



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:26 AM UTC

PDB ID : 5XBM / pdb_00005xbm
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

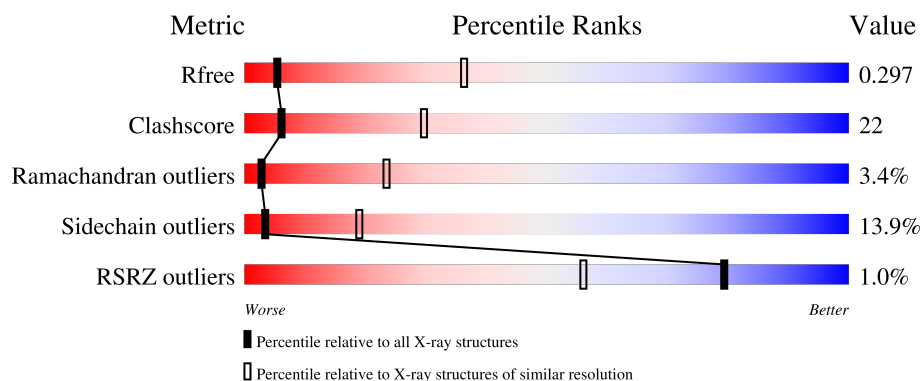
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



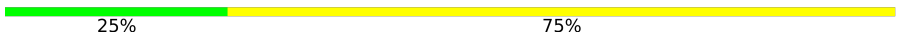
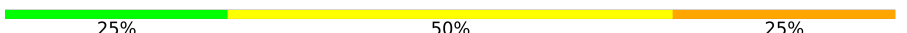
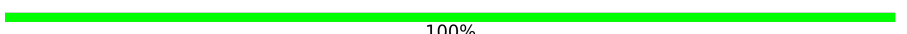
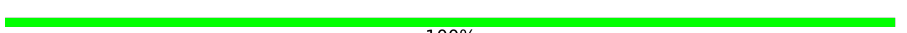
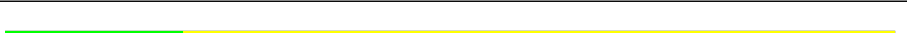
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	394	% 
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	

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.



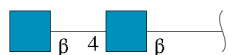
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

Continued on next page...

Continued from previous page...

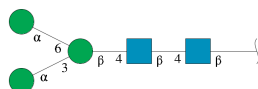
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



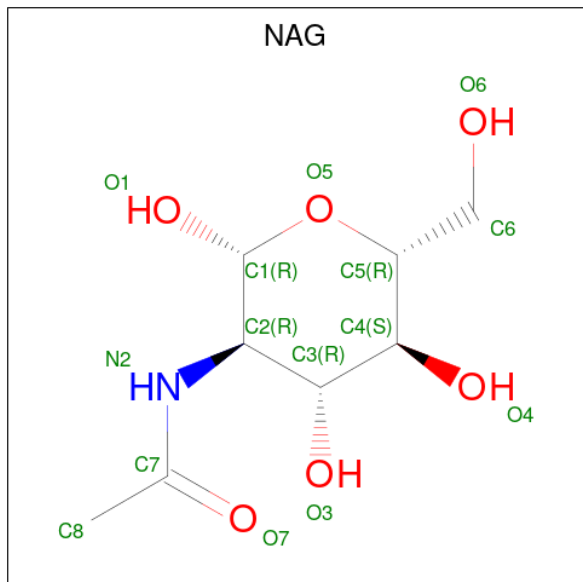
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

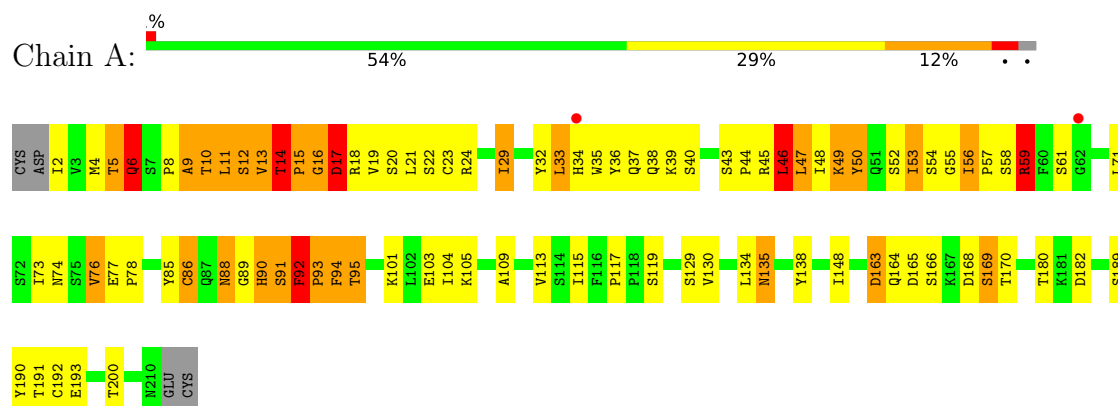


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		

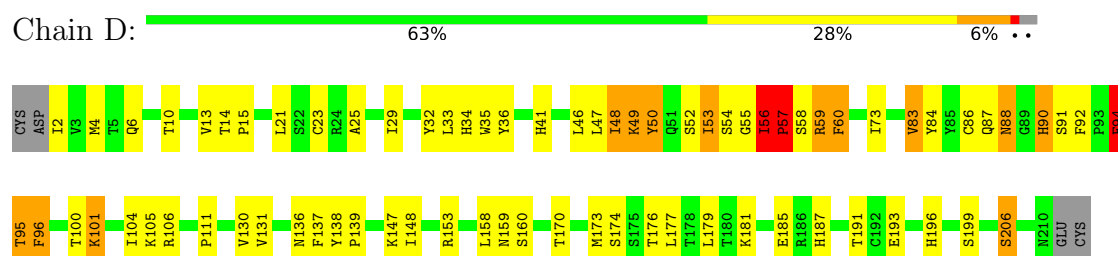
3 Residue-property plots [i](#)

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.

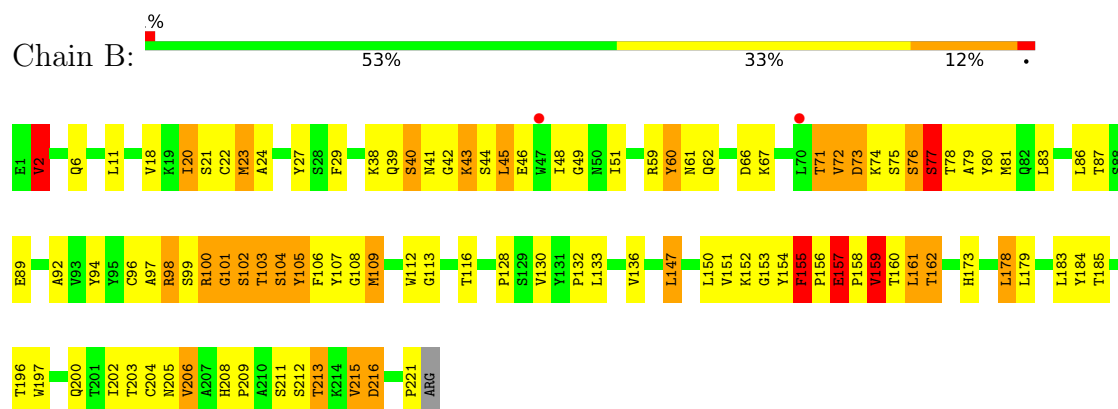
- Molecule 1: light chain of JL2



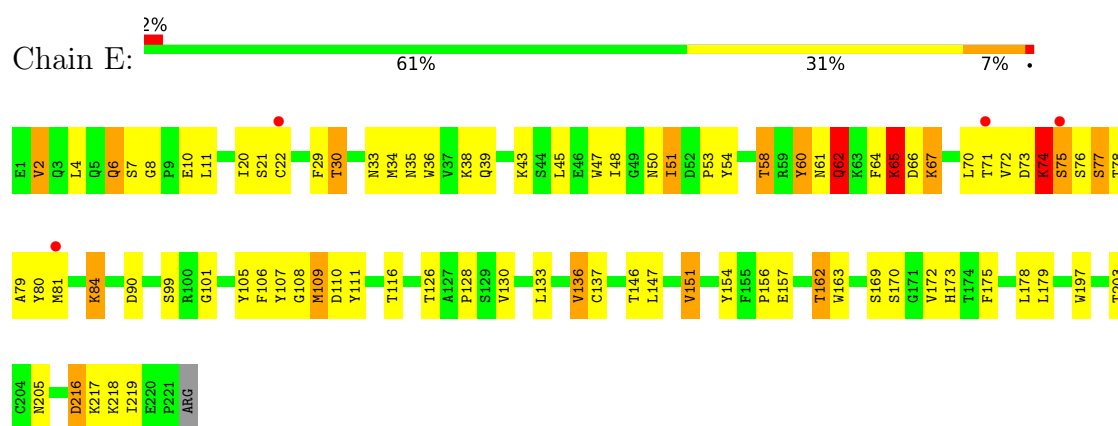
- Molecule 1: light chain of JL2



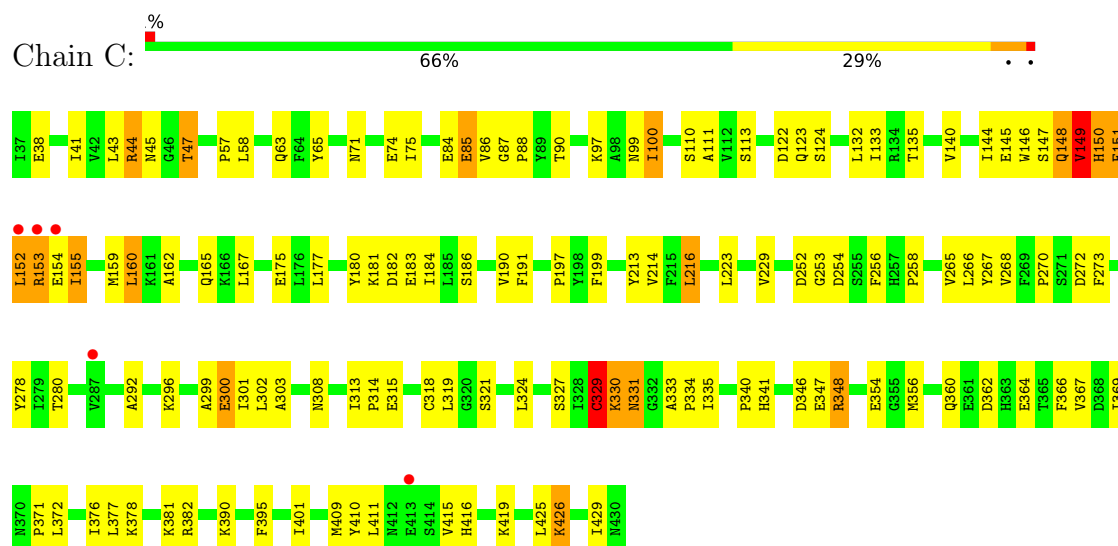
- Molecule 2: heavy chain of JL2



- Molecule 2: heavy chain of JL2



• Molecule 3: Lysosome membrane protein 2



• Molecule 3: Lysosome membrane protein 2



• 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%

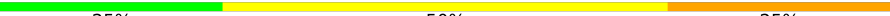


- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:  25% 50% 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:  50% 50%

