15,15	0.75	0	14,14,14	1.51	4 (28%)
8	1PE	D	7002	-	15,15,15	0.80	0	14,14,14	1.49	4 (28%)
9	NAG	B	5006	1	15,15,15	0.39	0	21,21,21	0.80	0
9	NAG	D	5015	1	15,15,15	0.46	0	21,21,21	1.00	1 (4%)
8	1PE	C	7001	-	15,15,15	0.79	0	14,14,14	1.49	4 (28%)
7	PO4	B	8001	-	4,4,4	1.66	0	6,6,6	0.43	0
7	PO4	A	8000	-	4,4,4	1.61	0	6,6,6	0.45	0
8	1PE	A	6000	-	15,15,15	0.79	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
8	1PE	B	7000	-	-	6/13/13/13	-
8	1PE	D	7002	-	-	6/13/13/13	-
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	A	6000	-	-	6/13/13/13	-

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 (27) 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
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
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.

9 monomers are involved in 13 short contacts:

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