



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 01:10 PM BST

PDB ID : 5XBM
Title : Structure of SCARB2-JL2 complex
Authors : Zhang, X.; Yang, P.; Wang, N.; Zhang, J.; Li, J.; Guo, H.; Yin, X.; Rao, Z.;
Wang, X.; Zhang, L.
Deposited on : 2017-03-20
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

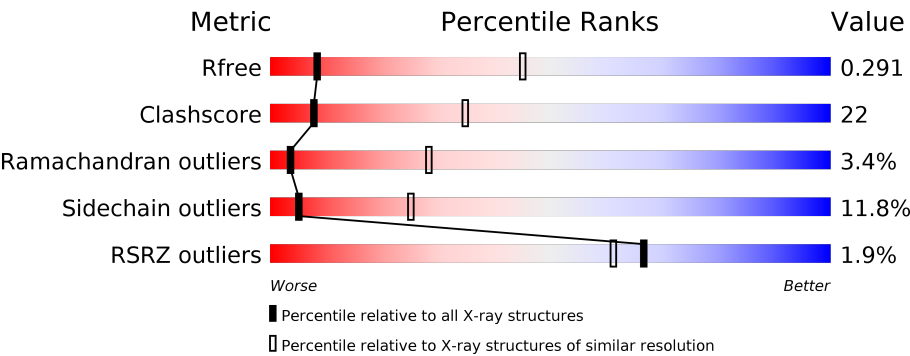
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	213	
1	D	213	
2	B	222	
2	E	222	
3	C	394	
3	F	394	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	G	4	
4	M	4	
4	R	4	
5	H	2	
5	I	2	
5	J	2	
5	N	2	
5	O	2	
5	P	2	
6	K	5	
6	L	5	
6	Q	5	

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
4	MAN	M	4	-	-	-	X
5	NAG	J	2	-	-	-	X
5	NAG	P	1	-	-	-	X
5	NAG	P	2	-	-	-	X
6	MAN	Q	4	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13343 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 light chain of JL2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1611	1003	273	329	6			
1	D	209	Total	C	N	O	S	0	0	0
			1615	1007	275	327	6			

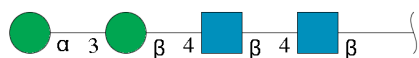
- Molecule 2 is a protein called heavy chain of JL2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	0	0	0
			1658	1046	269	334	9			
2	E	221	Total	C	N	O	S	0	0	0
			1654	1044	266	335	9			

- Molecule 3 is a protein called Lysosome membrane protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	394	Total	C	N	O	S	0	0	0
			3144	2028	509	596	11			
3	F	392	Total	C	N	O	S	0	0	0
			3132	2021	507	593	11			

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



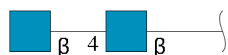
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

Continued on next page...

Continued from previous page...

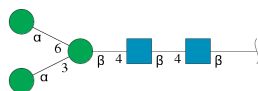
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 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
5	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	K	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	L	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	Q	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

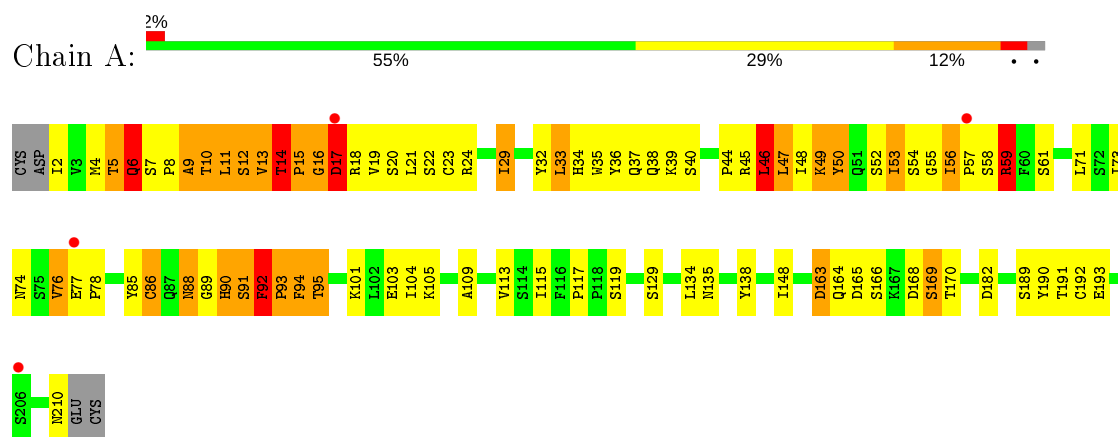


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		

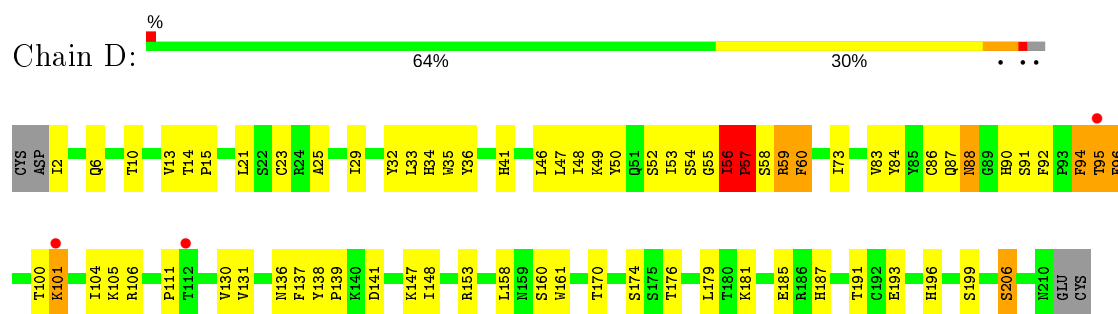
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

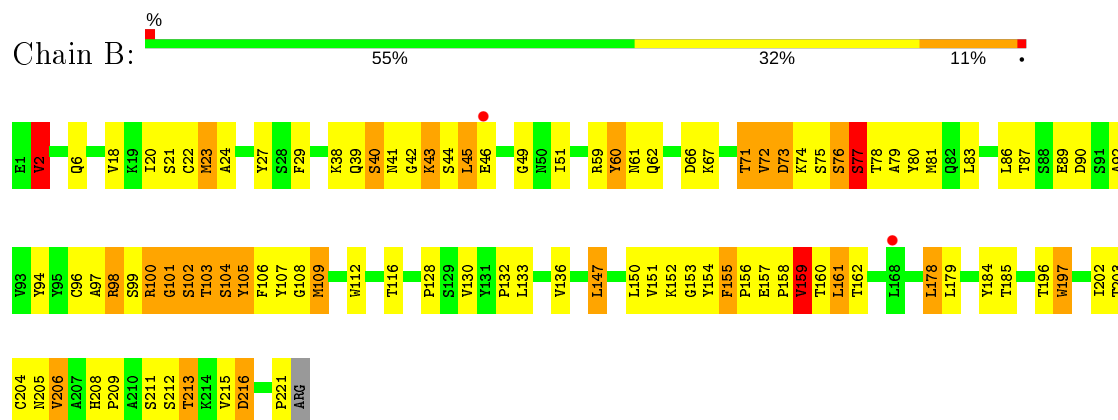
- Molecule 1: light chain of JL2



- Molecule 1: light chain of JL2



- Molecule 2: heavy chain of JL2



Chain E:

Category	Percentage
E1	4%
V2	61%
Q3	31%
L4	7%
Q5	
Q6	
S7	
G8	
P9	
F10	
L11	
T20	
S21	
C22	
F29	
T30	
N33	
M34	
N35	
I36	
I37	
K38	
K39	
L45	
F46	
W47	
L48	
F51	
D52	
P53	
Y54	
T58	
R59	
Y60	
M61	
Q62	
R63	
F64	
K65	
D66	
K67	
L70	
T71	
V72	
D73	
K74	
S75	
S76	
S77	
T78	
A79	
Y80	
M81	
K84	
D90	
R98	
S99	
G101	
S104	
F105	
F106	
Y107	
G108	
M109	
D110	
Y111	
T116	
T126	
A127	
P128	
S129	
V130	
L133	
V136	
C137	
G138	
D139	
T146	
L147	
V151	
F154	
F155	
P156	
E157	
T162	
W163	
S169	
S170	
G171	
V172	
H173	
T174	
F175	
L178	
L179	
V190	
W197	
I202	
T203	
C204	
K205	
V206	
D216	
K217	
K218	
I219	
E220	
P221	
ARG	

Chain C:

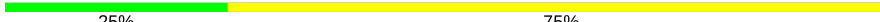
29% 69% 26%

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

Chain G:  50% 50%




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

Chain M:  25% 75%



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

Chain R:  75% 25%



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

Chain H:  100%



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

Chain I:  50% 50%



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

Chain J:  100%



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

Chain N:  100%



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

Chain O:



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

Chain P:



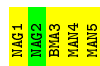
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain L:



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

Chain Q:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	199.86Å 75.65Å 164.31Å 90.00° 100.11° 90.00°	Depositor
Resolution (Å)	49.55 – 3.50 49.55 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.55-3.50) 98.8 (49.55-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.238 , 0.293 0.250 , 0.291	Depositor DCC
R_{free} test set	1516 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	93.0	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13343	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.39	0/1650	0.59	1/2243 (0.0%)
1	D	0.37	0/1654	0.61	2/2246 (0.1%)
2	B	0.37	0/1700	0.59	0/2320
2	E	0.28	0/1696	0.55	0/2315
3	C	0.32	0/3227	0.51	2/4397 (0.0%)
3	F	0.28	0/3215	0.48	0/4379
All	All	0.33	0/13142	0.54	5/17900 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	149	VAL	N-CA-C	-6.18	94.32	111.00
1	D	56	ILE	C-N-CD	5.73	140.43	128.40
1	D	57	PRO	CA-N-CD	-5.33	104.04	111.50
3	C	329	CYS	N-CA-C	-5.22	96.89	111.00
1	A	7	SER	C-N-CD	5.03	138.97	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1611	0	1520	152	0
1	D	1615	0	1540	90	0
2	B	1658	0	1596	117	0
2	E	1654	0	1585	91	0
3	C	3144	0	2989	83	0
3	F	3132	0	2985	71	0
4	G	50	0	43	2	0
4	M	50	0	43	0	0
4	R	50	0	43	1	0
5	H	28	0	25	0	0
5	I	28	0	25	2	0
5	J	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	5	0
5	P	28	0	25	2	0
6	K	61	0	52	3	0
6	L	61	0	52	0	0
6	Q	61	0	52	2	0
7	C	14	0	13	0	0
7	F	14	0	13	1	0
All	All	13343	0	12676	563	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 22.