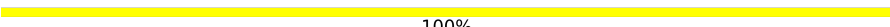
MAG1
MAG2

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

Chain P:  50% 50%

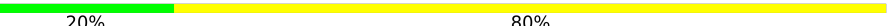
MAG1
MAG2

- 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:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

- 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:  20% 80%

MAG1
MAG2
BMA3
MAN4
MAN5

- 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:  80% 20%

MAG1
MAG2
BMA3
MAN4
MAN5

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 0.254 , 0.297	Depositor DCC
R_{free} test set	1516 reflections (4.91%)	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)	0.31 , 61.1	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	0.89	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: NAG, BMA, 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	0.38	0/1650	0.63	2/2243 (0.1%)
1	D	0.40	0/1654	0.72	4/2246 (0.2%)
2	B	0.34	0/1700	0.61	4/2320 (0.2%)
2	E	0.23	0/1696	0.62	4/2315 (0.2%)
3	C	0.27	0/3227	0.47	3/4397 (0.1%)
3	F	0.17	0/3215	0.41	0/4379
All	All	0.29	0/13142	0.55	17/17900 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	67	LYS	N-CA-C	10.84	123.10	111.28
1	D	49	LYS	N-CA-C	9.34	121.40	111.03
2	E	62	GLN	N-CA-C	7.84	119.45	111.07
2	B	155	PHE	C-N-CD	7.63	137.39	120.60
3	C	147	SER	N-CA-C	-7.56	103.67	113.12
2	B	157	GLU	C-N-CD	7.40	136.87	120.60
1	D	94	PHE	N-CA-C	-7.24	98.73	109.15
3	C	149	VAL	N-CA-C	-7.22	94.32	109.34
1	D	90	HIS	N-CA-C	7.03	119.03	111.36
1	A	92	PHE	C-N-CD	7.00	136.01	120.60
3	C	329	CYS	N-CA-C	-6.53	96.89	110.80
2	B	157	GLU	N-CA-C	-6.32	101.10	110.20
1	D	57	PRO	CA-N-CD	-5.68	104.04	112.00
2	E	43	LYS	CB-CA-C	-5.49	110.23	116.54
1	A	59	ARG	N-CA-C	5.48	122.47	110.80
2	B	155	PHE	N-CA-C	-5.24	99.75	108.23
2	E	65	LYS	N-CA-C	5.02	121.49	110.80

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	156	0
1	D	1615	0	1540	95	0
2	B	1658	0	1596	121	0
2	E	1654	0	1585	96	0
3	C	3144	0	2989	84	0
3	F	3132	0	2985	73	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	583	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 (583) 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	1.55	1.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:THR:C	1:A:11:LEU:HD23	1.45	1.39
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
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	1.27
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
2:B:157:GLU:HG3	2:B:158:PRO:HA	1.27	1.14
1:A:4:MET:HE2	1:A:86:CYS:HB2	1.24	1.13
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:10:THR:C	1:A:11:LEU:CD2	2.34	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4:MET:HE1	1:A:23:CYS:SG	2.05	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:86:CYS:CB	2.02	0.90
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
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:54:SER:OG	1:A:55:GLY:N	2.09	0.82
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:59:ARG:O	1:D:60:PHE:C	2.30	0.74
1:D:94:PHE:CD2	2:E:106:PHE:CD1	2.75	0.74
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
2:B:153:GLY:H	2:B:185:THR:CG2	1.95	0.73
1:A:4:MET:CE	1:A:86:CYS:HB2	2.11	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
2:E:74:LYS:C	2:E:74:LYS:HE3	2.15	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:54:SER:OG	1:D:55:GLY:N	2.23	0.71
1:D:160:SER:HB2	2:E:178:LEU:HD11	1.72	0.71
1:A:6:GLN:CG	1:A:22:SER:C	2.60	0.71
1:A:56:ILE:N	1:A:57:PRO:HD3	2.06	0.70
1:D:53:ILE:HD13	1:D:53:ILE:N	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
1:A:11:LEU:HD23	1:A:11:LEU:N	2.03	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:GLN:HA	3:C:148:GLN:HE21	1.56	0.70
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:71:THR:HG23	2:E:80:TYR:HD2	1.57	0.69
2:E:106:PHE:HZ	2:E:109:MET:HG2	1.56	0.69
3:F:391:LYS:HD2	3:F:400:ASP:HA	1.74	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
2:B:103:THR:O	2:B:104:SER:OG	2.09	0.68
1:A:12:SER:HB2	1:A:105:LYS:HG3	1.74	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
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
3:F:263:ASP:N	3:F:263:ASP:OD1	2.28	0.66
3:F:165:GLN:NE2	3:F:183:GLU:OE2	2.29	0.66
1:D:47:LEU:C	1:D:48:ILE:CD1	2.54	0.66
2:B:43:LYS:HD2	2:B:43:LYS:N	2.10	0.66
2:E:48:ILE:HG23	2:E:64:PHE:CE2	2.31	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:HD13	1:A:53:ILE:N	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:HD13	1:D:48:ILE:N	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:9:ALA:C	1:A:10:THR:HG1	1.94	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:319:LEU:HD21	6:K:1:NAG:H81	1.79	0.63
2:E:74:LYS:HA	2:E:74:LYS:CE	2.27	0.63
2:E:29:PHE:O	2:E:30:THR:OG1	2.15	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
1:A:35:TRP:O	1:A:47:LEU:HB2	1.99	0.62
1:D:57:PRO:C	1:D:58:SER:HG	2.03	0.62
1:A:13:VAL:HG13	1:A:14:THR:N	2.04	0.62
2:E:6:GLN:HB2	2:E:22:CYS:HA	1.82	0.62
2:E:72:VAL:C	2:E:74:LYS:H	2.07	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	0.61
3:F:149:VAL:HA	6:Q:3:BMA:H62	1.83	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
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
3:C:150:HIS:O	3:C:151:PHE:HB3	1.99	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:149:VAL:HG22	3:C:150:HIS:N	2.16	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
2:B:154:TYR:CZ	2:B:159:VAL:HG11	2.37	0.59

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:CD2	2.86	0.59
1:D:34:HIS:NE2	2:E:106:PHE:HD2	2.00	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
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:B:106:PHE:CE2	2:B:108:GLY:N	2.73	0.57
1:D:56:ILE:HG12	1:D:56:ILE:O	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:60:TYR:N	2:E:60:TYR:CD2	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:OD1	3:F:252:ASP:N	2.38	0.56
1:A:6:GLN:HB2	1:A:22:SER:C	2.29	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
1:A:4:MET:CE	1:A:86:CYS:CB	2.78	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:LEU:HB3	2:E:178:LEU:HD22	1.88	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
1:A:88:ASN:ND2	1:A:94:PHE:C	2.63	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
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
1:D:94:PHE:HD1	1:D:94:PHE:H	1.53	0.55
2:B:81:MET:HE2	2:B:83:LEU:HD21	1.89	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
2:B:106:PHE:CD2	2:B:106:PHE:C	2.85	0.54
2:B:75:SER:C	2:B:77:SER:H	2.15	0.54
1:D:13:VAL:HG12	1:D:15:PRO:HA	1.89	0.54
1:A:54:SER:HG	1:A:55:GLY:H	1.51	0.54
2:B:154:TYR:C	2:B:154:TYR:CD1	2.85	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:64:PHE:C	2:E:64:PHE:CD2	2.85	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
1:A:45:ARG:C	1:A:46:LEU:O	2.52	0.53
1:D:4:MET:HE3	1:D:25:ALA:HB2	1.90	0.53
2:E:62:GLN:N	2:E:62:GLN:OE1	2.42	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
1:A:94:PHE:N	1:A:94:PHE:CD1	2.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ARG:O	2:B:109:MET:HA	2.09	0.53
2:B:155:PHE:CD2	2:B:156:PRO:N	2.77	0.53
3:F:320:GLY:HA2	5:P:1:NAG:H82	1.91	0.53
1:A:13:VAL:HG23	1:A:17:ASP:CG	2.34	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
2:B:155:PHE:CD2	2:B:155:PHE:C	2.85	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
3:C:149:VAL:HG23	6:K:3:BMA:H62	1.90	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:32:TYR:CZ	2:B:105:TYR:HD1	2.27	0.52
1:A:13:VAL:HG22	1:A:14:THR:N	2.25	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
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:145:GLU:HG2	3:F:332:GLY:O	2.10	0.51
3:F:175:GLU:HB3	3:F:180:TYR:HB3	1.91	0.51
3:C:360:GLN:C	3:C:362:ASP:H	2.18	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:41:ILE:HG21	3:C:258:PRO:HG2	1.92	0.51
3:C:150:HIS:O	3:C:151:PHE:HB2	2.11	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:N	2:B:43:LYS:CD	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
2:B:76:SER:C	2:B:78:THR:H	2.19	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:92:PHE:C	1:A:92:PHE:CD2	2.85	0.50
1:A:129:SER:CB	2:B:152:LYS:NZ	2.74	0.50
2:E:65:LYS:HG3	2:E:66:ASP:N	2.24	0.50
1:A:135:ASN:OD1	1:A:135:ASN:N	2.42	0.50
1:A:93:PRO:HG3	2:B:61:ASN:ND2	2.27	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:106:PHE:CE2	2:B:107:TYR:C	2.91	0.49
3:F:298:PRO:HG2	3:F:301:ILE:HG12	1.94	0.49
1:A:9:ALA:O	1:A:10:THR:CB	2.58	0.49
1:A:46:LEU:HD22	1:A:47:LEU:H	1.77	0.49
3:C:330:LYS:N	3:C:330:LYS:CD	2.73	0.49
1:A:88:ASN:O	1:A:94:PHE:HA	2.13	0.49
2:B:2:VAL:HG13	2:B:2:VAL:O	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
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:F:242:THR:HG1	3:F:245:CYS:HG	1.60	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
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
3:F:360:GLN:C	3:F:362:ASP:H	2.21	0.48
2:B:97:ALA:HB1	2:B:109:MET:HB3	1.96	0.48
1:D:6:GLN:NE2	1:D:84:TYR:O	2.47	0.48
1:D:94:PHE:N	1:D:94:PHE:HD1	2.09	0.48
1:D:191:THR:HG22	1:D:206:SER:HB3	1.96	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:346:ASP:OD1	3:C:347:GLU:N	2.46	0.47
2:E:65:LYS:O	2:E:66:ASP:C	2.56	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
3:F:159:MET:HE1	3:F:187:LEU:HB2	1.96	0.47
1:A:4:MET:HE2	1:A:86:CYS:SG	2.53	0.47
1:A:37:GLN:OE1	1:A:45:ARG:NH1	2.46	0.47
1:A:6:GLN:N	1:A:6:GLN:CD	2.73	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:72:VAL:C	2:E:74:LYS:N	2.73	0.47
2:E:216:ASP:N	2:E:216:ASP:OD1	2.47	0.47
3:F:222:TYR:O	3:F:257:HIS:HB2	2.14	0.47
3:F:249:ASN:ND2	5:O:1:NAG:H61	2.30	0.47
1:A:6:GLN:CB	1:A:22:SER:C	2.87	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
2:B:76:SER:C	2:B:78:THR:N	2.73	0.47
2:B:42:GLY:C	2:B:43:LYS:CD	2.89	0.46
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
3:F:217:THR:OG1	3:F:218:GLY:N	2.43	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:48:ILE:HG21	2:B:81:MET:HE3	1.98	0.46
1:A:43:SER:OG	2:B:113:GLY:O	2.28	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
1:D:159:ASN:HB3	1:D:173:MET:HE3	1.97	0.46
3:F:242:THR:OG1	3:F:245:CYS:SG	2.66	0.46
1:A:14:THR:C	1:A:16:GLY:N	2.73	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:75:SER:C	2:B:77:SER:N	2.73	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
2:E:74:LYS:C	2:E:76:SER:N	2.73	0.46
1:A:168:ASP:OD1	1:A:168:ASP:N	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
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
2:B:102:SER:C	2:B:104:SER:N	2.73	0.45
3:C:63:GLN:HG2	3:C:90:THR:HG22	1.98	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:111:PRO:HD3	1:D:196:HIS:CD2	2.52	0.45
1:D:153:ARG:HA	1:D:153:ARG:HD3	1.83	0.45
3:F:151:PHE:CD1	3:F:151:PHE:C	2.94	0.45
3:F:323:VAL:HG23	3:F:338:SER:HB3	1.98	0.45
1:A:88:ASN:CG	1:A:94:PHE:HA	2.41	0.45
3:C:85:GLU:OE2	3:C:341:HIS:NE2	2.44	0.45
3:F:82:ARG:HA	3:F:354:GLU:HB2	1.97	0.45
3:F:224:ASN:OD1	3:F:224:ASN:N	2.49	0.45
2:B:40:SER:C	2:B:42:GLY:N	2.73	0.45
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
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:71:ASN:O	3:C:75:ILE:HG13	2.17	0.45
3:C:390:LYS:HB2	3:C:390:LYS:HE3	1.69	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:PHE:CD2	2:B:107:TYR:C	2.95	0.45
1:D:96:PHE:HD1	1:D:96:PHE:HA	1.59	0.45
2:E:74:LYS:HA	2:E:74:LYS:NZ	2.32	0.45
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:A:148:ILE:O	1:A:148:ILE:HG13	2.15	0.44
1:D:58:SER:CB	1:D:60:PHE:HE2	2.30	0.44
1:D:147:LYS:HG3	1:D:191:THR:OG1	2.16	0.44
2:B:21:SER:HA	2:B:79:ALA:O	2.17	0.44
3:C:148:GLN:NE2	3:C:148:GLN:CA	2.73	0.44
3:C:313:ILE:N	3:C:314:PRO:HD2	2.32	0.44
3:C:313:ILE:C	3:C:315:GLU:H	2.25	0.44
2:E:71:THR:HG23	2:E:80:TYR:CD2	2.45	0.44
3:F:249:ASN:N	3:F:249:ASN:OD1	2.49	0.44
3:F:376:ILE:HD11	3:F:379:ALA:HB2	1.99	0.44
1:A:19:VAL:CG1	1:A:20:SER:N	2.39	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
2:E:67:LYS:HE3	2:E:90:ASP:CG	2.40	0.44
3:C:74:GLU:N	3:C:74:GLU:OE1	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:O	1:D:92:PHE:CD1	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:72:VAL:HG23	2:B:73:ASP:N	2.31	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
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:C:330:LYS:H	3:C:330:LYS:CD	2.31	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:63:GLN:HA	3:F:90:THR:HA	2.01	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:155:PHE:C	2:B:155:PHE:HD2	2.26	0.42
1:D:2:ILE:O	1:D:95:THR:CG2	2.66	0.42
1:A:8:PRO:CA	1:A:9:ALA:CB	2.85	0.42
2:B:40:SER:O	2:B:42:GLY:N	2.53	0.42
2:B:100:ARG:NH1	3:C:395:PHE:O	2.52	0.42
2:B:109:MET:HB2	2:B:112:TRP:HE1	1.83	0.42
3:C:100:ILE:HA	3:C:110:SER:O	2.19	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:44:ARG:O	3:C:47:THR:OG1	2.36	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
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:HE2	3:C:419:LYS:HB2	1.88	0.42
2:B:161:LEU:CD2	2:B:161:LEU:C	2.85	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:151:PHE:C	3:F:151:PHE:HD1	2.26	0.42
3:F:230:GLU:OE2	3:F:234:LYS:N	2.52	0.42
1:A:47:LEU:HD23	1:A:47:LEU:HA	1.53	0.42
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
3:C:86:VAL:CG1	4:G:1:NAG:H82	2.50	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:LYS:HB2	2:B:67:LYS:HE3	1.82	0.42
2:E:34:MET:HE3	2:E:34:MET:HB3	1.93	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
2:E:67:LYS:O	2:E:84:LYS:HG2	2.20	0.41
1:A:4:MET:HE3	1:A:4:MET:HB3	1.95	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
2:E:35:ASN:ND2	2:E:47:TRP:HE1	2.19	0.41
2:E:128:PRO:HB2	2:E:151:VAL:HG23	2.01	0.41
3:F:318:CYS:C	3:F:320:GLY:H	2.27	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
2:E:62:GLN:CD	2:E:62:GLN:H	2.22	0.41
1:D:92:PHE:CD1	1:D:92:PHE:C	2.99	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
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:409:MET:HG2	3:C:410:TYR:N	2.35	0.41
3:C:426:LYS:H	3:C:426:LYS:HG3	1.59	0.41
2:E:50:ASN:C	2:E:51:ILE:HG13	2.46	0.41
1:A:33:LEU:C	1:A:34:HIS:HD1	2.29	0.41
1:A:105:LYS:HA	1:A:138:TYR:OH	2.20	0.41
2:B:105:TYR:CD2	2:B:105:TYR:N	2.87	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
1:D:6:GLN:NE2	1:D:100:THR:HG23	2.29	0.41
1:D:59:ARG:C	1:D:60:PHE:O	2.62	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
1:D:25:ALA:CB	1:D:29:ILE:HD11	2.50	0.40
1:A:12:SER:HA	1:A:103:GLU:C	2.46	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
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:60:TYR:N	2:E:60:TYR:HD2	2.17	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:147:LEU:HD22	2:E:219:ILE:HG21	2.03	0.40
1:A:45:ARG:O	1:A:46:LEU:C	2.65	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:H	2:B:178:LEU:HD13	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	6
1	D	207/213 (97%)	179 (86%)	22 (11%)	6 (3%)	3	26
2	B	219/222 (99%)	188 (86%)	18 (8%)	13 (6%)	1	12
2	E	219/222 (99%)	183 (84%)	28 (13%)	8 (4%)	2	21
3	C	392/394 (100%)	342 (87%)	45 (12%)	5 (1%)	9	39
3	F	390/394 (99%)	351 (90%)	36 (9%)	3 (1%)	16	49
All	All	1634/1658 (99%)	1396 (85%)	182 (11%)	56 (3%)	3	23

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
2	E	151	VAL
3	F	226	THR
1	D	199	SER
2	E	78	THR
1	A	95	THR
2	B	209	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 [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	186/193 (96%)	155 (83%)	31 (17%)	2	13
1	D	187/193 (97%)	168 (90%)	19 (10%)	7	28
2	B	187/192 (97%)	144 (77%)	43 (23%)	1	5
2	E	186/192 (97%)	158 (85%)	28 (15%)	3	16
3	C	341/355 (96%)	298 (87%)	43 (13%)	4	21
3	F	340/355 (96%)	305 (90%)	35 (10%)	7	28
All	All	1427/1480 (96%)	1228 (86%)	199 (14%)	3	19