All (563) 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:D:94:PHE:HE2	2:E:106:PHE:CB	1.20	1.55
1:D:94:PHE:CE2	2:E:106:PHE:HB2	1.03	1.52
1:A:4:MET:HE3	1:A:23:CYS:SG	1.51	1.50
1:A:4:MET:CE	1:A:23:CYS:SG	2.09	1.39
1:A:6:GLN:CG	1:A:22:SER:O	1.70	1.36
1:A:10:THR:C	1:A:11:LEU:HD23	1.45	1.35
2:E:106:PHE:CE2	2:E:108:GLY:HA2	1.63	1.34
1:D:94:PHE:CE2	2:E:106:PHE:CB	1.99	1.30
1:D:47:LEU:O	1:D:48:ILE:HD13	1.27	1.27
1:D:47:LEU:C	1:D:48:ILE:HD13	1.58	1.22
1:A:6:GLN:CB	1:A:23:CYS:HA	1.73	1.17
2:B:153:GLY:H	2:B:185:THR:HG22	1.06	1.17
1:A:6:GLN:HG2	1:A:22:SER:O	0.99	1.16
2:E:106:PHE:CE2	2:E:108:GLY:CA	2.29	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:GLU:HG3	2:B:158:PRO:HA	1.27	1.14
1:A:19:VAL:HG12	1:A:20:SER:H	0.95	1.10
1:D:59:ARG:HG2	1:D:60:PHE:N	1.65	1.09
2:E:61:ASN:O	2:E:65:LYS:HB3	1.49	1.09
1:A:6:GLN:CG	1:A:23:CYS:HA	1.83	1.08
1:D:94:PHE:CD2	2:E:106:PHE:HB2	1.87	1.08
2:E:21:SER:HA	2:E:79:ALA:O	1.54	1.08
2:E:106:PHE:HE2	2:E:108:GLY:CA	1.63	1.07
2:B:161:LEU:CD2	2:B:162:THR:H	1.68	1.07
1:A:92:PHE:HA	1:A:94:PHE:H	1.21	1.05
1:A:6:GLN:HG3	1:A:23:CYS:HA	1.38	1.04
1:A:92:PHE:HB2	1:A:93:PRO:HA	1.39	1.03
1:A:13:VAL:HG13	1:A:14:THR:H	1.23	1.03
2:E:58:THR:HB	2:E:60:TYR:CE2	1.94	1.03
2:B:155:PHE:CE2	2:B:156:PRO:HB3	1.91	1.03
3:F:313:ILE:HD12	3:F:314:PRO:HD3	1.35	1.02
2:E:71:THR:HG22	2:E:80:TYR:HB2	1.39	1.02
2:B:161:LEU:HD23	2:B:162:THR:H	1.23	1.01
1:D:36:TYR:CE2	1:D:87:GLN:OE1	2.13	1.01
1:A:19:VAL:HG12	1:A:20:SER:N	1.65	1.01
1:A:9:ALA:O	1:A:10:THR:OG1	1.78	1.00
2:B:39:GLN:HB2	2:B:45:LEU:CD1	1.91	1.00
1:D:59:ARG:HG2	1:D:60:PHE:H	1.24	0.99
1:A:19:VAL:CG1	1:A:20:SER:H	1.73	0.99
1:D:47:LEU:O	1:D:48:ILE:CD1	2.10	0.98
2:E:74:LYS:O	2:E:76:SER:N	1.96	0.97
1:A:33:LEU:O	1:A:49:LYS:O	1.82	0.97
2:B:161:LEU:CD2	2:B:162:THR:N	2.27	0.97
1:A:10:THR:C	1:A:11:LEU:CD2	2.34	0.96
2:B:161:LEU:HD22	2:B:162:THR:N	1.79	0.96
1:A:6:GLN:HG3	1:A:23:CYS:CA	1.97	0.95
1:A:14:THR:OG1	1:A:17:ASP:OD2	1.85	0.94
1:A:129:SER:OG	2:B:152:LYS:NZ	2.00	0.94
1:A:6:GLN:HB3	1:A:23:CYS:HA	1.44	0.94
2:E:67:LYS:HE3	2:E:90:ASP:OD2	1.69	0.93
1:D:36:TYR:HE2	1:D:87:GLN:OE1	1.49	0.92
1:A:93:PRO:O	1:A:95:THR:N	2.03	0.91
1:A:14:THR:O	1:A:16:GLY:N	2.03	0.91
2:E:106:PHE:HE2	2:E:108:GLY:HA2	0.77	0.90
2:B:71:THR:HG23	2:B:80:TYR:HB2	1.53	0.90
1:A:4:MET:HE2	1:A:23:CYS:SG	2.13	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:HIS:ND1	1:D:49:LYS:O	2.06	0.89
2:E:58:THR:HB	2:E:60:TYR:HE2	1.31	0.88
2:B:157:GLU:HG3	2:B:158:PRO:CA	2.02	0.88
2:B:43:LYS:O	2:B:45:LEU:N	2.07	0.87
2:B:106:PHE:HE2	2:B:108:GLY:HA2	1.38	0.87
2:B:39:GLN:HB2	2:B:45:LEU:HD13	1.54	0.87
1:D:57:PRO:O	1:D:58:SER:OG	1.91	0.87
1:A:8:PRO:HA	1:A:9:ALA:HB2	1.56	0.86
1:D:59:ARG:O	1:D:60:PHE:O	1.95	0.85
3:C:150:HIS:HD2	3:C:153:ARG:HG3	1.42	0.84
1:A:54:SER:OG	1:A:55:GLY:N	2.09	0.84
2:B:153:GLY:N	2:B:185:THR:HG22	1.89	0.84
2:E:106:PHE:CE2	2:E:108:GLY:N	2.45	0.84
1:A:92:PHE:CB	1:A:93:PRO:HA	2.07	0.83
2:E:71:THR:CG2	2:E:80:TYR:HB2	2.08	0.82
1:A:18:ARG:HG3	1:A:73:ILE:O	1.78	0.82
1:A:4:MET:HE1	1:A:86:CYS:HB2	1.63	0.81
1:A:13:VAL:HG11	1:A:76:VAL:HG11	1.61	0.81
1:A:88:ASN:ND2	1:A:94:PHE:HA	1.96	0.81
3:C:146:TRP:O	3:C:150:HIS:O	1.97	0.81
1:A:4:MET:CE	1:A:86:CYS:HB2	2.11	0.80
1:A:13:VAL:HG23	1:A:17:ASP:OD1	1.80	0.80
1:A:18:ARG:CG	1:A:73:ILE:O	2.30	0.80
2:B:71:THR:CG2	2:B:80:TYR:HB2	2.11	0.80
1:D:34:HIS:HB2	1:D:87:GLN:HB3	1.64	0.80
3:C:330:LYS:HD2	3:C:330:LYS:N	1.94	0.79
1:D:49:LYS:HB3	1:D:50:TYR:CE2	2.18	0.79
3:C:148:GLN:HA	3:C:148:GLN:NE2	1.96	0.79
1:A:10:THR:O	1:A:11:LEU:HD23	1.82	0.78
1:A:11:LEU:O	1:A:103:GLU:HB2	1.84	0.78
1:A:10:THR:CA	1:A:11:LEU:HD23	2.13	0.77
3:C:145:GLU:O	3:C:149:VAL:HG12	1.84	0.77
1:A:6:GLN:CB	1:A:23:CYS:CA	2.58	0.77
1:A:94:PHE:CZ	2:B:106:PHE:HB2	2.20	0.77
2:E:106:PHE:CD2	2:E:108:GLY:N	2.52	0.77
1:A:88:ASN:ND2	1:A:94:PHE:O	2.18	0.76
3:F:63:GLN:HB3	3:F:90:THR:HG22	1.66	0.76
1:A:8:PRO:CA	1:A:9:ALA:HB2	2.15	0.76
1:A:6:GLN:O	1:A:6:GLN:NE2	2.20	0.75
1:D:59:ARG:CG	1:D:60:PHE:N	2.48	0.74
1:D:94:PHE:CD2	2:E:106:PHE:CD1	2.75	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:PHE:CD2	2:B:156:PRO:HB3	2.23	0.74
2:B:156:PRO:HD2	2:B:208:HIS:HE2	1.53	0.74
1:A:10:THR:O	1:A:11:LEU:CD2	2.35	0.74
3:C:150:HIS:O	3:C:151:PHE:CB	2.35	0.74
1:A:11:LEU:N	1:A:11:LEU:HD23	2.03	0.73
2:B:153:GLY:H	2:B:185:THR:CG2	1.95	0.73
1:D:6:GLN:HE21	1:D:100:THR:HG23	1.52	0.73
3:F:382:ARG:HG2	3:F:412:ASN:HB3	1.71	0.73
2:B:156:PRO:HD2	2:B:208:HIS:NE2	2.03	0.73
1:D:94:PHE:CE2	2:E:106:PHE:CG	2.77	0.73
3:C:150:HIS:CD2	3:C:153:ARG:HG3	2.23	0.72
1:A:34:HIS:O	1:A:48:ILE:O	2.07	0.72
1:A:38:GLN:NE2	2:B:39:GLN:OE1	2.22	0.72
1:A:94:PHE:CE2	2:B:106:PHE:CD1	2.78	0.72
2:B:161:LEU:HG	2:B:206:VAL:HG12	1.72	0.72
1:D:94:PHE:CD2	2:E:106:PHE:CB	2.59	0.71
2:B:106:PHE:CE2	2:B:108:GLY:HA2	2.24	0.71
2:B:102:SER:OG	2:B:103:THR:N	2.18	0.71
1:D:32:TYR:OH	3:F:73:GLU:OE2	2.08	0.71
1:D:94:PHE:HE2	2:E:106:PHE:CA	2.03	0.71
1:D:160:SER:HB2	2:E:178:LEU:HD11	1.72	0.71
1:D:54:SER:OG	1:D:55:GLY:N	2.23	0.71
1:A:56:ILE:N	1:A:57:PRO:HD3	2.06	0.70
1:D:53:ILE:N	1:D:53:ILE:HD13	2.04	0.70
1:A:18:ARG:HG3	1:A:74:ASN:HA	1.72	0.70
1:D:56:ILE:H	1:D:57:PRO:CD	2.05	0.70
3:C:148:GLN:HE21	3:C:148:GLN:HA	1.56	0.70
1:D:59:ARG:O	1:D:60:PHE:C	2.30	0.69
3:F:322:GLY:HA3	3:F:345:ALA:HA	1.72	0.69
3:C:327:SER:O	3:C:330:LYS:O	2.10	0.69
1:D:49:LYS:HB3	1:D:50:TYR:CD2	2.27	0.69
2:E:106:PHE:HZ	2:E:109:MET:HG2	1.56	0.69
2:E:71:THR:HG23	2:E:80:TYR:HD2	1.57	0.69
3:F:391:LYS:HD2	3:F:400:ASP:HA	1.74	0.69
2:B:103:THR:O	2:B:104:SER:OG	2.09	0.69
1:A:6:GLN:HG3	1:A:23:CYS:CB	2.23	0.69
2:B:161:LEU:HD23	2:B:162:THR:N	1.99	0.69
1:A:12:SER:HB2	1:A:105:LYS:HG3	1.74	0.68
1:A:4:MET:HE1	1:A:86:CYS:CB	2.23	0.68
1:D:48:ILE:HG23	1:D:52:SER:O	1.93	0.68
2:E:71:THR:CG2	2:E:80:TYR:HD2	2.07	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:74:LYS:C	2:E:74:LYS:HE3	2.15	0.67
1:A:90:HIS:HD1	1:A:91:SER:HG	1.39	0.67
1:A:6:GLN:HG3	1:A:22:SER:O	1.89	0.67
2:B:206:VAL:HG22	2:B:215:VAL:HG22	1.77	0.67
2:B:197:TRP:HE1	2:B:221:PRO:HB3	1.59	0.67
1:A:92:PHE:HA	1:A:94:PHE:N	2.02	0.67
2:B:130:VAL:HG22	2:B:151:VAL:HG22	1.78	0.66
1:D:56:ILE:H	1:D:57:PRO:HD3	1.59	0.66
1:A:90:HIS:HD1	1:A:91:SER:H	1.39	0.66
1:A:6:GLN:CG	1:A:23:CYS:CA	2.61	0.66
1:A:6:GLN:CG	1:A:22:SER:C	2.60	0.66
3:F:263:ASP:OD1	3:F:263:ASP:N	2.28	0.66
3:F:165:GLN:NE2	3:F:183:GLU:OE2	2.29	0.66
2:B:43:LYS:N	2:B:43:LYS:HD2	2.10	0.66
2:E:48:ILE:HG23	2:E:64:PHE:CE2	2.31	0.65
1:A:13:VAL:HG13	1:A:14:THR:N	2.04	0.65
1:D:94:PHE:CD2	2:E:106:PHE:CG	2.85	0.65
1:A:15:PRO:HG3	1:A:104:ILE:HD11	1.77	0.65
3:C:327:SER:OG	3:C:333:ALA:O	2.09	0.65
1:A:53:ILE:N	1:A:53:ILE:HD13	2.11	0.65
1:A:117:PRO:HD3	2:B:136:VAL:HG22	1.79	0.65
2:B:157:GLU:CG	2:B:158:PRO:HA	2.16	0.65
2:E:29:PHE:HE2	2:E:34:MET:HG3	1.60	0.65
1:D:48:ILE:N	1:D:48:ILE:HD13	2.03	0.64
3:F:315:GLU:N	3:F:315:GLU:OE1	2.29	0.64
1:D:94:PHE:CE2	2:E:106:PHE:CD1	2.85	0.64
1:A:32:TYR:CZ	2:B:105:TYR:CD1	2.86	0.64
1:A:88:ASN:ND2	1:A:94:PHE:CA	2.60	0.64
1:A:6:GLN:CB	1:A:22:SER:O	2.43	0.63
3:C:319:LEU:HD21	6:K:1:NAG:H81	1.79	0.63
2:E:74:LYS:CE	2:E:74:LYS:HA	2.27	0.63
3:C:364:GLU:O	3:C:382:ARG:NH2	2.30	0.63
1:D:90:HIS:CE1	2:E:105:TYR:HE1	2.17	0.63
3:C:182:ASP:OD2	3:C:183:GLU:N	2.32	0.63
1:D:90:HIS:ND1	2:E:105:TYR:HE1	1.97	0.63
2:E:203:THR:HG22	2:E:218:LYS:HA	1.81	0.63
1:A:90:HIS:ND1	1:A:91:SER:OG	2.28	0.62
3:C:175:GLU:HG2	3:C:180:TYR:HB3	1.81	0.62
2:B:18:VAL:HG23	2:B:86:LEU:HD11	1.80	0.62
2:B:97:ALA:CB	2:B:109:MET:HB3	2.29	0.62
3:F:94:LEU:HB2	3:F:116:ALA:HB3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TRP:O	1:A:47:LEU:HB2	1.99	0.62
2:E:6:GLN:HB2	2:E:22:CYS:HA	1.82	0.62
1:D:2:ILE:O	1:D:95:THR:HG21	2.00	0.62
1:A:5:THR:O	1:A:6:GLN:HB3	1.99	0.62
3:F:149:VAL:HA	6:Q:3:BMA:H62	1.83	0.61
3:C:149:VAL:HG22	3:C:150:HIS:N	2.16	0.61
2:E:58:THR:CB	2:E:60:TYR:HE2	2.10	0.61
2:B:101:GLY:O	2:B:102:SER:HB3	1.99	0.61
2:B:156:PRO:O	2:B:208:HIS:NE2	2.32	0.61
1:A:39:LYS:NZ	1:A:166:SER:OG	2.33	0.61
3:F:216:LEU:HD11	7:F:507:NAG:H82	1.82	0.61
3:C:150:HIS:O	3:C:151:PHE:HB3	1.99	0.61
2:B:155:PHE:CD2	2:B:156:PRO:CA	2.84	0.61
2:B:42:GLY:O	2:B:43:LYS:HB2	2.01	0.60
1:A:18:ARG:HG2	1:A:73:ILE:O	2.02	0.60
3:C:300:GLU:O	3:C:308:ASN:ND2	2.27	0.60
3:F:249:ASN:HD22	5:O:1:NAG:H61	1.66	0.60
1:A:88:ASN:O	1:A:94:PHE:HB3	2.02	0.60
3:C:292:ALA:HB2	3:C:377:LEU:HD12	1.82	0.60
2:B:106:PHE:HE2	2:B:108:GLY:CA	2.11	0.59
3:C:330:LYS:HD2	3:C:330:LYS:H	1.67	0.59
2:B:106:PHE:CE2	2:B:108:GLY:CA	2.85	0.59
2:E:72:VAL:O	2:E:74:LYS:N	2.36	0.59
3:F:285:GLU:OE1	3:F:294:ARG:NE	2.35	0.59
1:A:4:MET:CE	1:A:86:CYS:CB	2.78	0.59
2:B:154:TYR:CZ	2:B:159:VAL:HG11	2.37	0.59
2:E:71:THR:CG2	2:E:80:TYR:CD2	2.86	0.59
1:D:34:HIS:NE2	2:E:106:PHE:HD2	2.00	0.59
1:D:57:PRO:C	1:D:58:SER:HG	1.99	0.59
3:C:301:ILE:HG22	3:C:302:LEU:HG	1.84	0.59
2:E:61:ASN:O	2:E:65:LYS:CB	2.40	0.58
1:D:56:ILE:N	1:D:57:PRO:HD3	2.17	0.58
3:F:276:SER:HB2	5:O:1:NAG:H82	1.83	0.58
3:F:75:ILE:HG22	3:F:401:ILE:HG13	1.83	0.58
1:A:93:PRO:HG2	1:A:95:THR:HG23	1.86	0.58
3:C:155:ILE:HD11	3:C:191:PHE:CD2	2.39	0.58
2:E:128:PRO:HB3	2:E:154:TYR:HB3	1.85	0.58
1:A:13:VAL:HG11	1:A:76:VAL:CG1	2.31	0.57
1:D:50:TYR:CD2	1:D:50:TYR:N	2.72	0.57
1:A:13:VAL:O	1:A:14:THR:HG23	2.02	0.57
1:A:4:MET:HE2	1:A:86:CYS:HB2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:ALA:HB3	2:B:109:MET:HB3	1.87	0.57
3:C:254:ASP:OD1	3:C:381:LYS:NZ	2.33	0.57
2:E:71:THR:HG22	2:E:80:TYR:CB	2.24	0.57
2:E:72:VAL:C	2:E:74:LYS:H	2.07	0.57
2:B:106:PHE:CE2	2:B:108:GLY:N	2.73	0.57
1:D:56:ILE:O	1:D:56:ILE:HG12	2.04	0.57
5:O:1:NAG:H5	5:O:2:NAG:N2	2.20	0.57
1:A:90:HIS:CG	1:A:91:SER:H	2.20	0.57
1:A:94:PHE:HE2	2:B:106:PHE:CD1	2.23	0.57
1:A:90:HIS:CE1	1:A:91:SER:HG	2.23	0.57
3:C:65:TYR:CD2	3:C:87:GLY:HA3	2.40	0.57
3:C:65:TYR:CZ	3:C:88:PRO:HB3	2.40	0.57
1:D:48:ILE:CG2	1:D:52:SER:O	2.53	0.57
2:E:29:PHE:O	2:E:30:THR:OG1	2.15	0.57
2:E:60:TYR:CD2	2:E:60:TYR:N	2.73	0.57
3:F:294:ARG:HD3	3:F:296:LYS:HE3	1.86	0.57
2:B:2:VAL:HG22	2:B:27:TYR:CD1	2.39	0.56
2:E:7:SER:OG	2:E:8:GLY:N	2.36	0.56
1:A:73:ILE:HB	1:A:76:VAL:HG22	1.87	0.56
3:C:302:LEU:HD22	3:C:324:LEU:HB2	1.87	0.56
1:D:23:CYS:SG	1:D:86:CYS:CB	2.94	0.56
3:F:252:ASP:N	3:F:252:ASP:OD1	2.38	0.56
1:D:55:GLY:O	1:D:56:ILE:HB	2.05	0.56
1:A:94:PHE:CE2	2:B:106:PHE:HB2	2.39	0.56
2:B:106:PHE:CD2	2:B:107:TYR:N	2.74	0.56
3:C:75:ILE:HG22	3:C:401:ILE:HG13	1.87	0.56
1:D:158:LEU:HB3	2:E:178:LEU:HD22	1.88	0.56
1:D:34:HIS:CD2	2:E:106:PHE:CD2	2.93	0.56
1:D:94:PHE:CD1	1:D:94:PHE:N	2.73	0.56
2:B:6:GLN:HE21	2:B:116:THR:HG23	1.71	0.56
2:B:39:GLN:CB	2:B:45:LEU:HD13	2.31	0.56
2:B:92:ALA:HB3	2:B:94:TYR:CE2	2.41	0.56
2:B:155:PHE:CD2	2:B:156:PRO:CB	2.89	0.56
1:D:90:HIS:HD1	2:E:105:TYR:HE1	1.51	0.56
2:E:38:LYS:HB3	2:E:48:ILE:HD11	1.88	0.56
1:A:11:LEU:O	1:A:103:GLU:CB	2.52	0.55
2:B:73:ASP:O	2:B:75:SER:N	2.39	0.55
1:A:19:VAL:CG1	1:A:20:SER:N	2.39	0.55
5:O:1:NAG:H5	5:O:2:NAG:HN2	1.71	0.55
1:D:59:ARG:HD2	1:D:73:ILE:HG23	1.88	0.55
2:B:109:MET:HB2	2:B:112:TRP:NE1	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:PHE:H	1:D:94:PHE:HD1	1.53	0.55
1:A:9:ALA:C	1:A:10:THR:HG1	1.97	0.55
1:A:45:ARG:O	1:A:46:LEU:O	2.25	0.55
3:C:97:LYS:HE2	3:C:113:SER:HB3	1.89	0.54
3:F:300:GLU:N	3:F:300:GLU:OE1	2.40	0.54
1:A:20:SER:O	1:A:21:LEU:HB2	2.08	0.54
1:D:13:VAL:HG12	1:D:15:PRO:HA	1.89	0.54
2:B:78:THR:HG22	2:B:79:ALA:N	2.22	0.54
2:E:74:LYS:CE	2:E:74:LYS:CA	2.86	0.54
1:A:85:TYR:OH	2:B:43:LYS:HB3	2.08	0.54
3:F:63:GLN:NE2	4:R:1:NAG:O7	2.40	0.54
1:A:6:GLN:HB3	1:A:23:CYS:CA	2.29	0.54
1:A:94:PHE:O	1:A:95:THR:OG1	2.24	0.54
2:E:33:ASN:HB2	2:E:99:SER:HB3	1.90	0.54
1:D:36:TYR:CZ	1:D:87:GLN:OE1	2.60	0.53
2:E:74:LYS:HE3	2:E:74:LYS:CA	2.38	0.53
2:E:62:GLN:N	2:E:62:GLN:OE1	2.42	0.53
2:B:81:MET:HE2	2:B:83:LEU:HD21	1.90	0.53
1:D:33:LEU:O	1:D:50:TYR:HA	2.08	0.53
2:E:72:VAL:O	2:E:72:VAL:HG23	2.09	0.53
3:C:267:TYR:CD2	3:C:278:TYR:HB3	2.44	0.53
3:F:159:MET:HE1	3:F:187:LEU:HB2	1.90	0.53
1:A:94:PHE:CD1	1:A:94:PHE:N	2.73	0.53
2:B:155:PHE:CD2	2:B:156:PRO:N	2.77	0.53
2:B:98:ARG:O	2:B:109:MET:HA	2.09	0.53
3:F:320:GLY:HA2	5:P:1:NAG:H82	1.91	0.53
1:A:148:ILE:HG22	1:A:190:TYR:HA	1.90	0.53