All (199) 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
1	A	12	SER
1	A	14	THR
1	A	17	ASP
1	A	29	ILE
1	A	33	LEU
1	A	46	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	130	VAL
1	A	135	ASN
1	A	163	ASP
1	A	165	ASP
1	A	180	THR
1	A	182	ASP
1	A	189	SER
1	A	191	THR
1	A	193	GLU
1	A	200	THR
2	B	2	VAL
2	B	11	LEU
2	B	20	ILE
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
2	B	98	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	100	ARG
2	B	103	THR
2	B	109	MET
2	B	147	LEU
2	B	155	PHE
2	B	157	GLU
2	B	159	VAL
2	B	160	THR
2	B	161	LEU
2	B	162	THR
2	B	173	HIS
2	B	178	LEU
2	B	179	LEU
2	B	183	LEU
2	B	196	THR
2	B	200	GLN
2	B	202	ILE
2	B	203	THR
2	B	206	VAL
2	B	213	THR
2	B	215	VAL
2	B	216	ASP
3	C	38	GLU
3	C	43	LEU
3	C	44	ARG
3	C	45	ASN
3	C	47	THR
3	C	84	GLU
3	C	85	GLU
3	C	100	ILE
3	C	132	LEU
3	C	133	ILE
3	C	135	THR
3	C	140	VAL
3	C	148	GLN
3	C	149	VAL
3	C	152	LEU
3	C	153	ARG
3	C	154	GLU
3	C	155	ILE
3	C	159	MET
3	C	160	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	167	LEU
3	C	177	LEU
3	C	181	LYS
3	C	213	TYR
3	C	214	VAL
3	C	216	LEU
3	C	223	LEU
3	C	252	ASP
3	C	272	ASP
3	C	300	GLU
3	C	318	CYS
3	C	329	CYS
3	C	330	LYS
3	C	331	ASN
3	C	348	ARG
3	C	354	GLU
3	C	356	MET
3	C	372	LEU
3	C	411	LEU
3	C	415	VAL
3	C	425	LEU
3	C	426	LYS
3	C	429	ILE
1	D	14	THR
1	D	41	HIS
1	D	46	LEU
1	D	48	ILE
1	D	50	TYR
1	D	53	ILE
1	D	56	ILE
1	D	59	ARG
1	D	83	VAL
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	177	LEU
1	D	193	GLU
1	D	206	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	2	VAL
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	70	LEU
2	E	74	LYS
2	E	81	MET
2	E	84	LYS
2	E	109	MET
2	E	116	THR
2	E	126	THR
2	E	133	LEU
2	E	136	VAL
2	E	137	CYS
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	43	LEU
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	214	VAL
3	F	216	LEU
3	F	217	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	219	GLU
3	F	222	TYR
3	F	223	LEU
3	F	224	ASN
3	F	249	ASN
3	F	259	LEU
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	369	ILE
3	F	400	ASP
3	F	417	ILE
3	F	420	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	88	ASN
3	C	148	GLN
3	C	150	HIS
3	C	344	GLN
2	E	33	ASN
2	E	35	ASN
3	F	357	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	0.46	0	17,19,21	0.61	0
4	NAG	G	2	4	14,14,15	0.26	0	17,19,21	0.48	0
4	BMA	G	3	4	11,11,12	0.72	0	15,15,17	0.64	0
4	MAN	G	4	4	11,11,12	0.94	1 (9%)	15,15,17	1.65	1 (6%)
5	NAG	H	1	5,3	14,14,15	0.35	0	17,19,21	0.44	0
5	NAG	H	2	5	14,14,15	0.21	0	17,19,21	0.46	0
5	NAG	I	1	5,3	14,14,15	0.85	1 (7%)	17,19,21	1.42	1 (5%)
5	NAG	I	2	5	14,14,15	0.34	0	17,19,21	0.57	0
5	NAG	J	1	5,3	14,14,15	0.34	0	17,19,21	0.61	0
5	NAG	J	2	5	14,14,15	0.23	0	17,19,21	0.35	0
6	NAG	K	1	6,3	14,14,15	0.41	0	17,19,21	0.55	0
6	NAG	K	2	6	14,14,15	0.80	1 (7%)	17,19,21	1.34	1 (5%)
6	BMA	K	3	6	11,11,12	0.64	0	15,15,17	0.79	0
6	MAN	K	4	6	11,11,12	0.66	0	15,15,17	1.11	2 (13%)
6	MAN	K	5	6	11,11,12	0.76	0	15,15,17	1.12	2 (13%)
6	NAG	L	1	6,3	14,14,15	0.18	0	17,19,21	1.03	2 (11%)
6	NAG	L	2	6	14,14,15	0.34	0	17,19,21	0.52	0
6	BMA	L	3	6	11,11,12	1.07	1 (9%)	15,15,17	0.87	0
6	MAN	L	4	6	11,11,12	1.05	0	15,15,17	0.99	2 (13%)
6	MAN	L	5	6	11,11,12	0.85	1 (9%)	15,15,17	1.66	2 (13%)
4	NAG	M	1	3,4	14,14,15	0.64	1 (7%)	17,19,21	0.56	0
4	NAG	M	2	4	14,14,15	0.29	0	17,19,21	0.47	0
4	BMA	M	3	4	11,11,12	1.12	2 (18%)	15,15,17	0.90	2 (13%)
4	MAN	M	4	4	11,11,12	0.92	0	15,15,17	1.49	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	N	1	5,3	14,14,15	0.39	0	17,19,21	0.50	0
5	NAG	N	2	5	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	O	1	5,3	14,14,15	0.59	0	17,19,21	1.13	1 (5%)
5	NAG	O	2	5	14,14,15	0.23	0	17,19,21	0.52	0
5	NAG	P	1	5,3	14,14,15	1.00	2 (14%)	17,19,21	1.12	1 (5%)
5	NAG	P	2	5	14,14,15	0.21	0	17,19,21	0.52	0
6	NAG	Q	1	6,3	14,14,15	0.63	0	17,19,21	0.87	1 (5%)
6	NAG	Q	2	6	14,14,15	0.72	1 (7%)	17,19,21	1.22	1 (5%)
6	BMA	Q	3	6	11,11,12	1.31	2 (18%)	15,15,17	1.57	4 (26%)
6	MAN	Q	4	6	11,11,12	1.17	2 (18%)	15,15,17	0.78	0
6	MAN	Q	5	6	11,11,12	0.79	0	15,15,17	1.15	2 (13%)
4	NAG	R	1	3,4	14,14,15	0.28	0	17,19,21	1.34	1 (5%)
4	NAG	R	2	4	14,14,15	0.57	0	17,19,21	0.40	0
4	BMA	R	3	4	11,11,12	1.14	1 (9%)	15,15,17	1.74	2 (13%)
4	MAN	R	4	4	11,11,12	0.96	0	15,15,17	1.14	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	5,3	-	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	5,3	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	NAG	J	1	5,3	-	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	6,3	-	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	6,3	-	1/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	5,3	-	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	5,3	-	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	5,3	-	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	6,3	-	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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	3	BMA	O5-C1	-3.24	1.38	1.43
5	I	1	NAG	O5-C1	3.08	1.48	1.43
5	P	1	NAG	C1-C2	2.96	1.56	1.52
6	K	2	NAG	O5-C1	2.87	1.48	1.43
6	Q	4	MAN	O5-C5	2.77	1.48	1.43
6	L	3	BMA	O5-C1	-2.77	1.39	1.43
6	Q	3	BMA	O5-C1	-2.53	1.39	1.43
6	Q	2	NAG	O5-C1	2.43	1.47	1.43
6	Q	3	BMA	C4-C5	2.36	1.58	1.53
4	M	1	NAG	O5-C1	-2.30	1.39	1.43
4	M	3	BMA	O5-C1	-2.22	1.40	1.43
4	G	4	MAN	O5-C5	2.21	1.47	1.43
6	L	5	MAN	O5-C5	2.16	1.47	1.43
5	P	1	NAG	O5-C1	2.11	1.47	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	3	BMA	C4-C5	2.11	1.57	1.53
6	Q	4	MAN	C1-C2	2.09	1.57	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	NAG	C1-O5-C5	5.59	119.67	112.19
4	G	4	MAN	C1-O5-C5	5.53	119.60	112.19
6	L	5	MAN	C1-O5-C5	5.28	119.26	112.19
6	K	2	NAG	C1-O5-C5	5.24	119.20	112.19
4	M	4	MAN	C1-O5-C5	4.85	118.69	112.19
6	Q	2	NAG	C1-O5-C5	4.80	118.62	112.19
4	R	3	BMA	C1-O5-C5	4.63	118.39	112.19
4	R	1	NAG	C1-O5-C5	4.49	118.20	112.19
5	O	1	NAG	C1-O5-C5	4.39	118.08	112.19
6	Q	3	BMA	C3-C4-C5	3.76	117.06	110.23
5	P	1	NAG	C1-O5-C5	3.50	116.87	112.19
4	R	3	BMA	O5-C5-C6	-3.30	101.23	107.66
6	K	4	MAN	C1-O5-C5	3.15	116.41	112.19
6	Q	1	NAG	C1-O5-C5	3.06	116.29	112.19
6	L	1	NAG	C1-O5-C5	2.58	115.64	112.19
4	R	4	MAN	O2-C2-C3	-2.48	105.02	110.15
6	L	4	MAN	C1-O5-C5	2.41	115.42	112.19
6	Q	5	MAN	C1-O5-C5	2.39	115.39	112.19
6	L	4	MAN	O2-C2-C3	-2.36	105.25	110.15
6	Q	3	BMA	C1-O5-C5	2.36	115.34	112.19
6	L	5	MAN	O2-C2-C3	-2.33	105.33	110.15
4	R	4	MAN	C1-O5-C5	2.30	115.28	112.19
6	K	4	MAN	O2-C2-C3	-2.26	105.47	110.15
4	R	4	MAN	C1-C2-C3	-2.22	106.41	109.64
6	K	5	MAN	C1-O5-C5	2.18	115.11	112.19
6	Q	5	MAN	O2-C2-C3	-2.16	105.68	110.15
6	Q	3	BMA	O3-C3-C4	-2.11	105.40	110.38
6	K	5	MAN	O2-C2-C3	-2.09	105.81	110.15
4	M	3	BMA	C3-C4-C5	2.07	113.98	110.23
4	M	3	BMA	O2-C2-C3	-2.04	105.93	110.15
6	Q	3	BMA	O2-C2-C3	-2.04	105.94	110.15
6	L	1	NAG	C2-N2-C7	2.03	125.62	122.90

There are no chirality outliers.

All (43) torsion outliers are listed below:

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

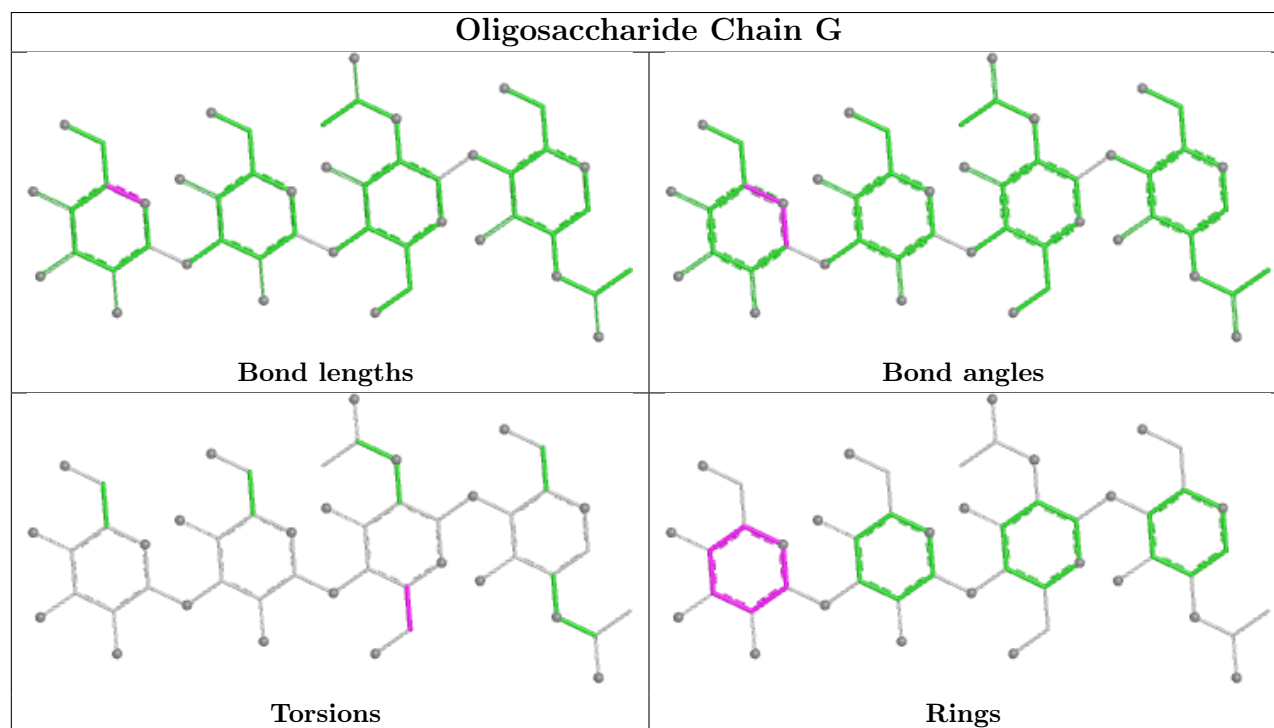
All (4) ring outliers are listed below:

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

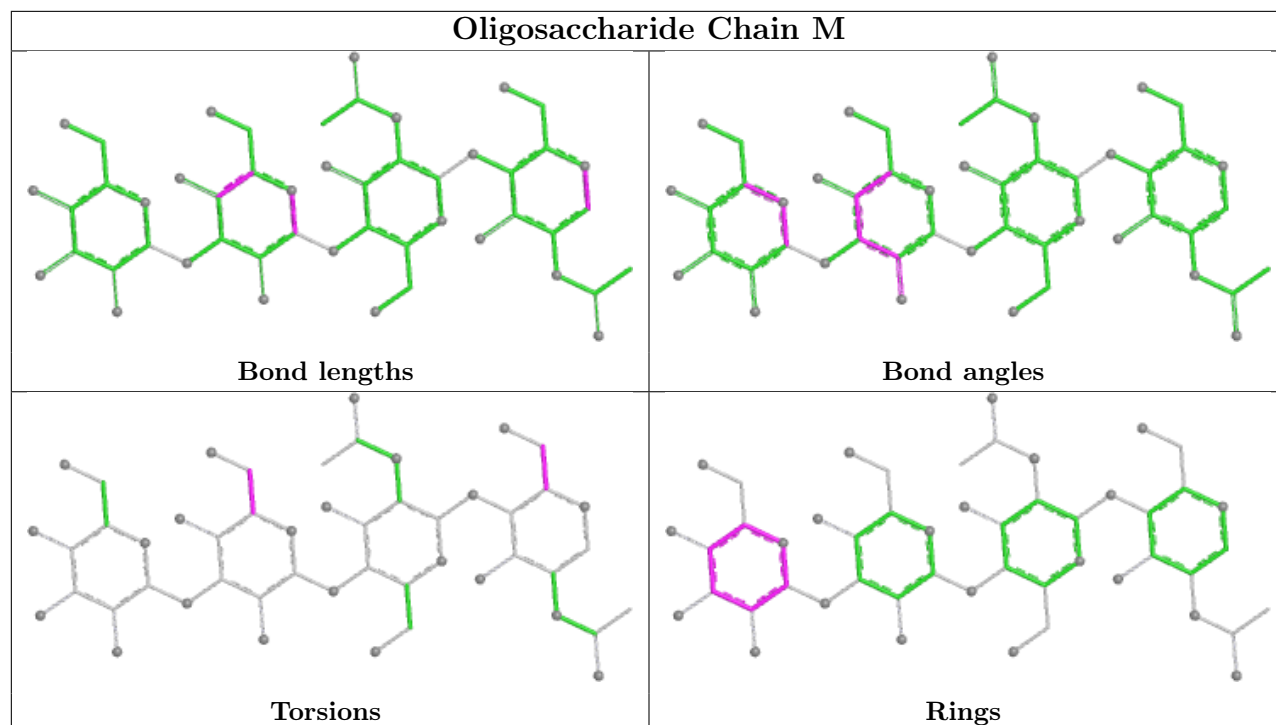
10 monomers are involved in 17 short contacts:

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

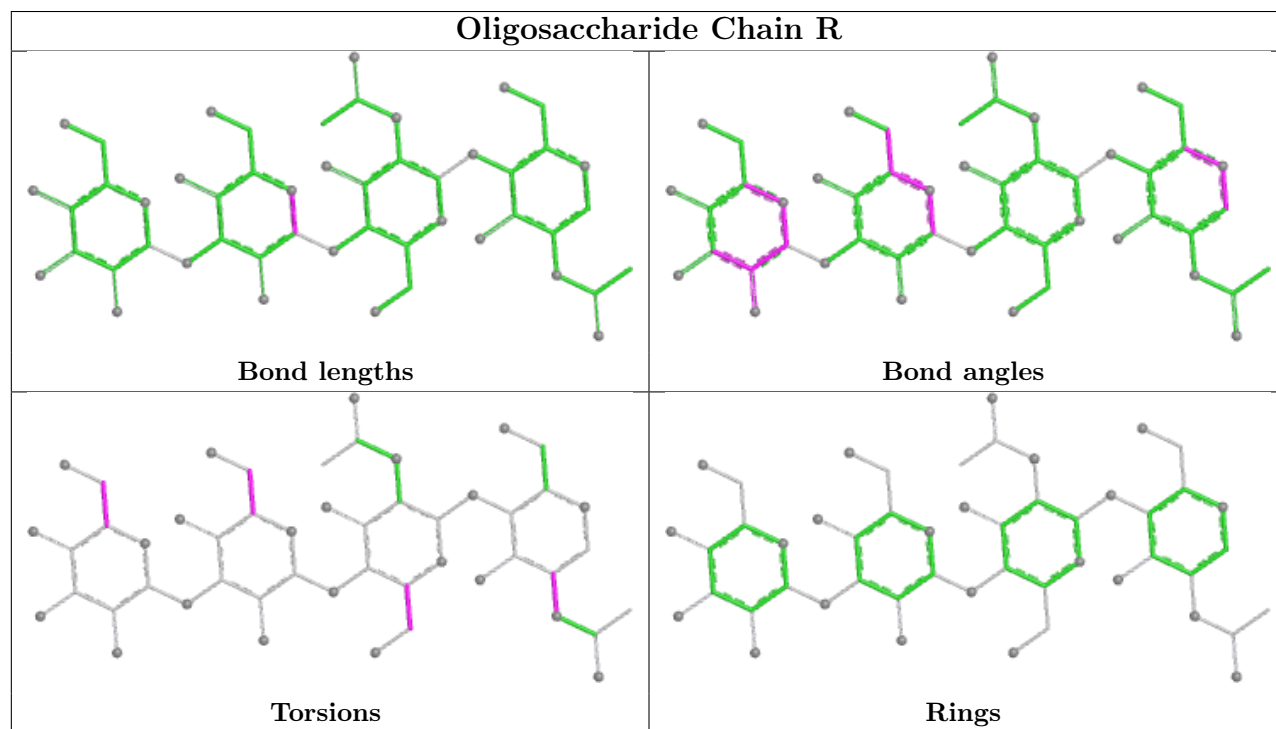
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