2:B:24:ALA:HB3	2:B:77:SER:HB3	1.91	0.52
3:C:190:VAL:HG11	3:F:190:VAL:HG21	1.91	0.52
3:F:228:ILE:HD11	3:F:252:ASP:HB3	1.91	0.52
1:A:6:GLN:HB2	1:A:22:SER:C	2.29	0.52
3:C:149:VAL:HG23	6:K:3:BMA:H62	1.90	0.52
1:A:13:VAL:HG22	1:A:14:THR:N	2.25	0.52
3:C:273:PHE:HE2	3:C:302:LEU:HD21	1.74	0.52
1:A:36:TYR:CE1	1:A:46:LEU:HD23	2.44	0.52
1:A:4:MET:CE	1:A:86:CYS:SG	2.97	0.52
1:A:4:MET:HE2	1:A:86:CYS:SG	2.50	0.52
1:A:32:TYR:CZ	2:B:105:TYR:HD1	2.27	0.52
3:F:217:THR:OG1	3:F:218:GLY:N	2.43	0.52
2:E:39:GLN:HB2	2:E:45:LEU:HD23	1.92	0.51
3:C:330:LYS:HG2	3:C:335:ILE:HD12	1.90	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:71:THR:CG2	2:E:80:TYR:CB	2.86	0.51
1:D:131:VAL:HG22	1:D:176:THR:HG22	1.91	0.51
3:F:100:ILE:HA	3:F:110:SER:O	2.11	0.51
1:D:88:ASN:HD22	1:D:95:THR:H	1.58	0.51
2:E:110:ASP:HB3	2:E:111:TYR:HD2	1.74	0.51
3:F:175:GLU:HB3	3:F:180:TYR:HB3	1.91	0.51
3:F:145:GLU:HG2	3:F:332:GLY:O	2.10	0.51
1:A:88:ASN:ND2	1:A:94:PHE:C	2.63	0.51
1:A:11:LEU:O	1:A:103:GLU:N	2.38	0.51
3:C:186:SER:HA	3:C:197:PRO:HB3	1.93	0.51
1:A:164:GLN:OE1	1:A:169:SER:HB3	2.11	0.51
2:B:76:SER:O	2:B:78:THR:N	2.43	0.51
3:C:150:HIS:O	3:C:151:PHE:HB2	2.11	0.51
3:C:41:ILE:HG21	3:C:258:PRO:HG2	1.92	0.51
1:D:49:LYS:HG3	1:D:54:SER:OG	2.11	0.51
3:F:85:GLU:OE2	3:F:341:HIS:NE2	2.41	0.51
3:C:299:ALA:O	3:C:303:ALA:HB2	2.11	0.50
2:B:43:LYS:CD	2:B:43:LYS:N	2.73	0.50
1:D:136:ASN:HA	1:D:170:THR:HB	1.93	0.50
3:F:141:LEU:HD13	3:F:387:ILE:HG21	1.94	0.50
1:A:50:TYR:CD2	1:A:50:TYR:N	2.80	0.50
3:C:190:VAL:HG21	3:F:190:VAL:HG11	1.93	0.50
1:A:89:GLY:O	2:B:106:PHE:N	2.43	0.50
1:A:129:SER:CB	2:B:152:LYS:NZ	2.74	0.50
1:A:36:TYR:CD1	1:A:46:LEU:HD23	2.46	0.50
1:A:92:PHE:CB	1:A:93:PRO:CA	2.86	0.50
2:E:65:LYS:HG3	2:E:66:ASP:N	2.24	0.50
3:F:242:THR:HG1	3:F:245:CYS:HG	1.59	0.50
1:A:135:ASN:OD1	1:A:135:ASN:N	2.42	0.50
2:B:106:PHE:C	2:B:106:PHE:CD2	2.85	0.49
1:A:93:PRO:HG3	2:B:61:ASN:ND2	2.27	0.49
2:B:75:SER:C	2:B:77:SER:H	2.15	0.49
1:D:181:LYS:NZ	1:D:185:GLU:OE2	2.41	0.49
1:A:8:PRO:HA	1:A:9:ALA:CB	2.22	0.49
2:B:154:TYR:CD1	2:B:154:TYR:C	2.85	0.49
2:B:155:PHE:CD2	2:B:155:PHE:C	2.85	0.49
3:F:298:PRO:HG2	3:F:301:ILE:HG12	1.94	0.49
1:A:46:LEU:HD22	1:A:47:LEU:H	1.77	0.49
1:A:9:ALA:O	1:A:10:THR:CB	2.58	0.49
2:E:64:PHE:C	2:E:64:PHE:CD2	2.85	0.49
3:C:330:LYS:CD	3:C:330:LYS:N	2.73	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ASN:O	1:A:94:PHE:HA	2.13	0.49
2:B:2:VAL:O	2:B:2:VAL:HG13	2.13	0.49
2:B:29:PHE:CE1	2:B:77:SER:O	2.66	0.49
1:D:58:SER:CB	1:D:60:PHE:CE2	2.96	0.49
1:A:45:ARG:C	1:A:46:LEU:O	2.52	0.48
3:C:99:ASN:O	3:C:111:ALA:HA	2.13	0.48
1:D:56:ILE:N	1:D:57:PRO:CD	2.73	0.48
3:C:90:THR:N	3:C:124:SER:OG	2.45	0.48
1:D:96:PHE:CD2	2:E:45:LEU:HB2	2.48	0.48
3:F:186:SER:HA	3:F:197:PRO:HB3	1.96	0.48
3:F:226:THR:HG21	3:F:255:SER:HB2	1.94	0.48
2:B:2:VAL:HG22	2:B:27:TYR:HD1	1.74	0.48
3:F:71:ASN:O	3:F:75:ILE:HG13	2.13	0.48
1:A:13:VAL:CG1	1:A:14:THR:H	2.03	0.48
2:B:147:LEU:HG	2:B:197:TRP:CZ3	2.49	0.48
2:E:2:VAL:HG21	2:E:111:TYR:CD2	2.49	0.48
3:C:148:GLN:HE21	3:C:148:GLN:CA	2.26	0.48
3:C:292:ALA:HA	3:C:371:PRO:HD3	1.95	0.48
1:A:13:VAL:HG23	1:A:17:ASP:CG	2.34	0.48
2:B:161:LEU:HD23	2:B:205:ASN:O	2.14	0.48
3:F:133:ILE:HD11	3:F:176:LEU:HD22	1.96	0.48
2:B:97:ALA:HB1	2:B:109:MET:HB3	1.96	0.48
1:D:191:THR:HG22	1:D:206:SER:HB3	1.96	0.48
1:D:6:GLN:NE2	1:D:84:TYR:O	2.47	0.48
1:D:94:PHE:HD1	1:D:94:PHE:N	2.09	0.48
3:F:149:VAL:HA	6:Q:3:BMA:C6	2.42	0.48
2:B:87:THR:HG22	2:B:89:GLU:H	1.79	0.48
1:A:8:PRO:CA	1:A:9:ALA:CB	2.85	0.47
3:C:346:ASP:OD1	3:C:347:GLU:N	2.46	0.47
2:E:76:SER:O	2:E:77:SER:OG	2.19	0.47
1:D:174:SER:HB3	2:E:175:PHE:CD1	2.49	0.47
2:B:100:ARG:HG3	2:B:101:GLY:N	2.30	0.47
3:F:265:VAL:HG12	3:F:278:TYR:HB2	1.96	0.47
1:A:92:PHE:HA	1:A:94:PHE:CD1	2.49	0.47
1:A:37:GLN:OE1	1:A:45:ARG:NH1	2.46	0.47
3:C:378:LYS:HE3	3:C:416:HIS:ND1	2.30	0.47
2:E:74:LYS:HE3	2:E:75:SER:N	2.28	0.47
3:F:222:TYR:HD2	3:F:223:LEU:N	2.12	0.47
1:D:34:HIS:NE2	2:E:106:PHE:CD2	2.83	0.47
2:E:216:ASP:OD1	2:E:216:ASP:N	2.47	0.47
3:F:222:TYR:O	3:F:257:HIS:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:249:ASN:ND2	5:O:1:NAG:H61	2.30	0.47
1:A:113:VAL:HG22	1:A:134:LEU:HD22	1.97	0.47
2:B:6:GLN:NE2	2:B:116:THR:HG23	2.29	0.47
3:C:144:ILE:O	3:C:148:GLN:HG2	2.15	0.46
3:C:296:LYS:HG2	3:C:366:PHE:HB3	1.97	0.46
2:E:11:LEU:HD23	2:E:156:PRO:HG3	1.96	0.46
2:E:110:ASP:HB3	2:E:111:TYR:CD2	2.51	0.46
1:D:34:HIS:CD2	2:E:106:PHE:CE2	3.03	0.46
3:F:44:ARG:HA	3:F:102:PHE:HZ	1.80	0.46
2:B:155:PHE:O	2:B:208:HIS:HE1	1.97	0.46
3:F:313:ILE:HD11	3:F:325:ASN:ND2	2.30	0.46
1:A:19:VAL:CG1	1:A:21:LEU:HD13	2.46	0.46
3:F:242:THR:OG1	3:F:245:CYS:SG	2.66	0.46
1:A:88:ASN:O	1:A:94:PHE:CB	2.62	0.46
2:B:156:PRO:HD2	2:B:208:HIS:CE1	2.50	0.46
3:C:57:PRO:HG2	3:C:58:LEU:HD12	1.97	0.46
1:A:109:ALA:HB3	1:A:138:TYR:N	2.30	0.46
1:A:168:ASP:O	1:A:170:THR:N	2.48	0.46
2:B:128:PRO:HB3	2:B:154:TYR:CB	2.46	0.46
1:D:83:VAL:HG13	1:D:101:LYS:HB2	1.96	0.46
1:A:168:ASP:N	1:A:168:ASP:OD1	2.49	0.46
2:B:154:TYR:O	2:B:184:TYR:HB2	2.15	0.46
3:C:267:TYR:CZ	5:I:1:NAG:H62	2.51	0.46
3:F:152:LEU:HB3	3:F:156:ILE:HG12	1.97	0.46
3:F:340:PRO:HG2	3:F:382:ARG:HB3	1.98	0.46
1:A:8:PRO:CB	1:A:9:ALA:HB2	2.45	0.46
2:B:76:SER:C	2:B:78:THR:H	2.19	0.46
1:D:34:HIS:HD2	2:E:106:PHE:CE2	2.34	0.46
3:C:253:GLY:HA2	3:C:268:VAL:HG23	1.98	0.45
2:E:29:PHE:CE1	2:E:53:PRO:HG3	2.51	0.45
3:C:63:GLN:HG2	3:C:90:THR:HG22	1.98	0.45
1:A:92:PHE:C	1:A:92:PHE:CD2	2.85	0.45
2:B:154:TYR:O	2:B:154:TYR:CG	2.68	0.45
3:C:216:LEU:HD23	3:C:229:VAL:HG11	1.97	0.45
1:D:153:ARG:HA	1:D:153:ARG:HD3	1.83	0.45
1:D:111:PRO:HD3	1:D:196:HIS:CD2	2.52	0.45
3:F:323:VAL:HG23	3:F:338:SER:HB3	1.98	0.45
2:B:72:VAL:HG23	2:B:73:ASP:N	2.31	0.45
3:C:85:GLU:OE2	3:C:341:HIS:NE2	2.44	0.45
3:F:224:ASN:N	3:F:224:ASN:OD1	2.49	0.45
3:F:82:ARG:HA	3:F:354:GLU:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:CYS:O	2:B:216:ASP:HA	2.16	0.45
3:F:409:MET:HG2	3:F:410:TYR:N	2.32	0.45
3:C:360:GLN:C	3:C:362:ASP:H	2.18	0.45
2:E:30:THR:HG22	2:E:54:TYR:HD1	1.81	0.45
3:F:151:PHE:HD1	3:F:152:LEU:HB2	1.82	0.45
1:A:19:VAL:HG11	1:A:21:LEU:HD13	1.97	0.45
3:C:390:LYS:HE3	3:C:390:LYS:HB2	1.69	0.45
3:C:71:ASN:O	3:C:75:ILE:HG13	2.17	0.45
3:F:132:LEU:HA	3:F:172:THR:HA	1.99	0.45
3:C:314:PRO:HG3	6:K:1:NAG:O7	2.17	0.45
1:A:56:ILE:N	1:A:57:PRO:CD	2.75	0.45
1:A:92:PHE:CA	1:A:94:PHE:H	2.10	0.45
2:B:100:ARG:O	2:B:107:TYR:CD2	2.70	0.45
1:D:96:PHE:HD1	1:D:96:PHE:HA	1.59	0.45
2:E:74:LYS:NZ	2:E:74:LYS:HA	2.32	0.45
1:A:148:ILE:O	1:A:148:ILE:HG13	2.15	0.44
1:A:40:SER:OG	1:A:163:ASP:OD2	2.34	0.44
1:A:94:PHE:HE2	2:B:106:PHE:HD1	1.63	0.44
1:D:147:LYS:HG3	1:D:191:THR:OG1	2.16	0.44
1:D:58:SER:CB	1:D:60:PHE:HE2	2.30	0.44
2:B:106:PHE:CE2	2:B:107:TYR:C	2.91	0.44
2:B:21:SER:HA	2:B:79:ALA:O	2.17	0.44
3:C:148:GLN:CA	3:C:148:GLN:NE2	2.73	0.44
3:C:313:ILE:N	3:C:314:PRO:HD2	2.32	0.44
2:E:71:THR:HG23	2:E:80:TYR:CD2	2.45	0.44
3:F:249:ASN:OD1	3:F:249:ASN:N	2.49	0.44
3:F:376:ILE:HD11	3:F:379:ALA:HB2	1.99	0.44
2:B:67:LYS:NZ	2:B:90:ASP:OD2	2.46	0.44
1:D:111:PRO:HB3	1:D:137:PHE:HB3	1.98	0.44
1:D:138:TYR:CG	1:D:139:PRO:HA	2.51	0.44
2:E:20:ILE:O	2:E:80:TYR:HA	2.17	0.44
3:C:74:GLU:OE1	3:C:74:GLU:N	2.50	0.44
1:D:94:PHE:CE2	2:E:106:PHE:HD1	2.36	0.44
1:D:21:LEU:HD22	1:D:100:THR:HG21	1.98	0.44
1:D:92:PHE:CD1	1:D:92:PHE:O	2.70	0.44
2:E:163:TRP:NE1	2:E:172:VAL:HG21	2.32	0.44
2:E:101:GLY:HA2	2:E:107:TYR:CD2	2.52	0.44
1:A:119:SER:HB3	2:B:132:PRO:O	2.18	0.43
2:B:133:LEU:HD11	2:B:150:LEU:HB2	1.99	0.43
3:F:370:ASN:HB2	3:F:377:LEU:HD11	1.99	0.43
1:A:10:THR:HG22	1:A:11:LEU:N	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:ALA:CB	3:F:155:ILE:HD11	2.48	0.43
3:F:290:LEU:HD22	3:F:290:LEU:H	1.82	0.43
1:D:33:LEU:HD12	1:D:86:CYS:HB2	2.01	0.43
3:F:360:GLN:C	3:F:362:ASP:H	2.21	0.43
3:C:330:LYS:CD	3:C:330:LYS:H	2.31	0.43
2:E:65:LYS:O	2:E:66:ASP:C	2.56	0.43
2:B:39:GLN:CG	2:B:43:LYS:HA	2.49	0.43
3:C:86:VAL:HG13	4:G:1:NAG:H82	2.01	0.43
3:C:149:VAL:CG2	3:C:150:HIS:N	2.79	0.43
3:F:198:TYR:HB2	3:F:203:TYR:CZ	2.53	0.43
3:F:236:SER:OG	3:F:246:ASN:O	2.31	0.43
3:F:63:GLN:HA	3:F:90:THR:HA	2.01	0.43
2:B:20:ILE:O	2:B:80:TYR:HA	2.17	0.43
5:I:1:NAG:H5	5:I:2:NAG:N2	2.34	0.43
2:B:23:MET:HA	2:B:78:THR:HA	2.00	0.43
2:B:78:THR:CG2	2:B:79:ALA:N	2.82	0.43
3:C:151:PHE:CE1	3:C:152:LEU:HG	2.53	0.43
1:D:2:ILE:O	1:D:95:THR:CG2	2.66	0.42
2:B:109:MET:HB2	2:B:112:TRP:HE1	1.83	0.42
2:B:40:SER:O	2:B:42:GLY:N	2.53	0.42
3:C:100:ILE:HA	3:C:110:SER:O	2.19	0.42
2:B:100:ARG:NH1	3:C:395:PHE:O	2.52	0.42
1:D:10:THR:HA	1:D:101:LYS:O	2.19	0.42
3:F:74:GLU:N	3:F:74:GLU:OE1	2.52	0.42
3:F:320:GLY:CA	5:P:1:NAG:H82	2.50	0.42
1:A:59:ARG:CD	1:A:59:ARG:H	2.31	0.42
3:C:165:GLN:HE21	3:C:184:ILE:HG12	1.83	0.42
3:C:348:ARG:H	3:C:348:ARG:HG3	1.40	0.42
3:C:44:ARG:O	3:C:47:THR:OG1	2.36	0.42
1:D:105:LYS:HB2	1:D:105:LYS:HE3	1.81	0.42
1:D:153:ARG:HH22	1:D:179:LEU:HD11	1.84	0.42
3:F:140:VAL:HA	3:F:143:VAL:HG22	2.02	0.42
3:F:384:GLN:HG3	3:F:410:TYR:HB3	2.01	0.42
2:B:49:GLY:HA2	2:B:60:TYR:HA	2.01	0.42
2:B:99:SER:OG	2:B:100:ARG:N	2.53	0.42
3:C:419:LYS:HB2	3:C:419:LYS:HE2	1.88	0.42
2:E:101:GLY:HA2	2:E:107:TYR:CG	2.54	0.42
2:E:162:THR:HG22	2:E:205:ASN:HB2	2.02	0.42
3:F:230:GLU:OE2	3:F:234:LYS:N	2.52	0.42
1:A:6:GLN:CB	1:A:22:SER:C	2.87	0.42
1:A:47:LEU:HD23	1:A:47:LEU:HA	1.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:82:ARG:HG2	3:F:354:GLU:HB2	2.02	0.42
2:B:128:PRO:HB3	2:B:154:TYR:HB2	2.02	0.42
2:B:40:SER:C	2:B:42:GLY:N	2.73	0.42
1:D:58:SER:HB3	1:D:60:PHE:CE2	2.55	0.42
2:E:130:VAL:HG23	2:E:217:LYS:HG3	2.01	0.42
3:C:86:VAL:CG1	4:G:1:NAG:H82	2.50	0.42
1:A:6:GLN:N	1:A:6:GLN:CD	2.73	0.42
3:C:160:LEU:HD13	3:C:160:LEU:HA	1.89	0.42
3:C:256:PHE:CD1	3:C:266:LEU:HD13	2.54	0.42
1:D:15:PRO:HB3	1:D:104:ILE:HD11	2.01	0.42
1:A:10:THR:O	1:A:11:LEU:HD22	2.19	0.42
2:B:42:GLY:C	2:B:43:LYS:CD	2.89	0.42
2:B:67:LYS:HB2	2:B:67:LYS:HE3	1.82	0.42
1:A:6:GLN:HB2	1:A:23:CYS:CA	2.45	0.42
1:A:6:GLN:HB3	1:A:24:ARG:H	1.85	0.41
3:C:409:MET:HG2	3:C:410:TYR:N	2.35	0.41
2:E:67:LYS:O	2:E:84:LYS:HG2	2.20	0.41
2:E:72:VAL:C	2:E:74:LYS:N	2.73	0.41
1:A:56:ILE:H	1:A:57:PRO:HD3	1.82	0.41
1:A:59:ARG:CD	1:A:59:ARG:N	2.83	0.41
1:A:90:HIS:CG	1:A:91:SER:N	2.86	0.41
2:E:128:PRO:HB2	2:E:151:VAL:HG23	2.01	0.41
2:E:35:ASN:ND2	2:E:47:TRP:HE1	2.19	0.41
1:A:38:GLN:HE21	1:A:44:PRO:HG3	1.85	0.41
2:B:21:SER:HB3	2:B:80:TYR:CE1	2.55	0.41
3:C:265:VAL:HG22	3:C:280:THR:HG22	2.03	0.41
3:C:303:ALA:HA	3:C:321:SER:HB3	2.01	0.41
1:A:14:THR:C	1:A:16:GLY:N	2.73	0.41
2:B:75:SER:C	2:B:77:SER:N	2.73	0.41
2:B:76:SER:C	2:B:78:THR:N	2.73	0.41
3:F:293:PHE:CE2	3:F:371:PRO:HB3	2.55	0.41
1:A:10:THR:HA	1:A:101:LYS:O	2.20	0.41
2:B:102:SER:C	2:B:104:SER:N	2.73	0.41
3:C:270:PRO:HG2	3:C:273:PHE:HB2	2.02	0.41
1:A:115:ILE:HD13	1:A:192:CYS:SG	2.61	0.41
1:A:13:VAL:O	1:A:14:THR:OG1	2.37	0.41
3:C:426:LYS:H	3:C:426:LYS:HG3	1.59	0.41
2:B:105:TYR:CD2	2:B:105:TYR:N	2.87	0.41
1:D:6:GLN:NE2	1:D:100:THR:HG23	2.29	0.41
1:D:148:ILE:HD13	1:D:187:HIS:ND1	2.36	0.41
3:F:150:HIS:HA	3:F:153:ARG: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:105:LYS:HA	1:A:138:TYR:OH	2.20	0.41
2:B:211:SER:O	2:B:213:THR:HG23	2.21	0.41
3:C:180:TYR:HE1	3:C:199:PHE:HD2	1.69	0.41
3:F:151:PHE:CD1	3:F:151:PHE:C	2.94	0.41
1:D:25:ALA:CB	1:D:29:ILE:HD11	2.50	0.40
1:A:77:GLU:HB3	1:A:78:PRO:HD2	2.03	0.40
1:A:94:PHE:CE2	2:B:106:PHE:HD1	2.31	0.40
1:A:88:ASN:CG	1:A:94:PHE:HA	2.41	0.40
3:C:122:ASP:OD1	3:C:123:GLN:N	2.53	0.40
3:C:367:VAL:HG12	3:C:369:ILE:HG23	2.03	0.40
2:E:147:LEU:HD22	2:E:219:ILE:HG21	2.03	0.40
2:E:60:TYR:HD2	2:E:60:TYR:N	2.17	0.40
3:C:340:PRO:HG2	3:C:382:ARG:HB3	2.03	0.40
2:E:36:TRP:HZ2	2:E:79:ALA:HB1	1.86	0.40
2:B:178:LEU:HD13	2:B:178:LEU:H	1.86	0.40
3:C:369:ILE:HG22	3:C:376:ILE:HA	2.02	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	207/213 (97%)	153 (74%)	33 (16%)	21 (10%)	0	7
1	D	207/213 (97%)	179 (86%)	22 (11%)	6 (3%)	4	31
2	B	219/222 (99%)	188 (86%)	18 (8%)	13 (6%)	1	15
2	E	219/222 (99%)	183 (84%)	28 (13%)	8 (4%)	3	26
3	C	392/394 (100%)	342 (87%)	45 (12%)	5 (1%)	12	48
3	F	390/394 (99%)	351 (90%)	36 (9%)	3 (1%)	19	58
All	All	1634/1658 (99%)	1396 (85%)	182 (11%)	56 (3%)	3	28