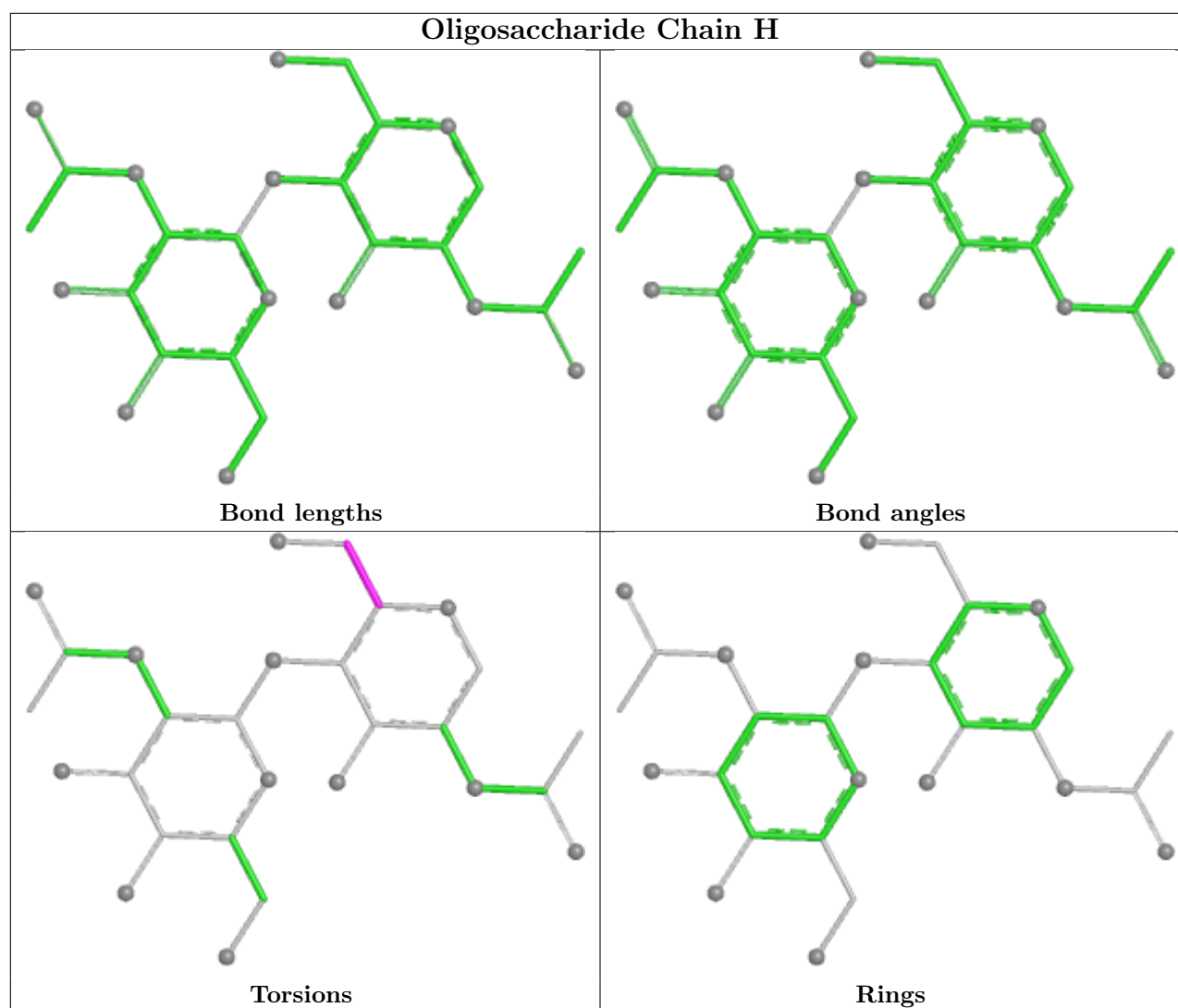


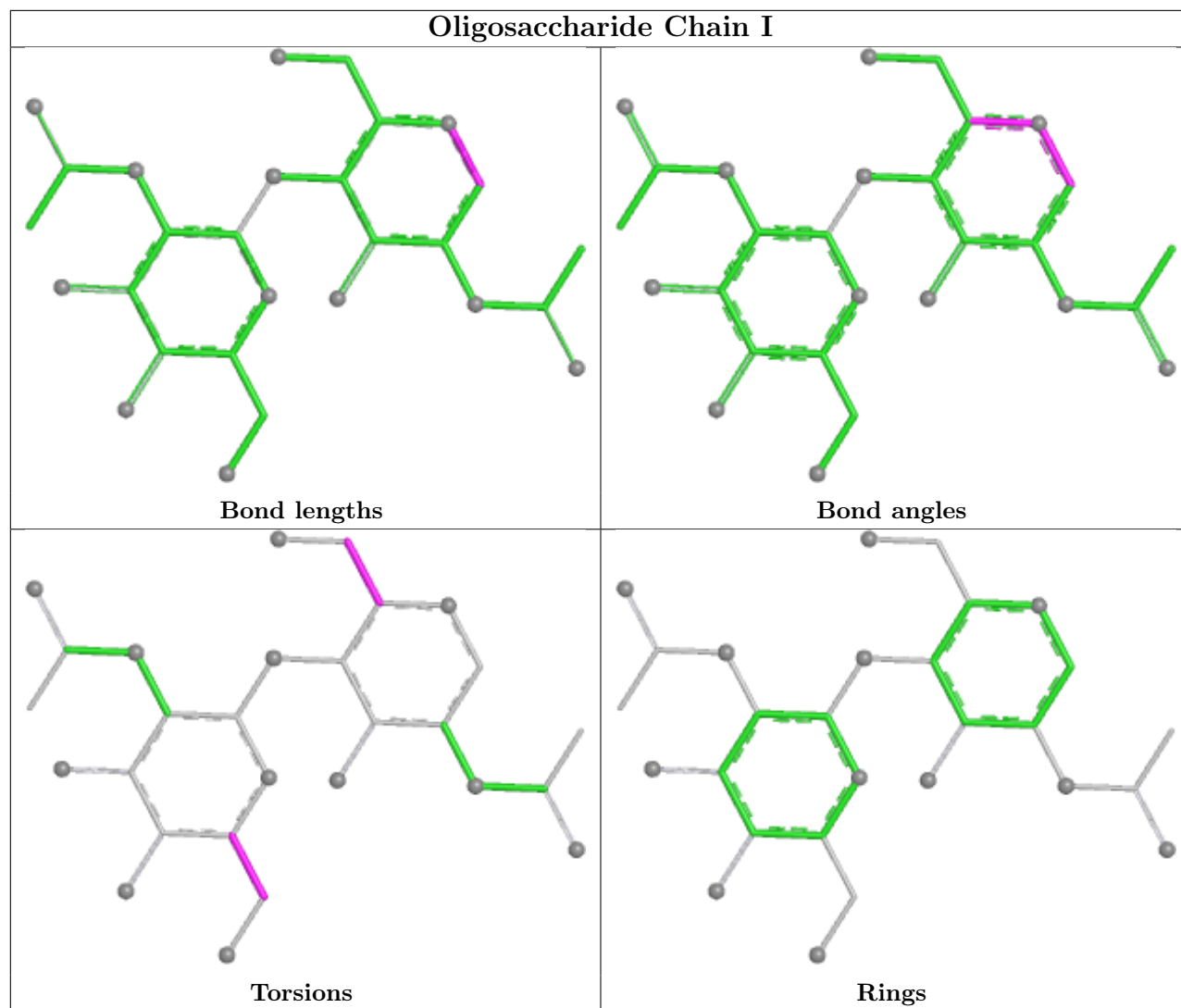
Oligosaccharide Chain M

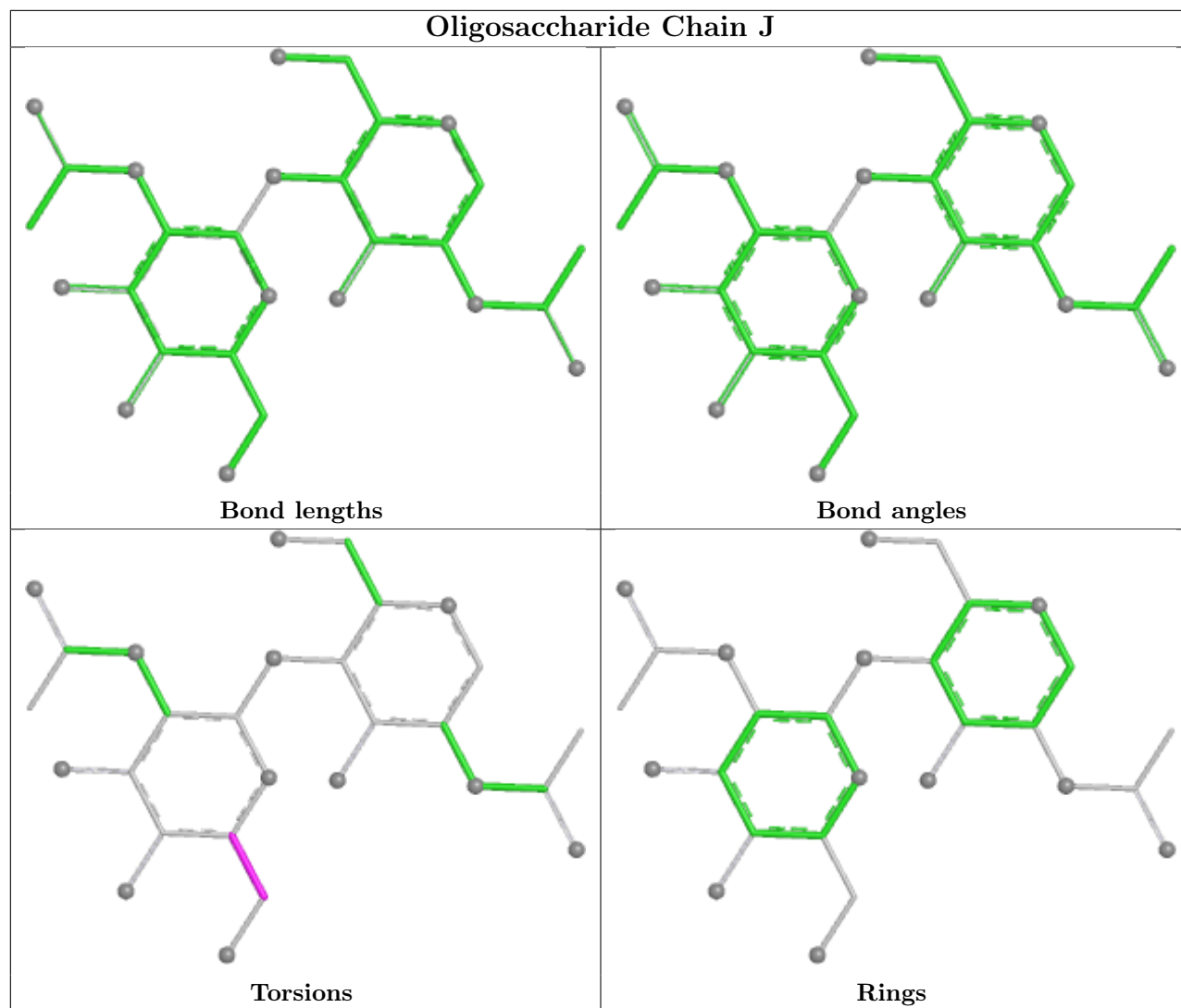


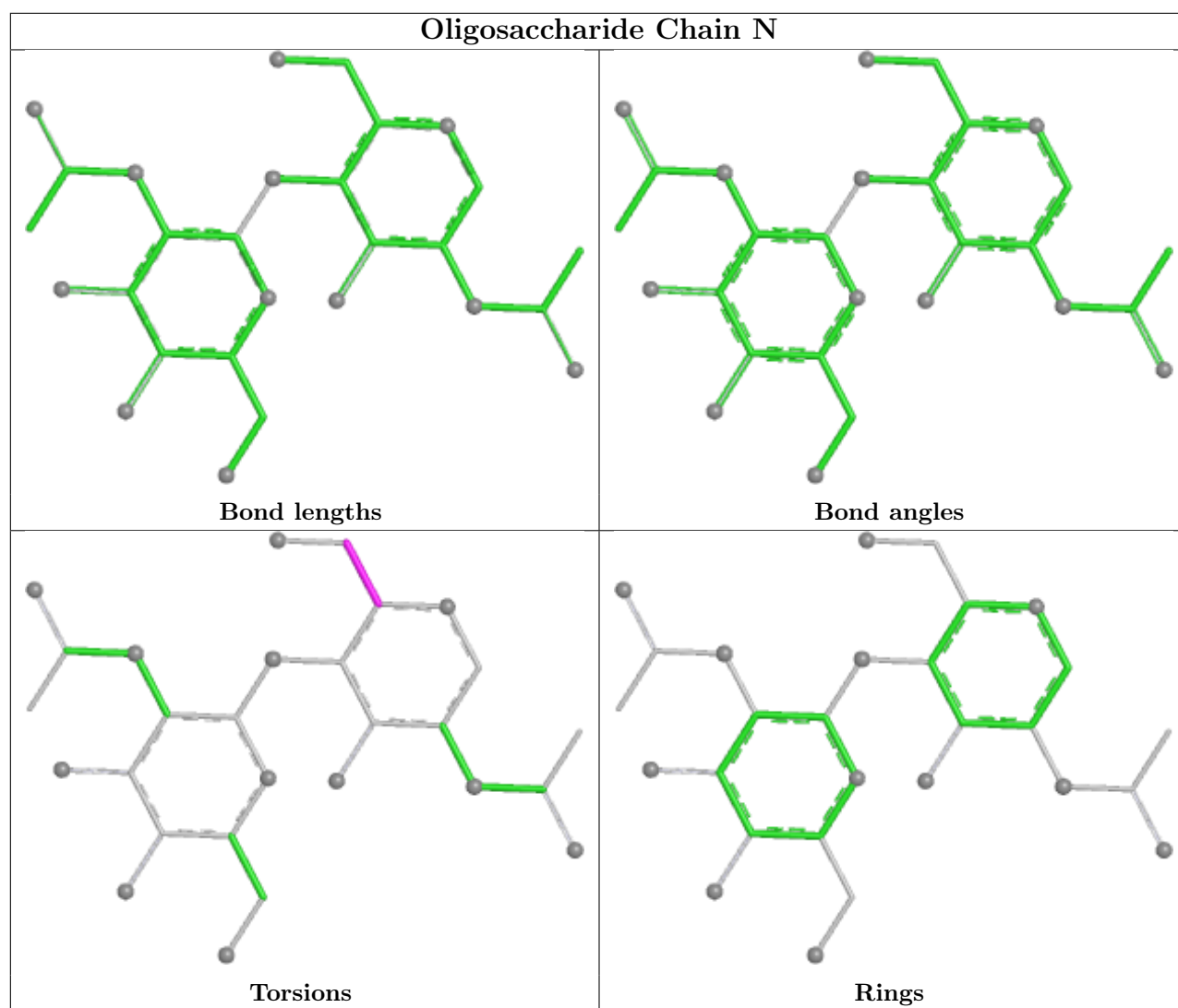
Oligosaccharide Chain R

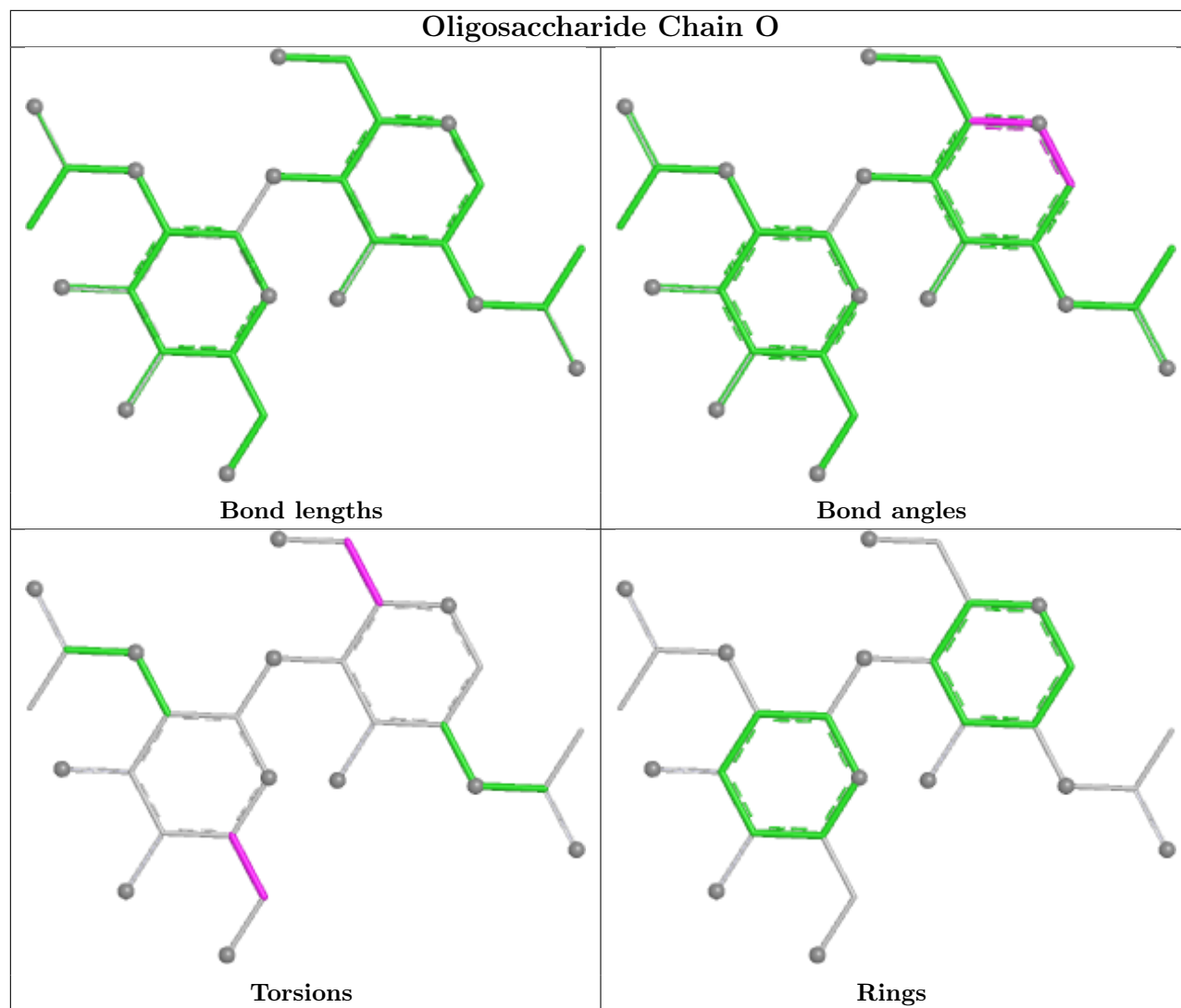


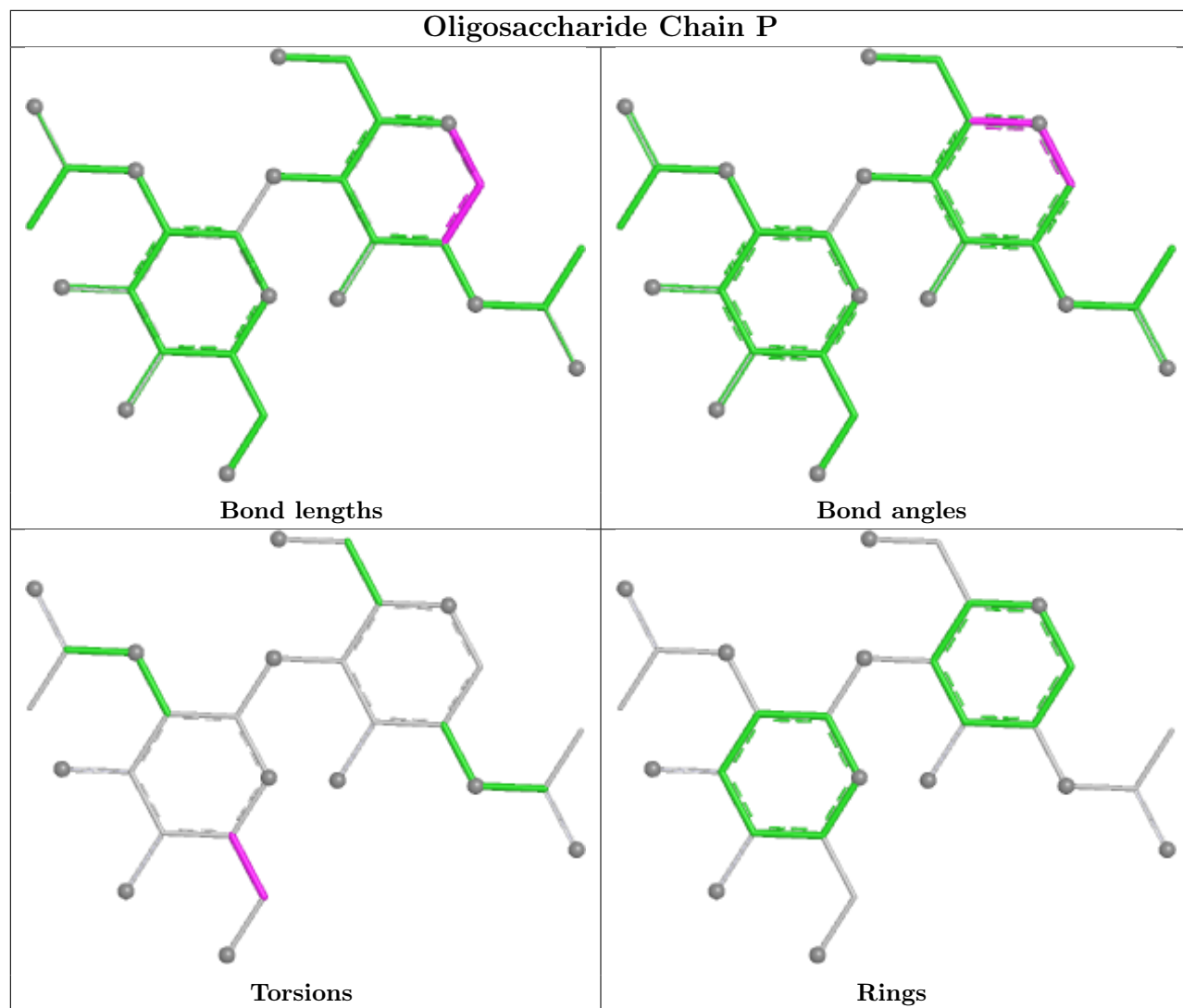


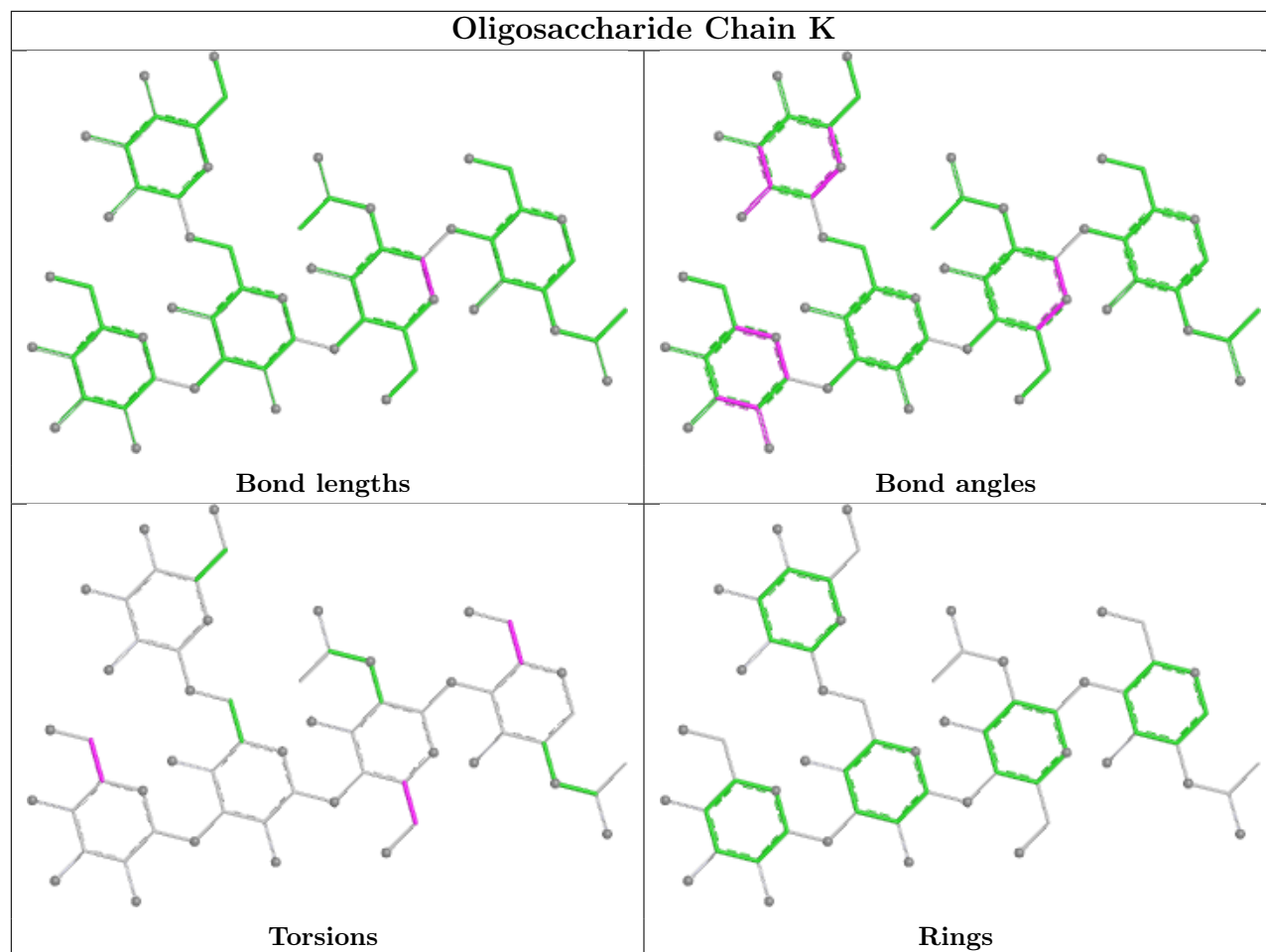


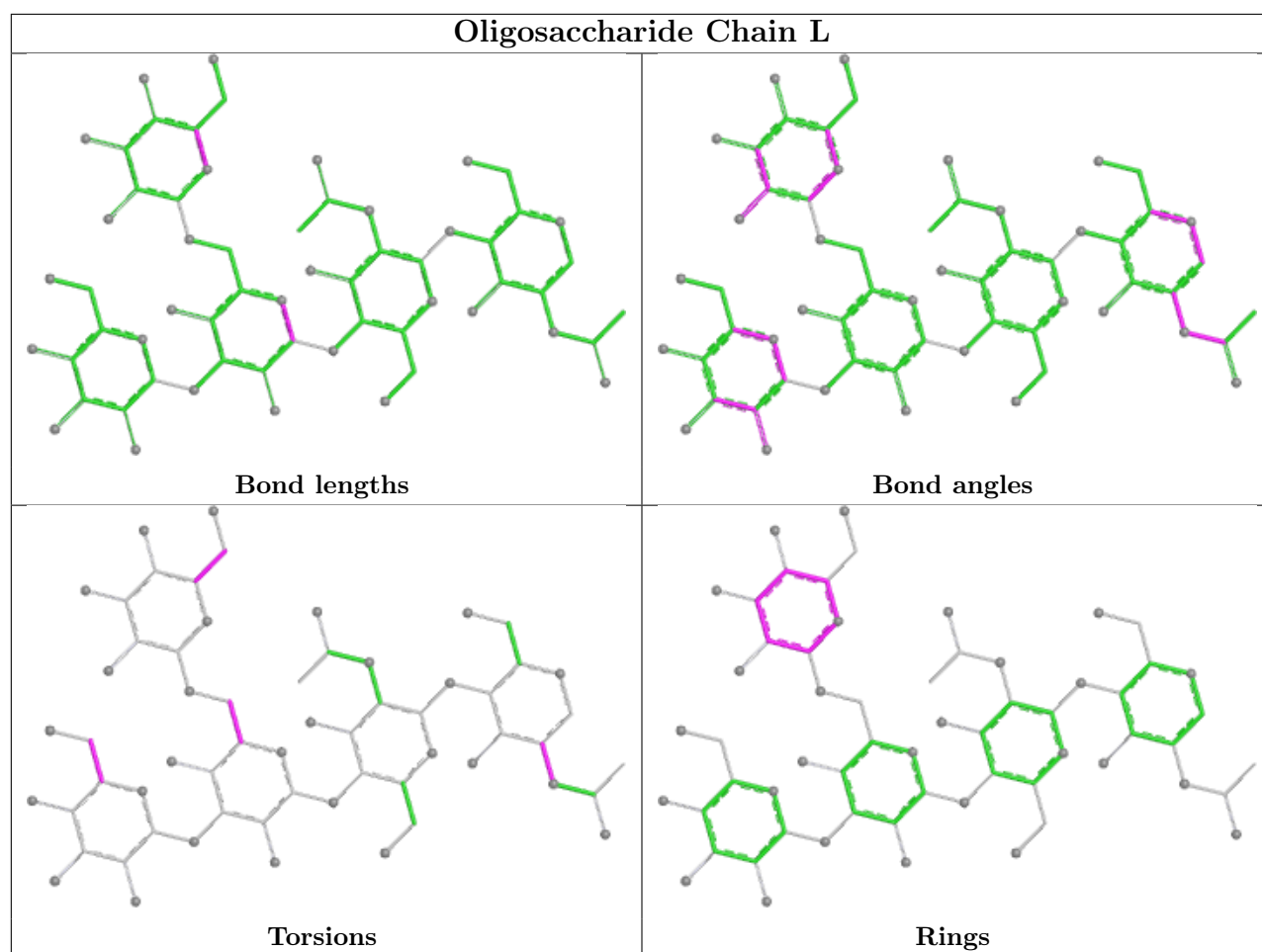


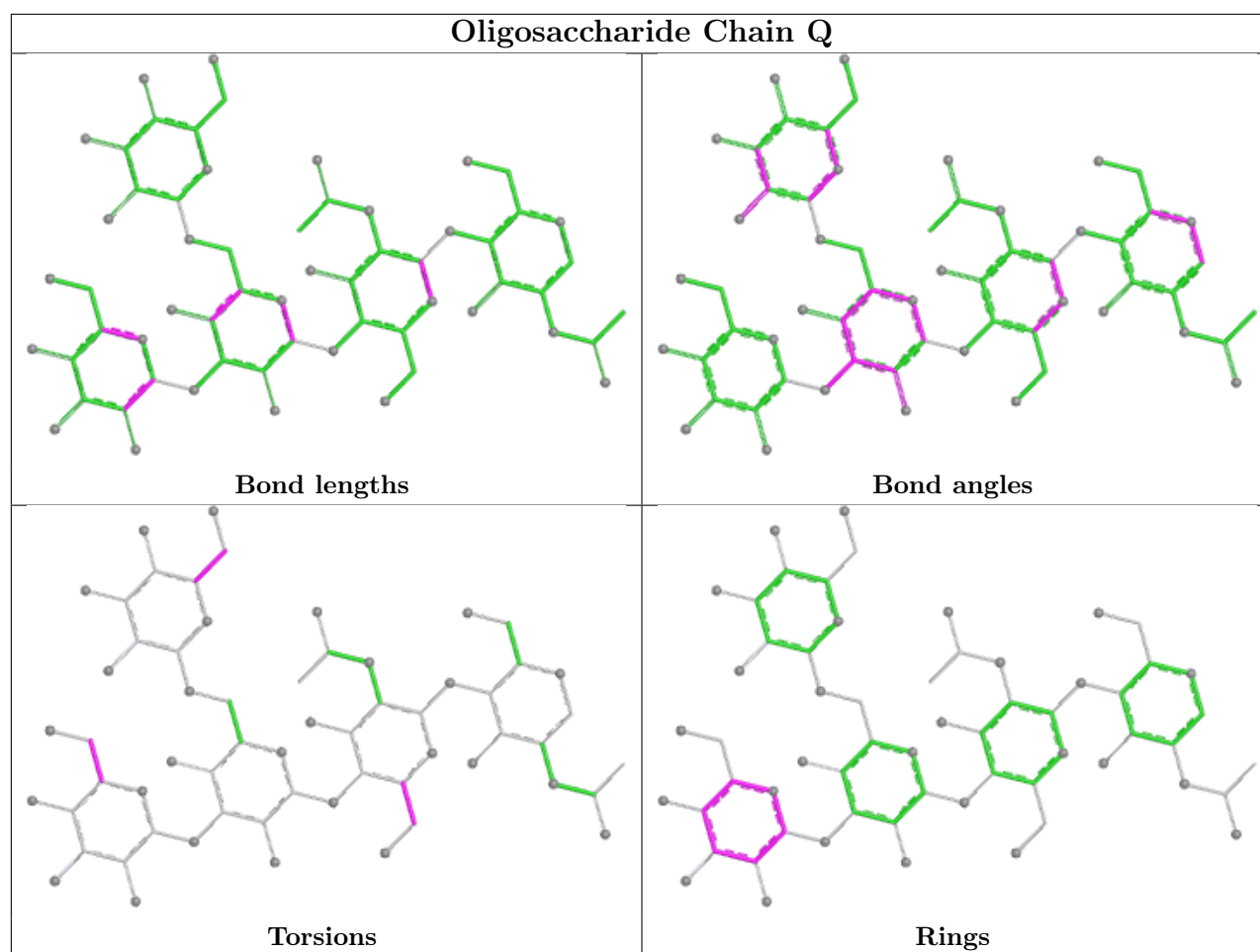












5.6 Ligand geometry [i](#)

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	1.01	1 (5%)