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	14	THR
1	A	46	LEU
1	A	59	ARG
1	A	94	PHE
2	B	44	SER
2	B	77	SER
2	B	102	SER
2	B	104	SER
3	C	150	HIS
3	C	151	PHE
3	C	331	ASN
1	D	56	ILE
1	D	60	PHE
2	E	73	ASP
2	E	75	SER
2	E	77	SER
1	A	6	GLN
1	A	9	ALA
1	A	29	ILE
1	A	58	SER
1	A	90	HIS
2	B	73	ASP
2	B	74	LYS
2	B	212	SER
1	D	57	PRO
2	E	30	THR
2	E	136	VAL
3	F	149	VAL
1	A	10	THR
1	A	17	ASP
1	A	169	SER
2	B	105	TYR
2	B	159	VAL
1	A	15	PRO
1	A	49	LYS
1	A	52	SER
1	A	76	VAL
3	C	329	CYS
1	D	35	TRP
1	D	101	LYS
2	E	74	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	151	VAL
3	F	226	THR
1	D	199	SER
2	E	78	THR
1	A	95	THR
2	B	209	PRO
3	C	334	PRO
1	A	16	GLY
2	B	72	VAL
1	A	92	PHE
2	B	2	VAL
2	B	101	GLY
3	F	314	PRO
1	A	93	PRO

5.3.2 Protein sidechains ⓘ

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	186/193 (96%)	158 (85%)	28 (15%)	3	17
1	D	187/193 (97%)	171 (91%)	16 (9%)	10	38
2	B	187/192 (97%)	151 (81%)	36 (19%)	1	7
2	E	186/192 (97%)	156 (84%)	30 (16%)	2	14
3	C	341/355 (96%)	312 (92%)	29 (8%)	10	39
3	F	340/355 (96%)	310 (91%)	30 (9%)	10	38
All	All	1427/1480 (96%)	1258 (88%)	169 (12%)	5	25

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	5	THR
1	A	6	GLN
1	A	11	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	12	SER
1	A	14	THR
1	A	17	ASP
1	A	29	ILE
1	A	33	LEU
1	A	46	LEU
1	A	47	LEU
1	A	50	TYR
1	A	53	ILE
1	A	56	ILE
1	A	59	ARG
1	A	61	SER
1	A	71	LEU
1	A	86	CYS
1	A	88	ASN
1	A	91	SER
1	A	92	PHE
1	A	163	ASP
1	A	165	ASP
1	A	182	ASP
1	A	189	SER
1	A	191	THR
1	A	193	GLU
1	A	210	ASN
2	B	2	VAL
2	B	22	CYS
2	B	23	MET
2	B	38	LYS
2	B	40	SER
2	B	41	ASN
2	B	43	LYS
2	B	45	LEU
2	B	46	GLU
2	B	51	ILE
2	B	59	ARG
2	B	60	TYR
2	B	62	GLN
2	B	66	ASP
2	B	71	THR
2	B	76	SER
2	B	77	SER
2	B	96	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	98	ARG
2	B	100	ARG
2	B	103	THR
2	B	109	MET
2	B	147	LEU
2	B	155	PHE
2	B	159	VAL
2	B	160	THR
2	B	161	LEU
2	B	178	LEU
2	B	179	LEU
2	B	196	THR
2	B	197	TRP
2	B	202	ILE
2	B	203	THR
2	B	206	VAL
2	B	213	THR
2	B	216	ASP
3	C	43	LEU
3	C	44	ARG
3	C	47	THR
3	C	84	GLU
3	C	100	ILE
3	C	133	ILE
3	C	153	ARG
3	C	155	ILE
3	C	159	MET
3	C	160	LEU
3	C	167	LEU
3	C	177	LEU
3	C	181	LYS
3	C	213	TYR
3	C	216	LEU
3	C	252	ASP
3	C	272	ASP
3	C	273	PHE
3	C	300	GLU
3	C	318	CYS
3	C	329	CYS
3	C	330	LYS
3	C	331	ASN
3	C	348	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	354	GLU
3	C	372	LEU
3	C	411	LEU
3	C	426	LYS
3	C	429	ILE
1	D	14	THR
1	D	41	HIS
1	D	46	LEU
1	D	56	ILE
1	D	59	ARG
1	D	88	ASN
1	D	91	SER
1	D	94	PHE
1	D	95	THR
1	D	96	PHE
1	D	106	ARG
1	D	130	VAL
1	D	141	ASP
1	D	161	TRP
1	D	193	GLU
1	D	206	SER
2	E	4	LEU
2	E	6	GLN
2	E	10	GLU
2	E	51	ILE
2	E	58	THR
2	E	60	TYR
2	E	62	GLN
2	E	65	LYS
2	E	66	ASP
2	E	70	LEU
2	E	74	LYS
2	E	81	MET
2	E	84	LYS
2	E	98	ARG
2	E	109	MET
2	E	110	ASP
2	E	116	THR
2	E	126	THR
2	E	133	LEU
2	E	136	VAL
2	E	137	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	146	THR
2	E	157	GLU
2	E	162	THR
2	E	169	SER
2	E	170	SER
2	E	173	HIS
2	E	179	LEU
2	E	197	TRP
2	E	216	ASP
3	F	52	SER
3	F	54	GLU
3	F	63	GLN
3	F	151	PHE
3	F	157	GLU
3	F	160	LEU
3	F	164	GLN
3	F	166	LYS
3	F	167	LEU
3	F	205	LYS
3	F	216	LEU
3	F	217	THR
3	F	219	GLU
3	F	222	TYR
3	F	223	LEU
3	F	224	ASN
3	F	249	ASN
3	F	263	ASP
3	F	290	LEU
3	F	306	SER
3	F	313	ILE
3	F	319	LEU
3	F	323	VAL
3	F	329	CYS
3	F	331	ASN
3	F	356	MET
3	F	365	THR
3	F	368	ASP
3	F	400	ASP
3	F	420	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
3	C	148	GLN
3	C	150	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

39 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	$\# Z > 2$
4	NAG	G	1	3,4	14,14,15	0.48	0	17,19,21	0.58	0
4	NAG	G	2	4	14,14,15	0.26	0	17,19,21	0.46	0
4	BMA	G	3	4	11,11,12	0.74	0	15,15,17	0.68	0
4	MAN	G	4	4	11,11,12	0.93	1 (9%)	15,15,17	1.71	3 (20%)
5	NAG	H	1	3,5	14,14,15	0.37	0	17,19,21	0.43	0
5	NAG	H	2	5	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	I	1	3,5	14,14,15	0.89	1 (7%)	17,19,21	1.40	1 (5%)
5	NAG	I	2	5	14,14,15	0.33	0	17,19,21	0.56	0
5	NAG	J	1	3,5	14,14,15	0.32	0	17,19,21	0.60	0
5	NAG	J	2	5	14,14,15	0.24	0	17,19,21	0.33	0
6	NAG	K	1	3,6	14,14,15	0.39	0	17,19,21	0.53	0
6	NAG	K	2	6	14,14,15	0.83	1 (7%)	17,19,21	1.32	1 (5%)
6	BMA	K	3	6	11,11,12	0.63	0	15,15,17	0.89	0
6	MAN	K	4	6	11,11,12	0.66	0	15,15,17	1.15	2 (13%)
6	MAN	K	5	6	11,11,12	0.79	0	15,15,17	1.26	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	L	1	3,6	14,14,15	0.18	0	17,19,21	0.99	1 (5%)
6	NAG	L	2	6	14,14,15	0.36	0	17,19,21	0.49	0
6	BMA	L	3	6	11,11,12	1.12	1 (9%)	15,15,17	0.88	0
6	MAN	L	4	6	11,11,12	1.06	0	15,15,17	1.03	2 (13%)
6	MAN	L	5	6	11,11,12	0.84	1 (9%)	15,15,17	1.74	3 (20%)
4	NAG	M	1	3,4	14,14,15	0.67	1 (7%)	17,19,21	0.55	0
4	NAG	M	2	4	14,14,15	0.30	0	17,19,21	0.46	0
4	BMA	M	3	4	11,11,12	1.15	2 (18%)	15,15,17	0.93	2 (13%)
4	MAN	M	4	4	11,11,12	0.92	0	15,15,17	1.56	2 (13%)
5	NAG	N	1	3,5	14,14,15	0.40	0	17,19,21	0.48	0
5	NAG	N	2	5	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	O	1	3,5	14,14,15	0.59	0	17,19,21	1.12	1 (5%)
5	NAG	O	2	5	14,14,15	0.22	0	17,19,21	0.50	0
5	NAG	P	1	3,5	14,14,15	0.96	2 (14%)	17,19,21	1.11	1 (5%)
5	NAG	P	2	5	14,14,15	0.20	0	17,19,21	0.50	0
6	NAG	Q	1	3,6	14,14,15	0.62	0	17,19,21	0.86	1 (5%)
6	NAG	Q	2	6	14,14,15	0.74	1 (7%)	17,19,21	1.21	1 (5%)
6	BMA	Q	3	6	11,11,12	1.34	2 (18%)	15,15,17	1.63	4 (26%)
6	MAN	Q	4	6	11,11,12	1.16	2 (18%)	15,15,17	0.89	0
6	MAN	Q	5	6	11,11,12	0.83	0	15,15,17	1.25	3 (20%)
4	NAG	R	1	3,4	14,14,15	0.30	0	17,19,21	1.31	1 (5%)
4	NAG	R	2	4	14,14,15	0.60	1 (7%)	17,19,21	0.39	0
4	BMA	R	3	4	11,11,12	1.19	1 (9%)	15,15,17	1.83	2 (13%)
4	MAN	R	4	4	11,11,12	0.97	0	15,15,17	1.23	3 (20%)

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
4	NAG	G	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	1/1/1/1
5	NAG	H	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	NAG	I	1	3,5	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	3	BMA	O5-C1	-3.42	1.38	1.43
5	I	1	NAG	O5-C1	3.23	1.48	1.43
6	K	2	NAG	O5-C1	3.01	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	3	BMA	O5-C1	-2.92	1.39	1.43
5	P	1	NAG	C1-C2	2.71	1.56	1.52
6	Q	3	BMA	O5-C1	-2.67	1.39	1.43
6	Q	4	MAN	O5-C5	2.66	1.48	1.43
6	Q	2	NAG	O5-C1	2.54	1.47	1.43
4	M	1	NAG	O5-C1	-2.43	1.39	1.43
6	Q	3	BMA	C4-C5	2.39	1.58	1.53
4	M	3	BMA	O5-C1	-2.35	1.40	1.43
5	P	1	NAG	O5-C1	2.21	1.47	1.43
6	Q	4	MAN	C1-C2	2.19	1.57	1.52
4	M	3	BMA	C4-C5	2.13	1.57	1.53
4	G	4	MAN	O5-C5	2.12	1.47	1.43
6	L	5	MAN	O5-C5	2.07	1.47	1.43
4	R	2	NAG	O5-C1	-2.06	1.40	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	NAG	C1-O5-C5	5.52	119.67	112.19
4	G	4	MAN	C1-O5-C5	5.47	119.60	112.19
6	L	5	MAN	C1-O5-C5	5.22	119.26	112.19
6	K	2	NAG	C1-O5-C5	5.18	119.20	112.19
4	M	4	MAN	C1-O5-C5	4.80	118.69	112.19
6	Q	2	NAG	C1-O5-C5	4.74	118.62	112.19
4	R	3	BMA	C1-O5-C5	4.57	118.39	112.19
4	R	1	NAG	C1-O5-C5	4.44	118.20	112.19
5	O	1	NAG	C1-O5-C5	4.34	118.08	112.19
6	Q	3	BMA	C3-C4-C5	3.82	117.06	110.24
4	R	3	BMA	O5-C5-C6	-3.81	101.23	107.20
5	P	1	NAG	C1-O5-C5	3.45	116.87	112.19
6	K	4	MAN	C1-O5-C5	3.12	116.41	112.19
6	Q	1	NAG	C1-O5-C5	3.02	116.29	112.19
4	R	4	MAN	C1-C2-C3	-2.65	106.41	109.67
4	R	4	MAN	O2-C2-C3	-2.55	105.02	110.14
6	L	1	NAG	C1-O5-C5	2.55	115.64	112.19
6	L	4	MAN	O2-C2-C3	-2.44	105.25	110.14
6	L	5	MAN	O5-C1-C2	2.42	114.50	110.77
6	L	5	MAN	O2-C2-C3	-2.40	105.33	110.14
6	L	4	MAN	C1-O5-C5	2.38	115.42	112.19
6	K	5	MAN	O5-C1-C2	2.36	114.42	110.77
6	Q	5	MAN	C1-O5-C5	2.36	115.39	112.19
6	K	4	MAN	O2-C2-C3	-2.33	105.47	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	3	BMA	C1-O5-C5	2.33	115.34	112.19
4	R	4	MAN	C1-O5-C5	2.28	115.28	112.19
6	Q	5	MAN	O2-C2-C3	-2.23	105.68	110.14
6	K	5	MAN	O2-C2-C3	-2.16	105.81	110.14
6	K	5	MAN	C1-O5-C5	2.16	115.11	112.19
6	Q	3	BMA	O3-C3-C4	-2.14	105.40	110.35
4	M	3	BMA	O2-C2-C3	-2.10	105.93	110.14
4	M	3	BMA	C3-C4-C5	2.10	113.98	110.24
6	Q	3	BMA	O2-C2-C3	-2.10	105.94	110.14
4	G	4	MAN	O5-C1-C2	2.08	113.99	110.77
4	M	4	MAN	O2-C2-C3	-2.06	106.02	110.14
6	Q	5	MAN	O5-C1-C2	2.05	113.94	110.77
4	G	4	MAN	O2-C2-C3	-2.02	106.08	110.14

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	R	3	BMA	O5-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
6	Q	2	NAG	C4-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6
6	Q	5	MAN	O5-C5-C6-O6
4	R	3	BMA	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
6	Q	5	MAN	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
6	K	4	MAN	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6
4	M	3	BMA	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	K	1	NAG	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	K	4	MAN	O5-C5-C6-O6
6	L	3	BMA	C4-C5-C6-O6
6	L	5	MAN	C4-C5-C6-O6
4	R	4	MAN	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
6	L	4	MAN	O5-C5-C6-O6
4	R	1	NAG	C3-C2-N2-C7
6	L	1	NAG	C3-C2-N2-C7
6	K	1	NAG	C4-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	Q	4	MAN	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6

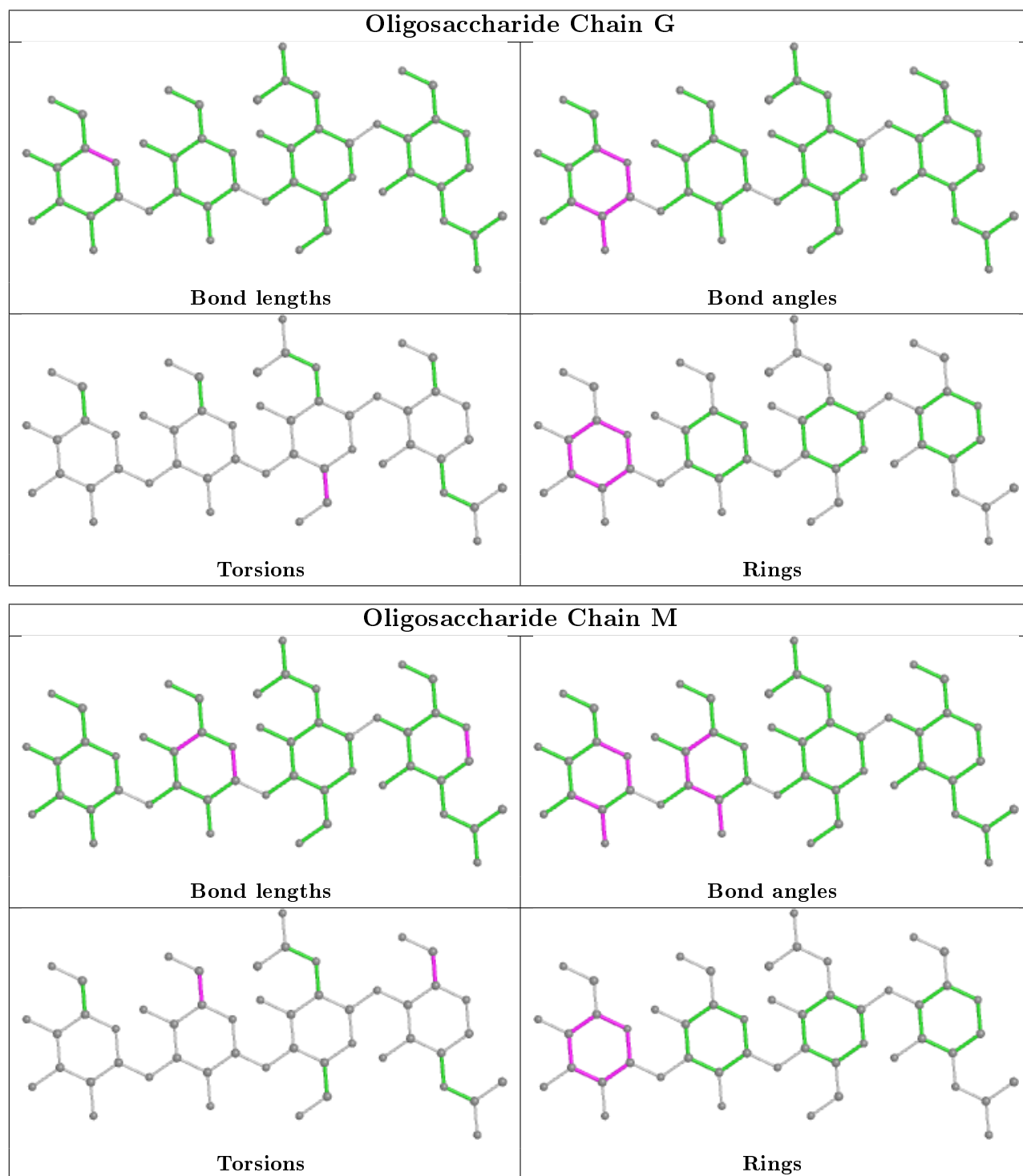
All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	5	MAN	C1-C2-C3-C4-C5-O5
4	G	4	MAN	C1-C2-C3-C4-C5-O5
4	M	4	MAN	C1-C2-C3-C4-C5-O5
6	Q	4	MAN	C1-C2-C3-C4-C5-O5

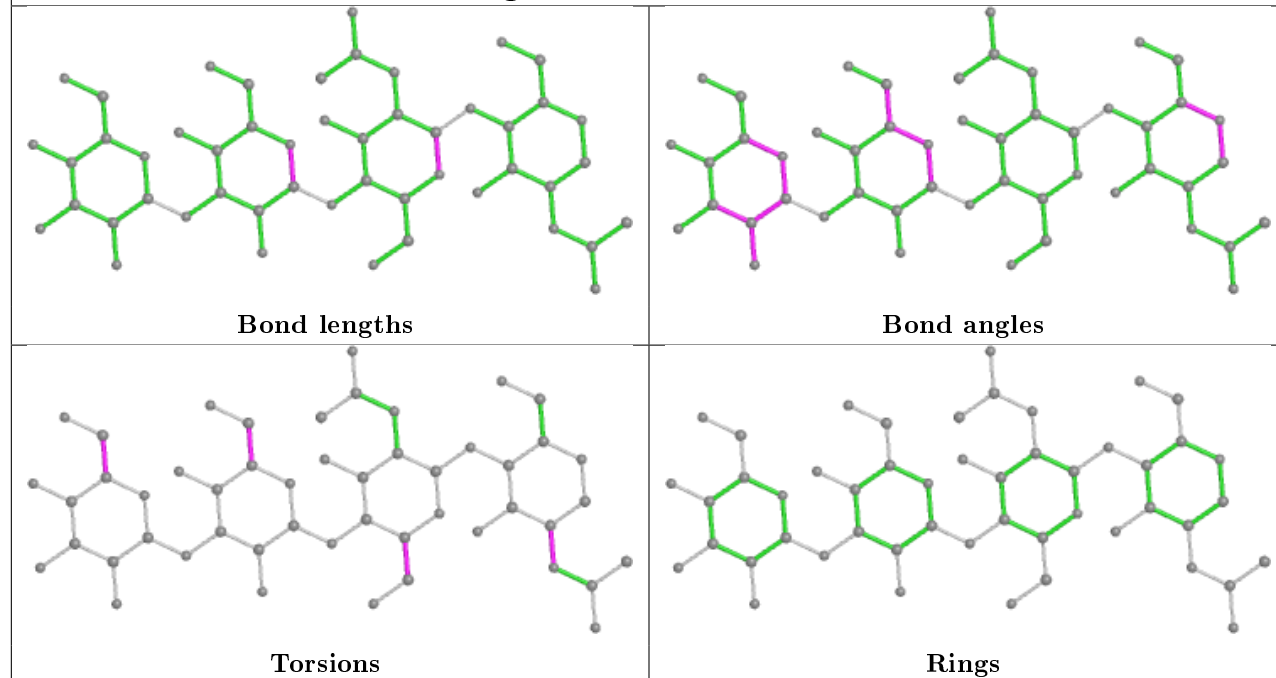
10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	1	NAG	2	0
5	O	2	NAG	2	0
5	O	1	NAG	5	0
5	I	1	NAG	2	0
4	R	1	NAG	1	0
6	K	3	BMA	1	0
5	I	2	NAG	1	0
6	K	1	NAG	2	0
6	Q	3	BMA	2	0
4	G	1	NAG	2	0

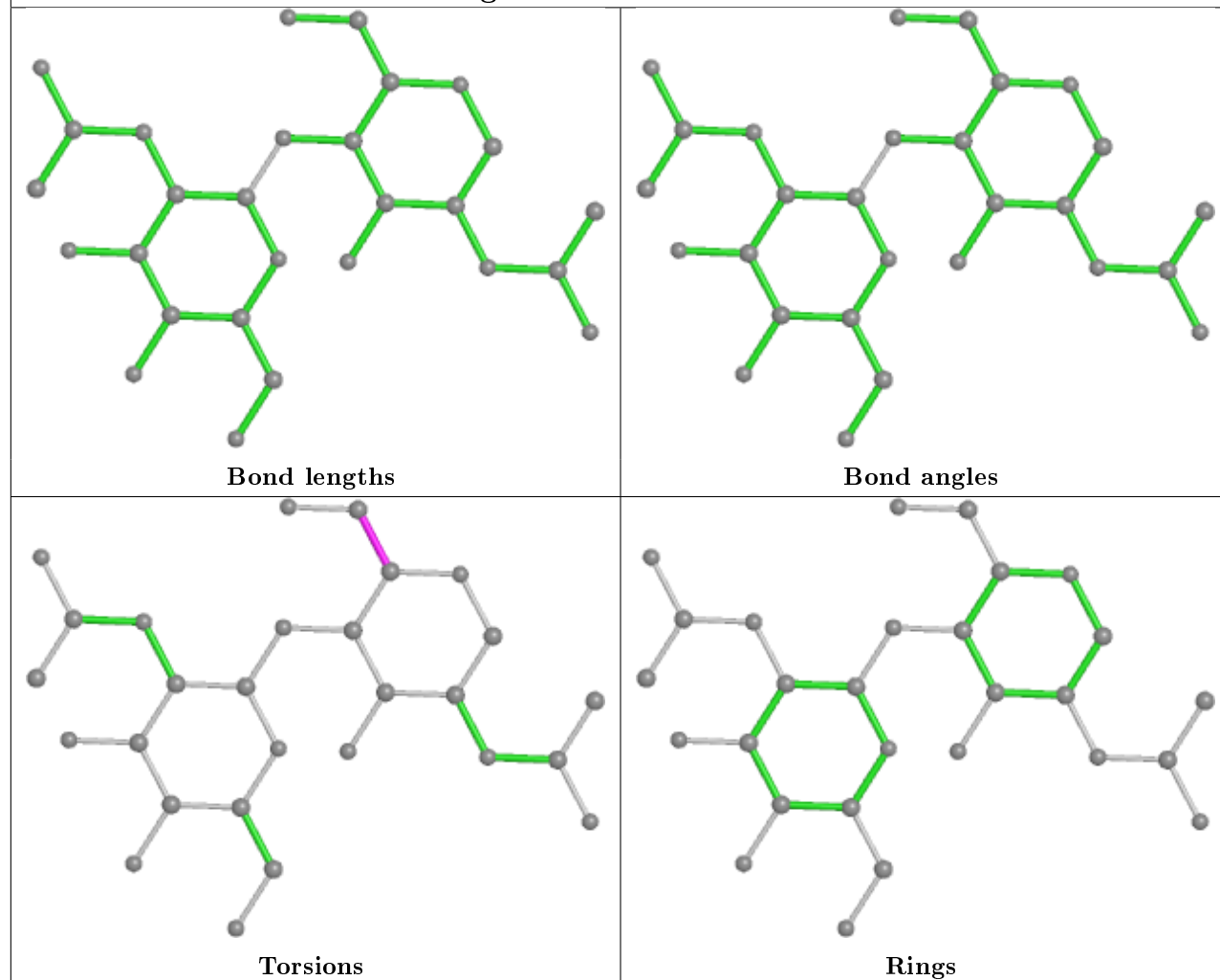
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

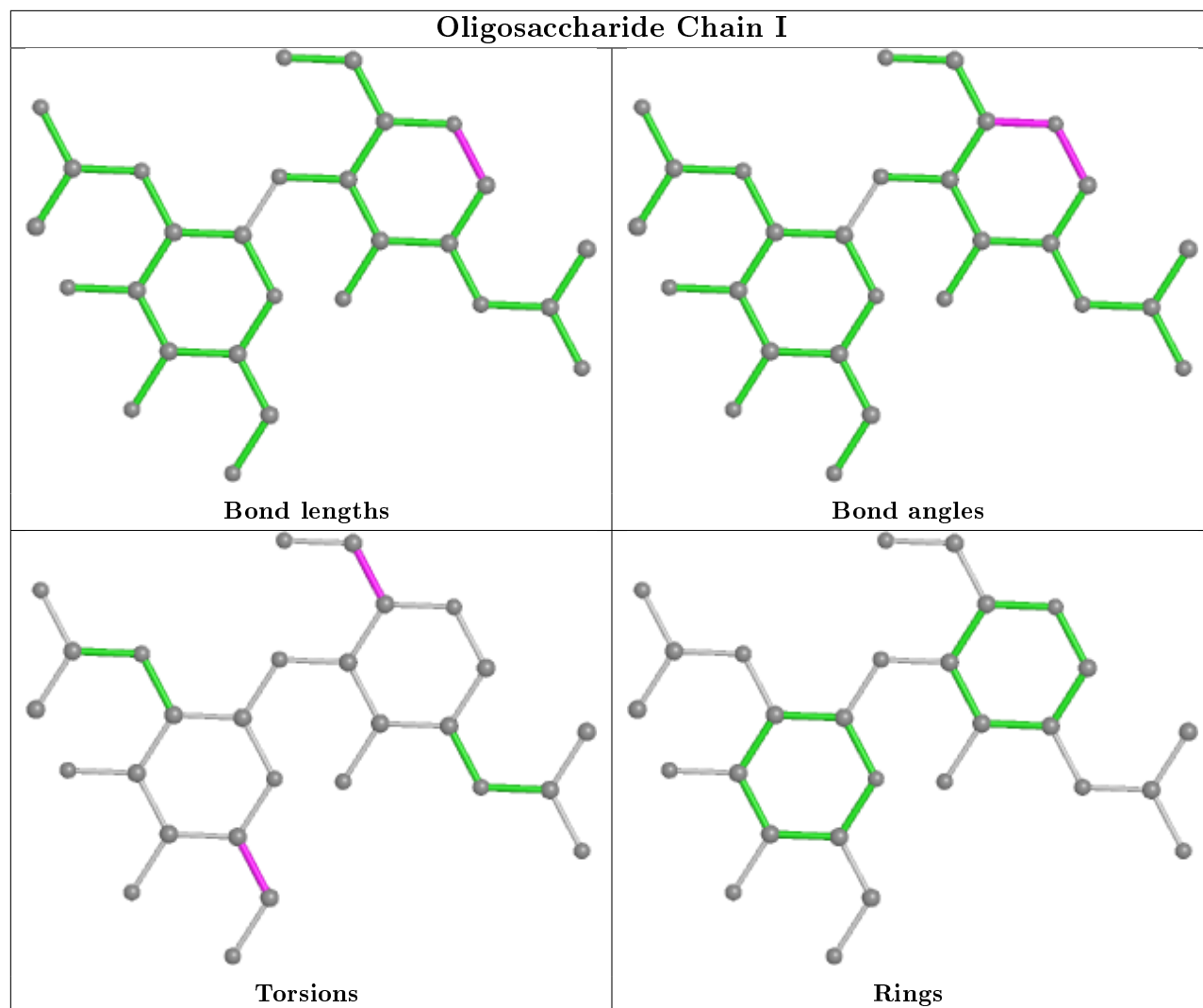


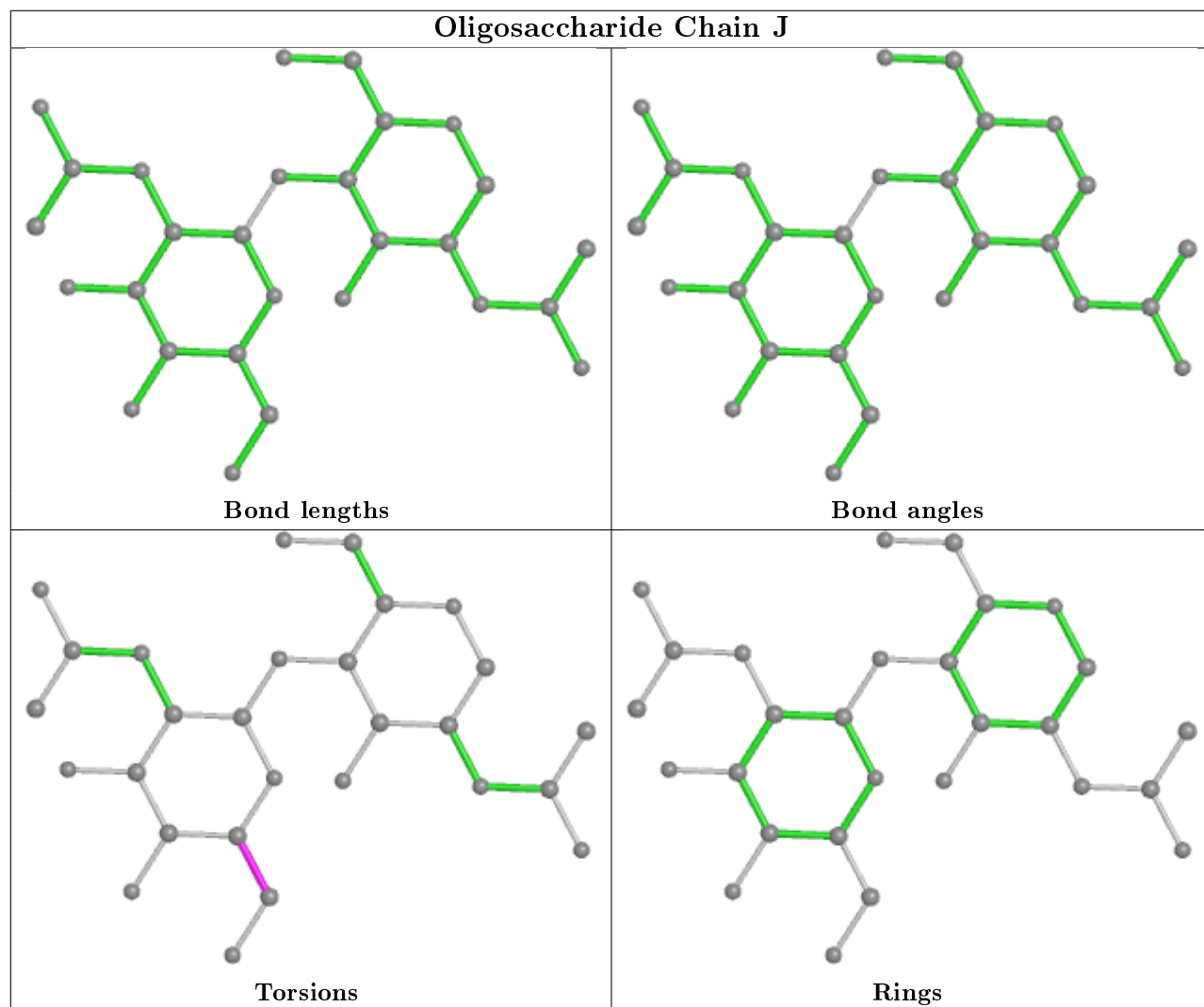
Oligosaccharide Chain R

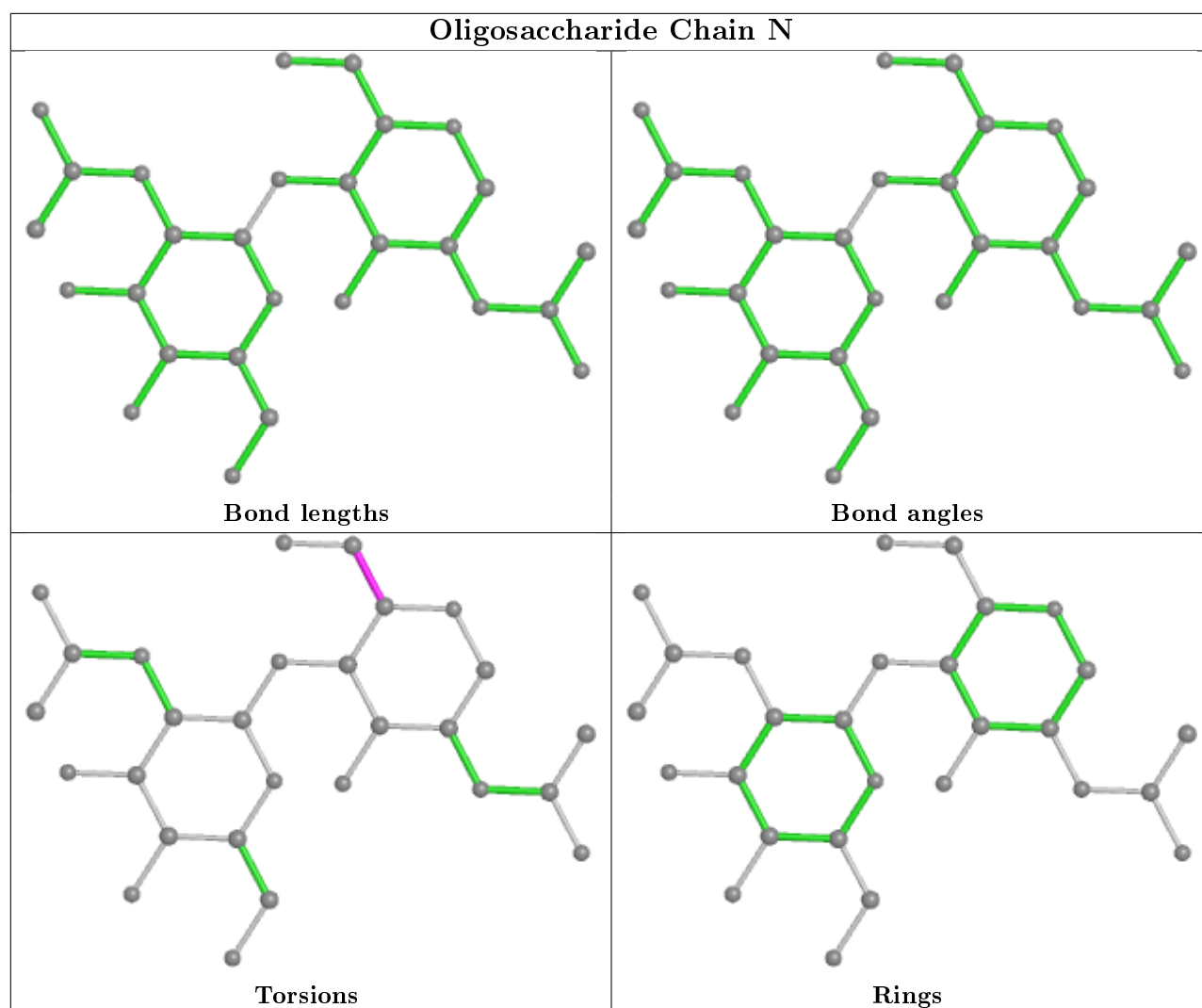


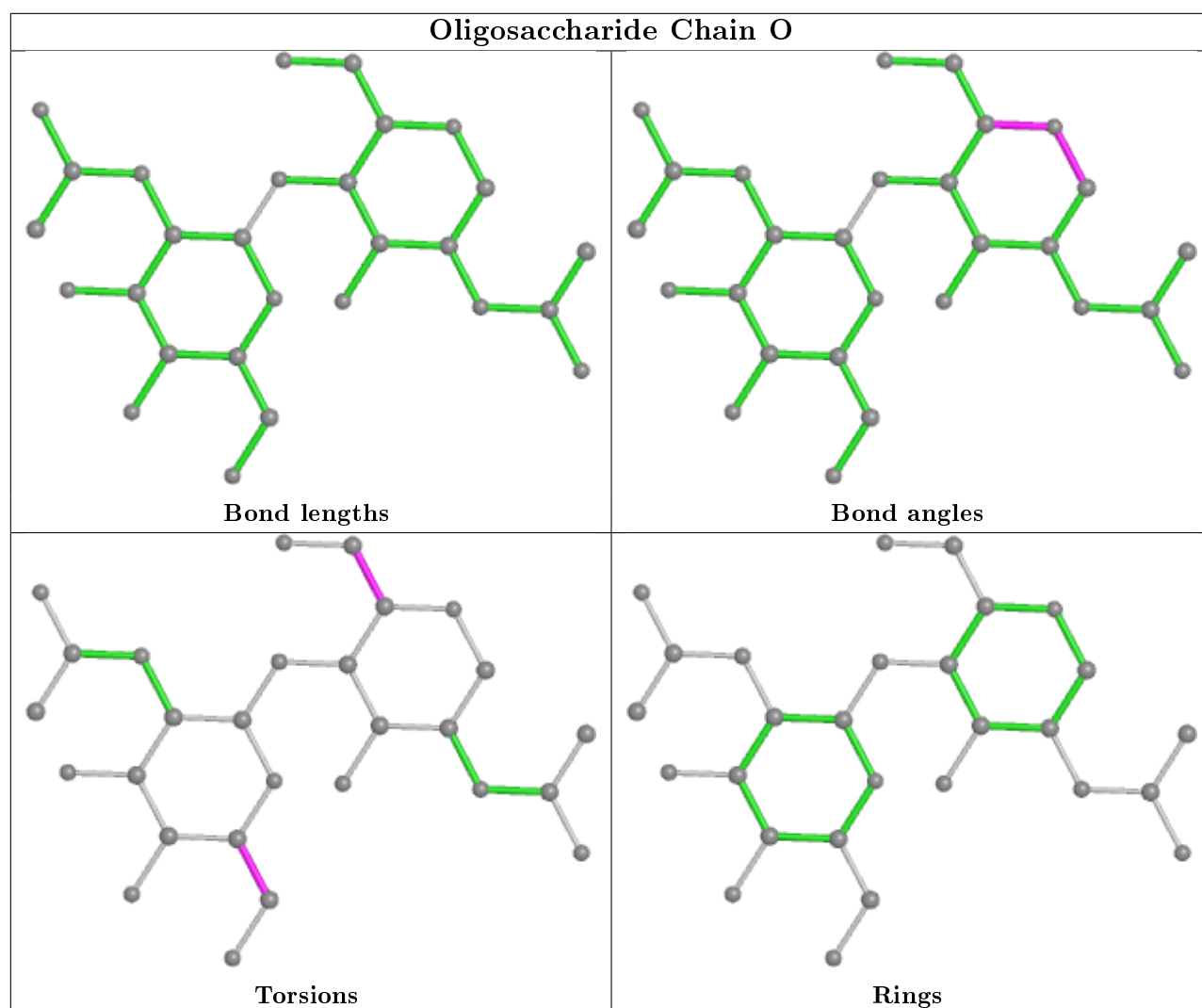
Oligosaccharide Chain H

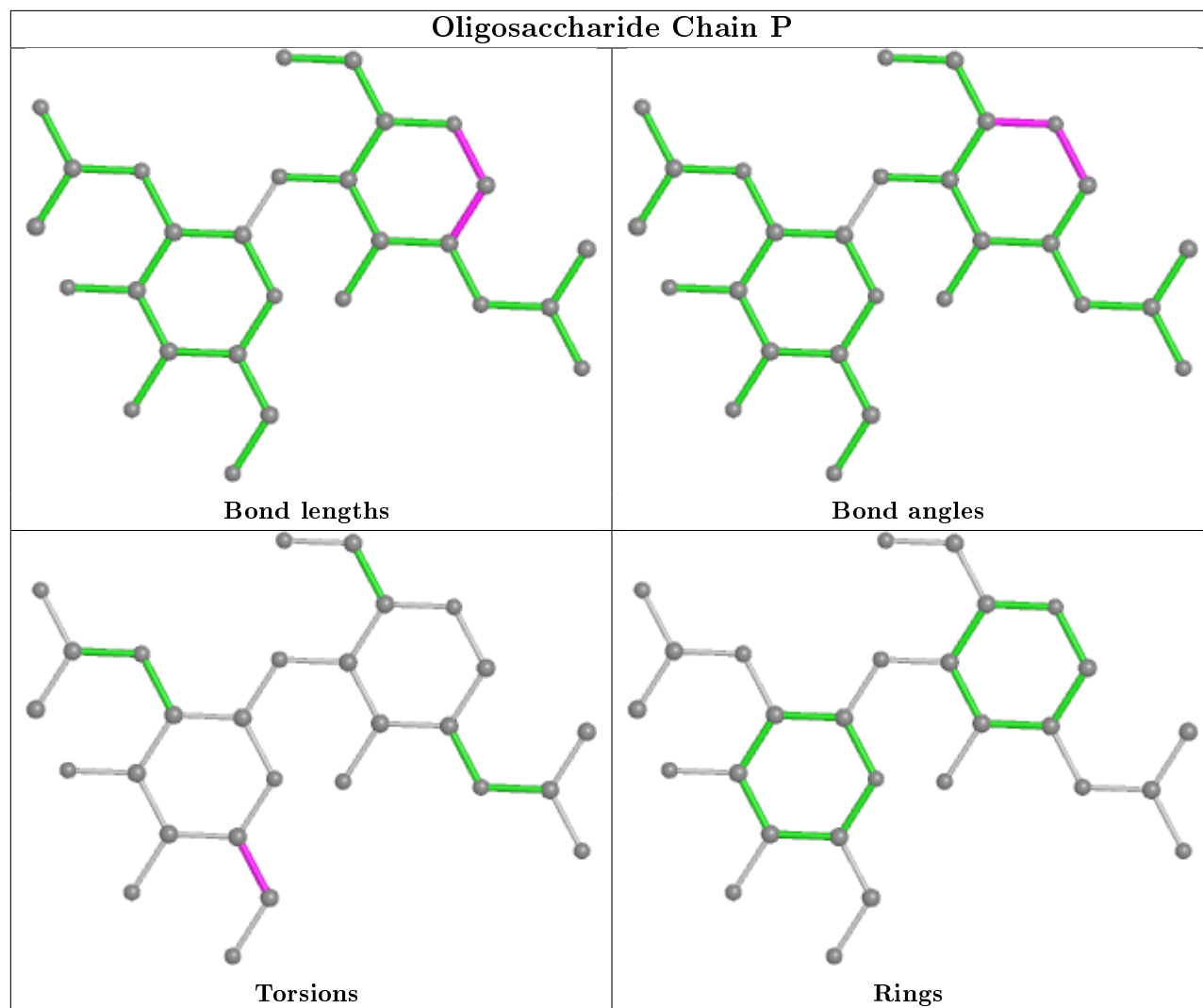


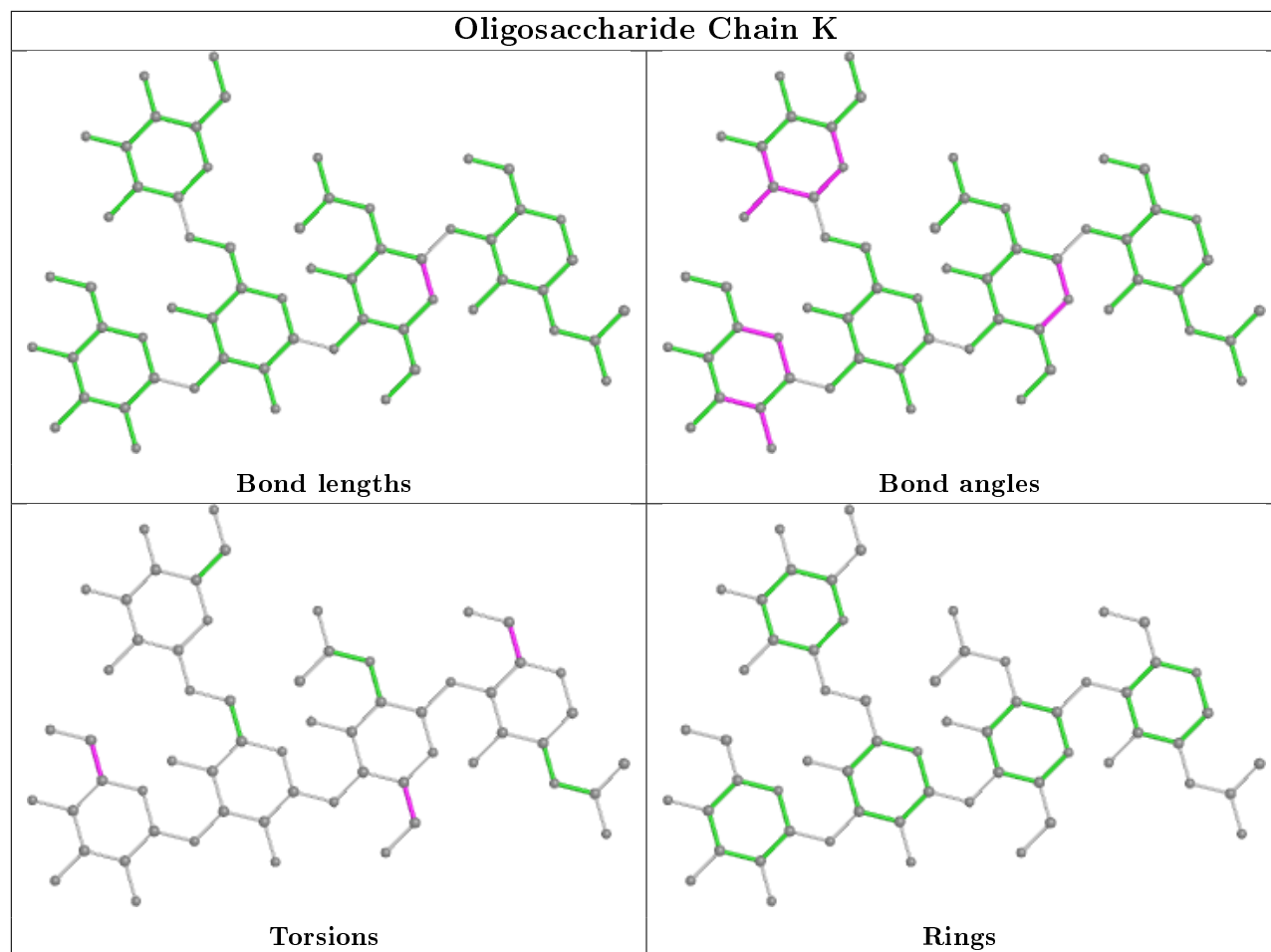


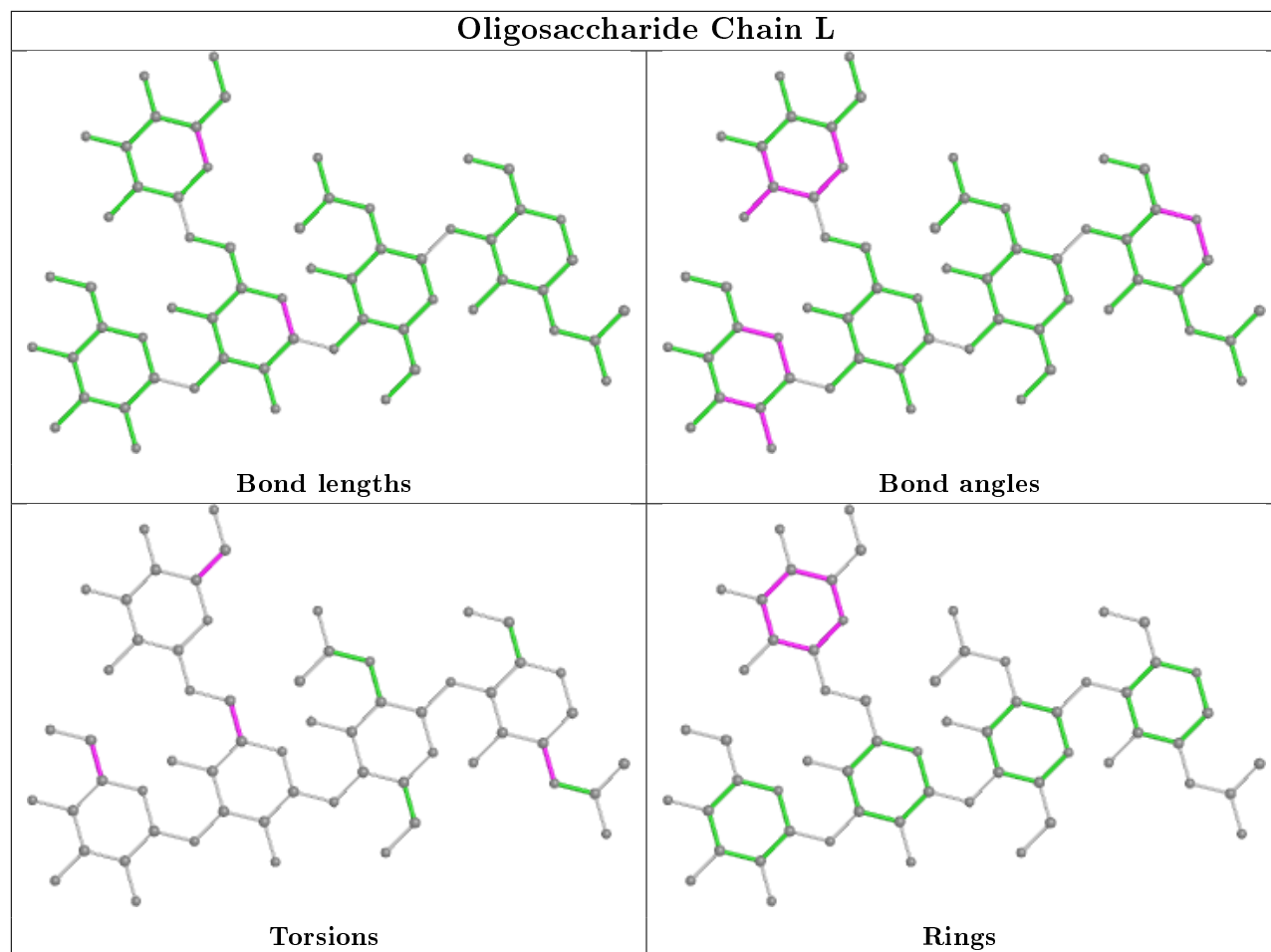


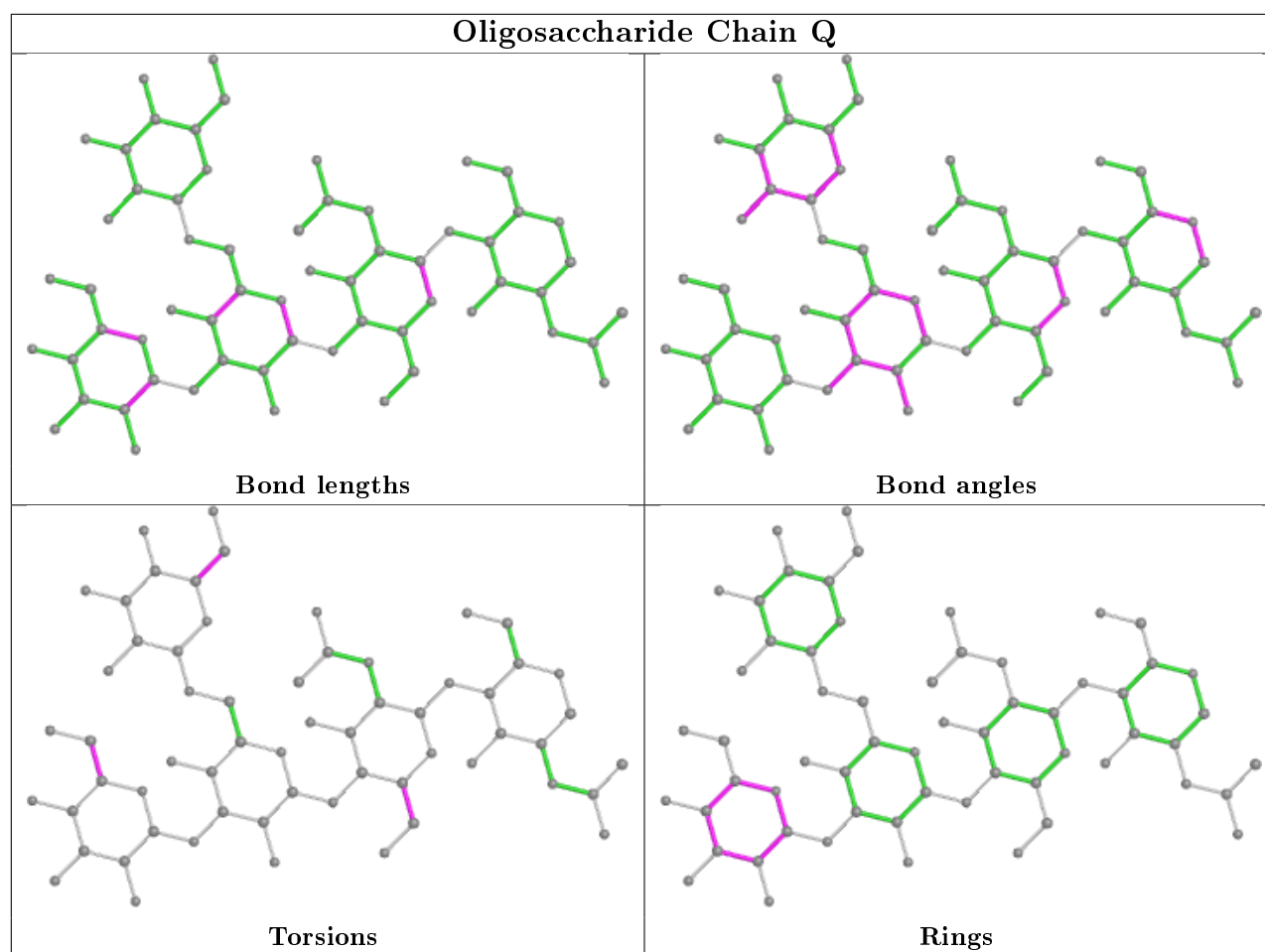












5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	NAG	C	507	3	14,14,15	0.77	1 (7%)	17,19,21	1.00	1 (5%)
7	NAG	F	507	3	14,14,15	0.28	0	17,19,21	0.75	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
7	NAG	C	507	3	-	2/6/23/26	0/1/1/1
7	NAG	F	507	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	507	NAG	O5-C1	2.37	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	507	NAG	C1-O5-C5	3.90	117.47	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	507	NAG	C4-C5-C6-O6
7	C	507	NAG	O5-C5-C6-O6
7	F	507	NAG	C4-C5-C6-O6
7	F	507	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	507	NAG	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	209/213 (98%)	0.19	4 (1%)	66 61	30, 89, 113, 167	0
1	D	209/213 (98%)	0.10	3 (1%)	75 69	30, 87, 107, 132	0
2	B	221/222 (99%)	0.02	2 (0%)	84 79	56, 85, 116, 144	0
2	E	221/222 (99%)	0.25	8 (3%)	42 38	63, 88, 125, 155	0
3	C	394/394 (100%)	0.05	7 (1%)	68 62	53, 86, 122, 136	0
3	F	392/394 (99%)	0.11	8 (2%)	65 60	50, 88, 131, 154	0
All	All	1646/1658 (99%)	0.11	32 (1%)	66 61	30, 87, 123, 167	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	46	GLU	3.3
3	F	216	LEU	3.0
3	C	42	VAL	3.0
3	C	44	ARG	2.8
1	A	77	GLU	2.8
3	F	41	ILE	2.6
1	D	95	THR	2.5
2	E	202	ILE	2.5
2	B	46	GLU	2.5
3	F	215	PHE	2.4
2	E	139	ASP	2.4
2	E	216	ASP	2.4
2	E	104	SER	2.4
3	C	182	ASP	2.4
1	A	17	ASP	2.3
2	B	168	LEU	2.3
1	A	206	SER	2.3
3	F	228	ILE	2.3
3	F	46	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	204	CYS	2.2
3	F	44	ARG	2.2
3	F	226	THR	2.2
2	E	206	VAL	2.2
3	C	255	SER	2.2
3	F	245	CYS	2.2
1	D	112	THR	2.1
3	C	97	LYS	2.1
1	D	101	LYS	2.1
3	C	202	PHE	2.1
3	C	244	LYS	2.1
1	A	57	PRO	2.0
2	E	190	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	G	4	11/12	0.35	0.39	121,132,140,142	0
4	BMA	G	3	11/12	0.36	0.37	115,127,135,136	0
5	NAG	P	2	14/15	0.48	0.96	128,142,146,147	0
6	MAN	K	5	11/12	0.53	0.34	121,123,131,134	0
6	MAN	Q	4	11/12	0.57	0.53	134,139,142,143	0
5	NAG	P	1	14/15	0.59	0.47	133,141,146,152	0
6	MAN	Q	5	11/12	0.60	0.33	118,127,135,140	0
5	NAG	J	2	14/15	0.66	0.51	123,138,144,145	0
6	BMA	Q	3	11/12	0.67	0.33	124,131,134,143	0
4	BMA	M	3	11/12	0.68	0.27	104,116,123,128	0
4	MAN	M	4	11/12	0.68	0.61	119,125,134,139	0
5	NAG	J	1	14/15	0.68	0.25	106,130,137,141	0
6	MAN	L	4	11/12	0.69	0.39	113,118,120,122	0
6	MAN	L	5	11/12	0.71	0.26	91,115,122,136	0
5	NAG	I	2	14/15	0.72	0.23	96,107,111,111	0

Continued on next page...

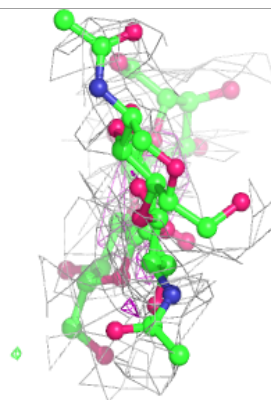
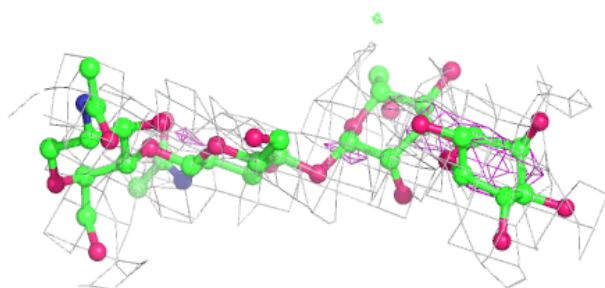
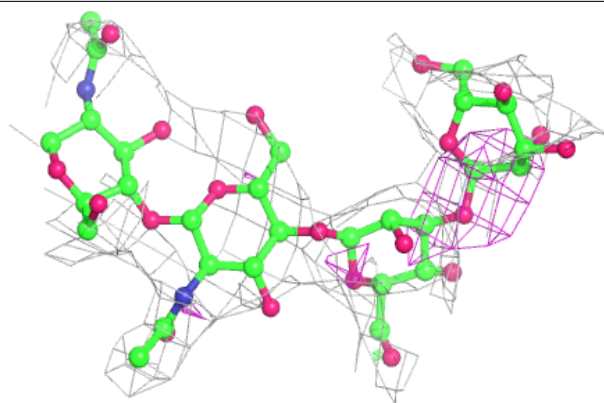
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	O	2	14/15	0.75	0.26	109,116,122,127	0
4	MAN	R	4	11/12	0.76	0.36	95,112,127,127	0
5	NAG	H	2	14/15	0.77	0.29	100,120,128,134	0
4	NAG	G	2	14/15	0.77	0.30	94,108,120,124	0
6	BMA	K	3	11/12	0.78	0.20	113,120,124,126	0
4	BMA	R	3	11/12	0.79	0.31	89,100,107,107	0
5	NAG	N	2	14/15	0.81	0.28	106,114,121,122	0
6	NAG	Q	2	14/15	0.82	0.24	99,108,117,126	0
6	NAG	L	2	14/15	0.83	0.25	81,92,95,104	0
6	MAN	K	4	11/12	0.84	0.20	106,117,125,129	0
6	BMA	L	3	11/12	0.86	0.34	104,109,118,122	0
4	NAG	R	1	14/15	0.86	0.29	70,77,84,85	0
6	NAG	K	2	14/15	0.87	0.32	98,104,117,117	0
4	NAG	R	2	14/15	0.87	0.28	76,86,96,101	0
5	NAG	H	1	14/15	0.87	0.28	88,94,100,106	0
5	NAG	N	1	14/15	0.88	0.34	87,99,108,112	0
6	NAG	L	1	14/15	0.89	0.25	74,79,86,93	0
5	NAG	I	1	14/15	0.89	0.26	79,83,93,95	0
4	NAG	M	2	14/15	0.89	0.18	91,99,102,109	0
4	NAG	G	1	14/15	0.90	0.22	74,86,94,95	0
6	NAG	Q	1	14/15	0.91	0.16	79,98,103,105	0
6	NAG	K	1	14/15	0.91	0.24	95,100,102,107	0
5	NAG	O	1	14/15	0.92	0.20	94,98,105,111	0
4	NAG	M	1	14/15	0.92	0.21	72,78,94,104	0

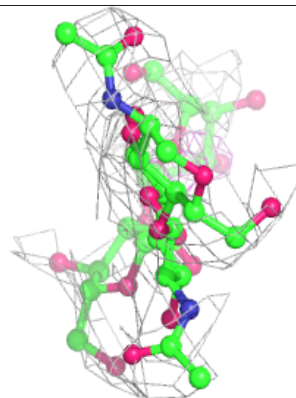
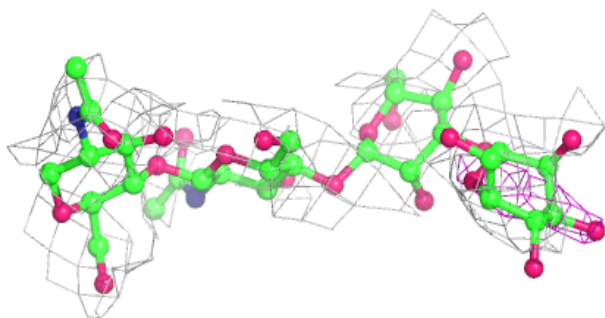
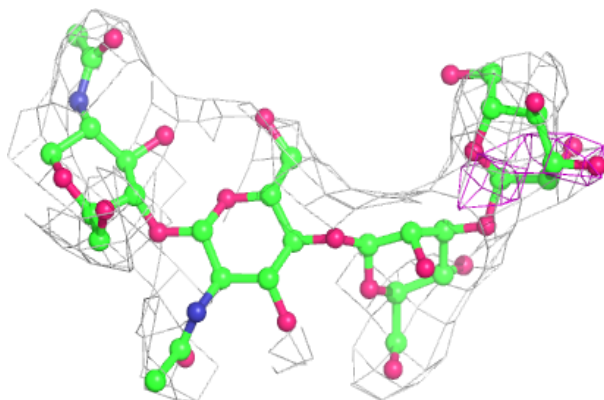
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

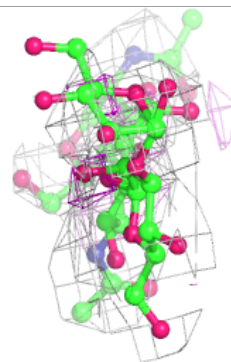
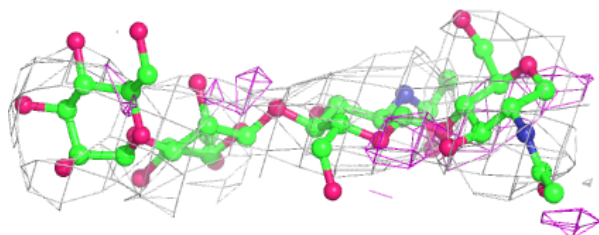
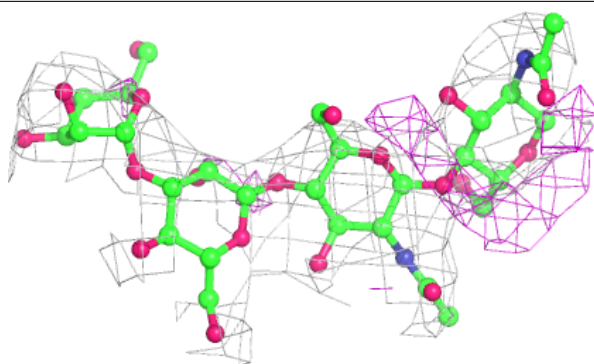
**Electron density around Chain M:**

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

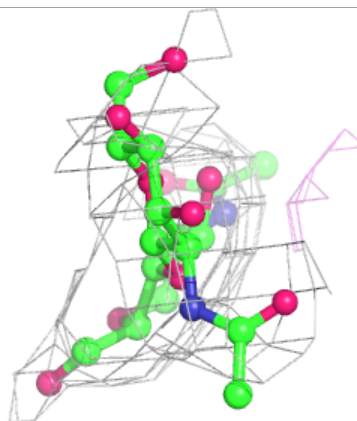
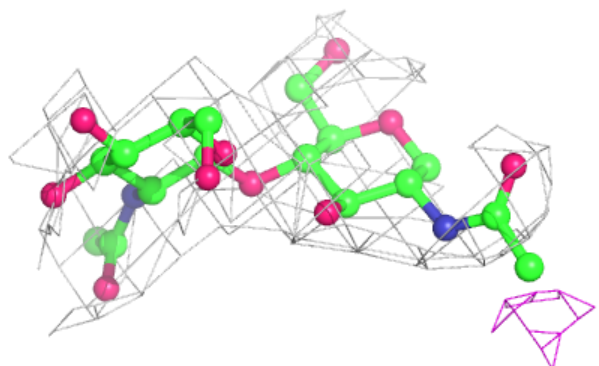
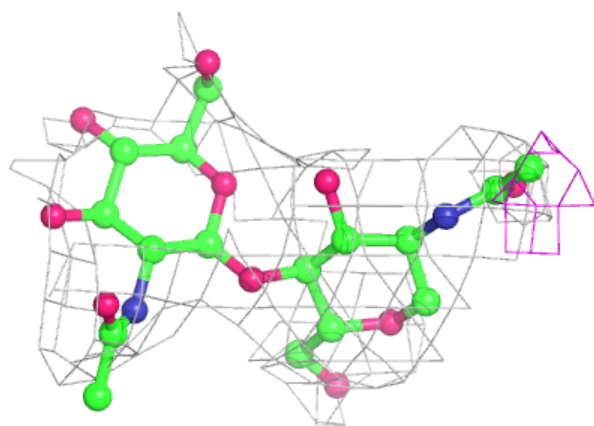


Electron density around Chain R:

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

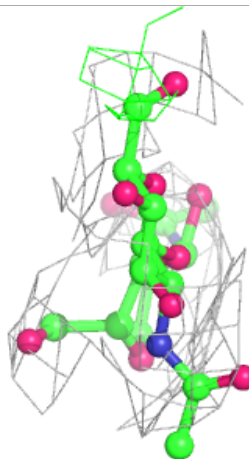
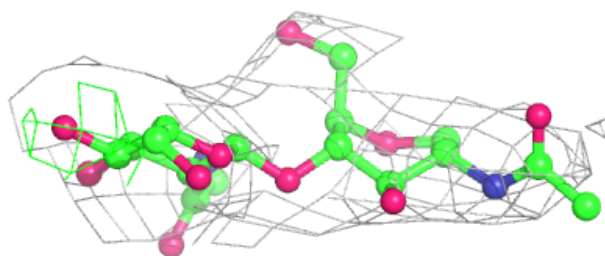
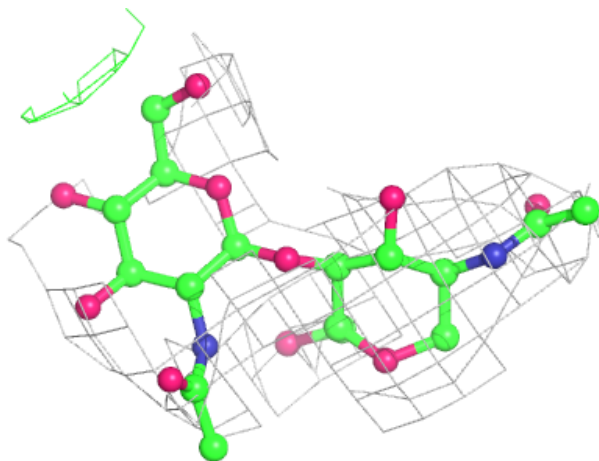
**Electron density around Chain H:**

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



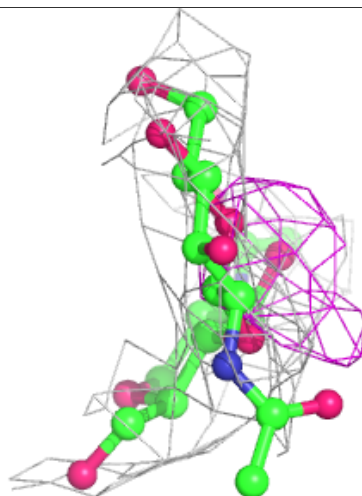
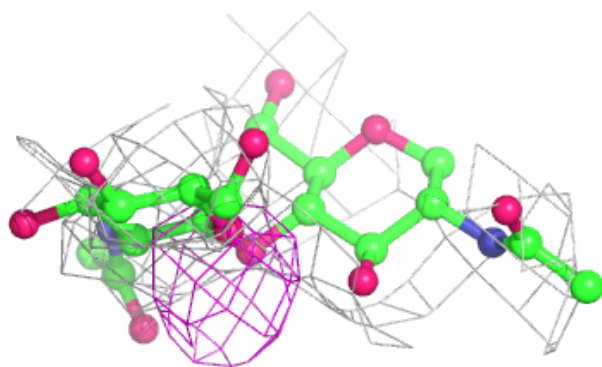
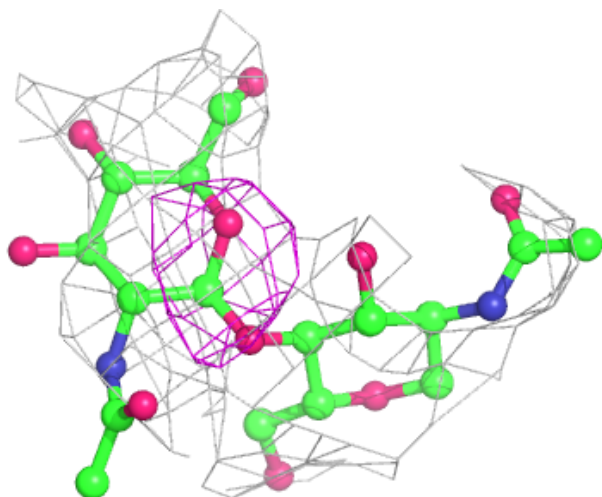
Electron density around Chain I:

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



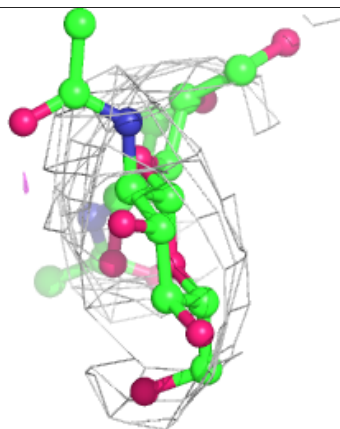
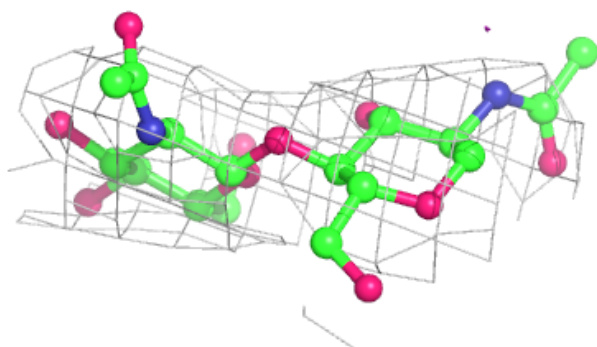
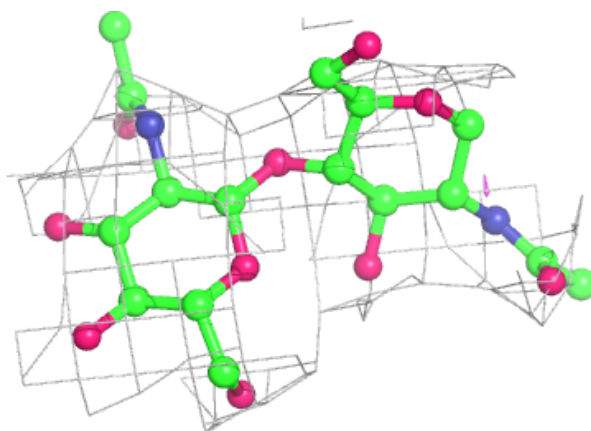
Electron density around Chain J:

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



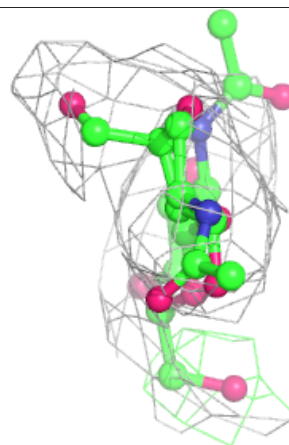
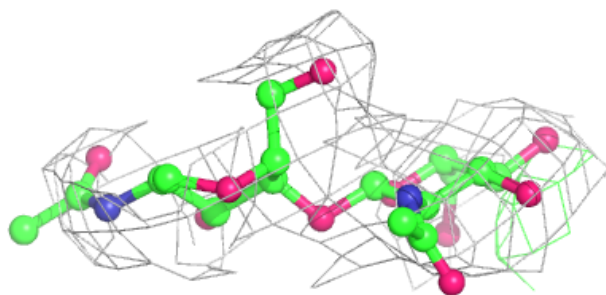
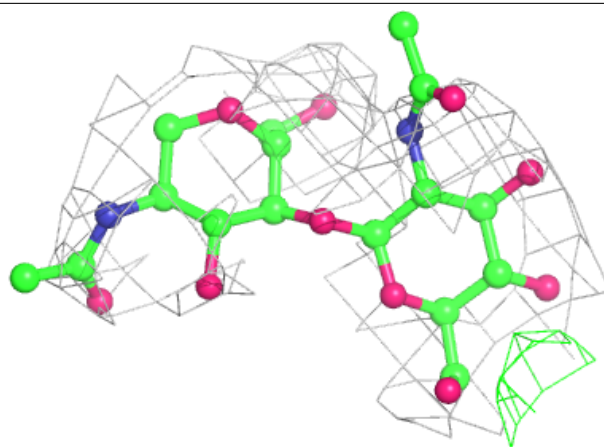
Electron density around Chain N:

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



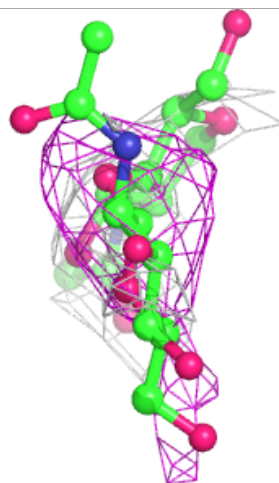
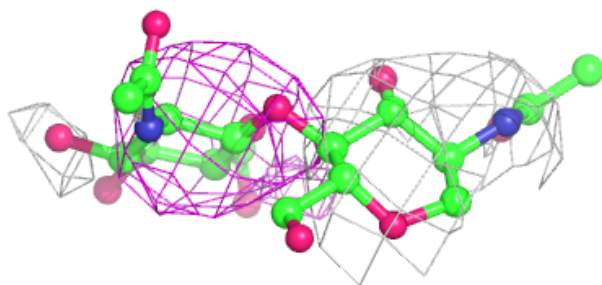
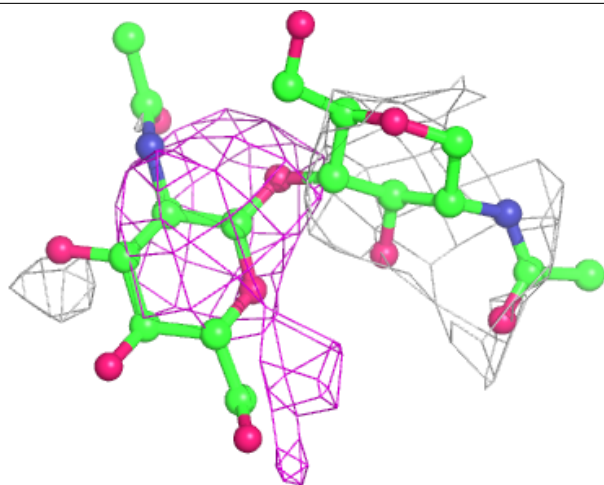
Electron density around Chain O:

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



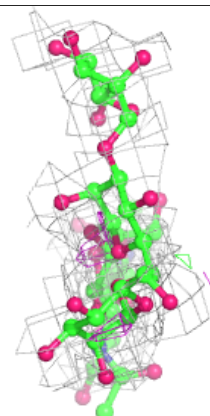
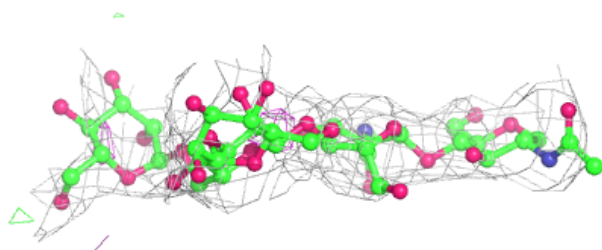
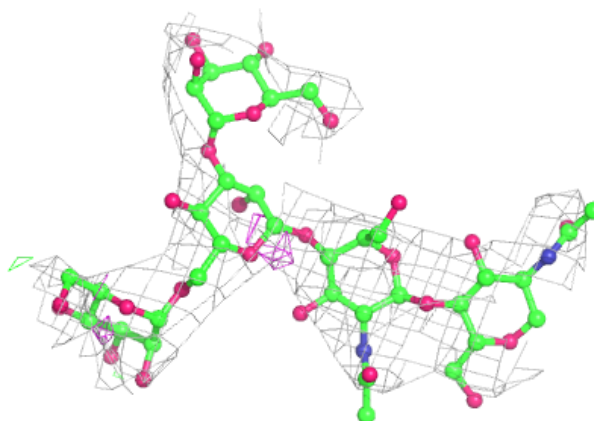
Electron density around Chain P:

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



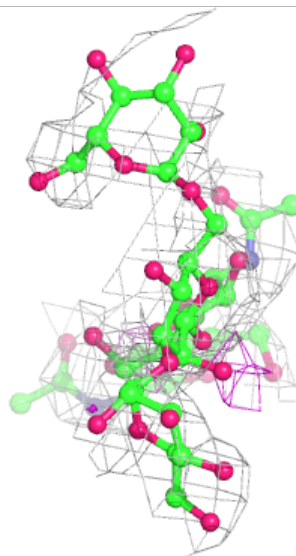
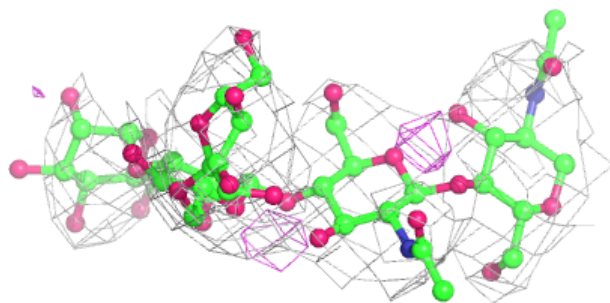
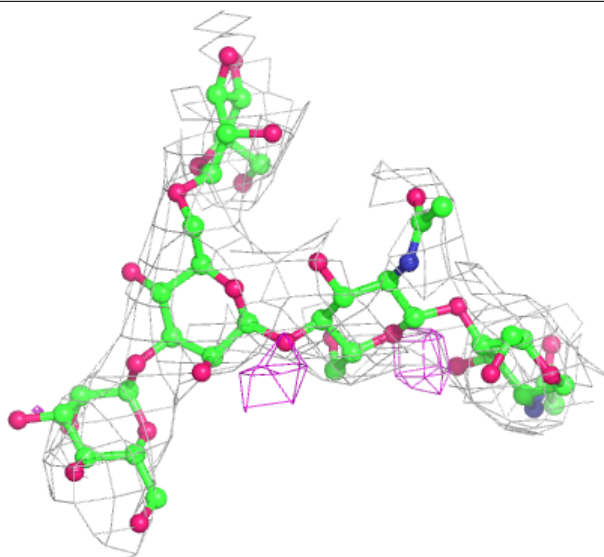
Electron density around Chain K:

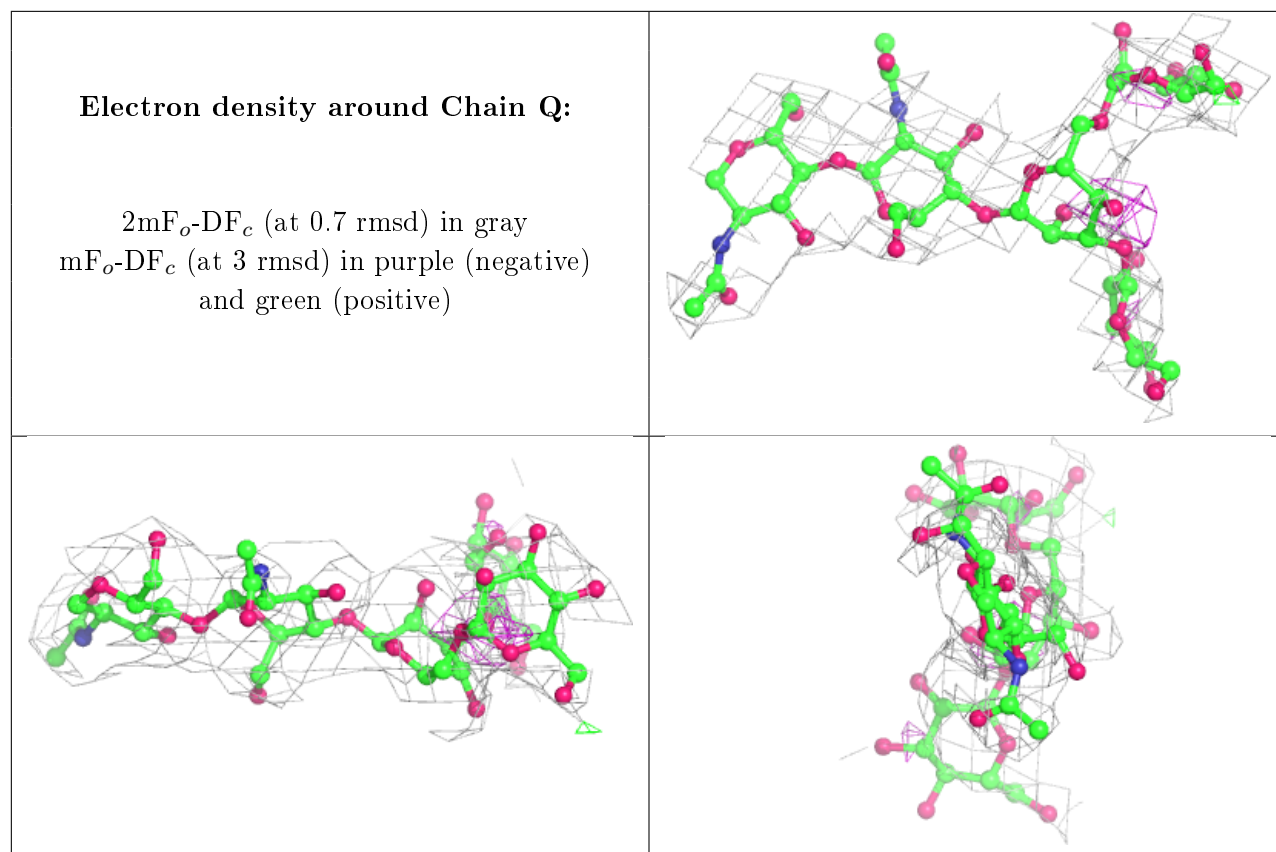
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	NAG	C	507	14/15	0.78	0.39	108,114,122,123	0
7	NAG	F	507	14/15	0.86	0.20	112,117,122,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.