7	NAG	F	507	3	14,14,15	0.27	0	17,19,21	0.79	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	2.26	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	3.94	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%)	0.17	2 (0%) 79 56	30, 89, 113, 167	0
1	D	209/213 (98%)	0.03	0 100 100	30, 87, 107, 132	0
2	B	221/222 (99%)	0.11	2 (0%) 81 58	56, 85, 116, 144	0
2	E	221/222 (99%)	0.11	4 (1%) 67 42	63, 88, 125, 155	0
3	C	394/394 (100%)	-0.01	5 (1%) 75 50	53, 86, 122, 136	0
3	F	392/394 (99%)	0.02	4 (1%) 79 56	50, 88, 131, 154	0
All	All	1646/1658 (99%)	0.06	17 (1%) 79 56	30, 87, 123, 167	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	154	GLU	3.4
2	E	22	CYS	2.3
3	C	413	GLU	2.3
2	E	71	THR	2.3
3	F	64	PHE	2.2
2	E	81	MET	2.2
1	A	34	HIS	2.2
2	B	47	TRP	2.1
3	F	253	GLY	2.1
3	F	154	GLU	2.1
2	B	70	LEU	2.1
1	A	62	GLY	2.1
3	C	287	VAL	2.1
3	C	153	ARG	2.0
3	F	228	ILE	2.0
3	C	152	LEU	2.0
2	E	75	SER	2.0

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

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

6.3 Carbohydrates ⓘ

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.

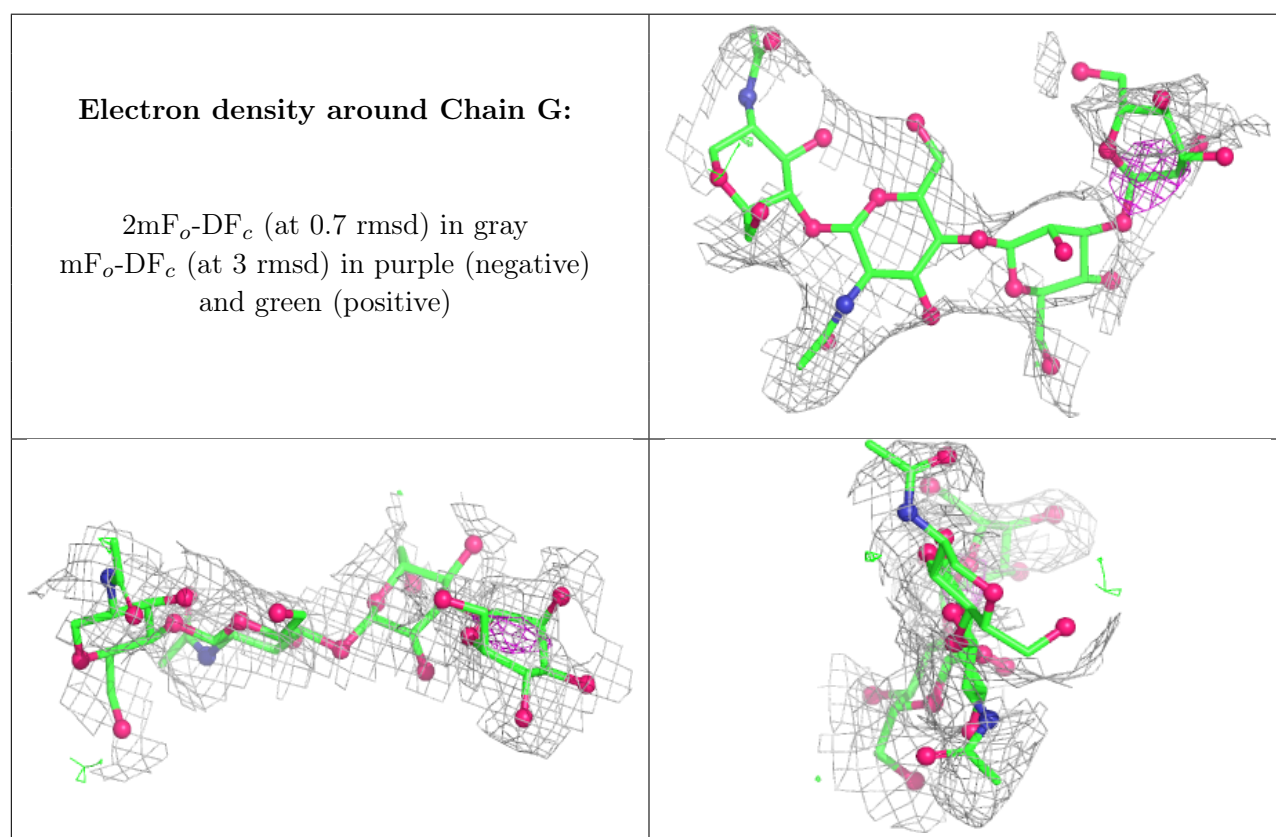
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MAN	K	5	11/12	0.24	0.14	121,123,131,134	0
6	MAN	Q	5	11/12	0.24	0.12	118,127,135,140	0
5	NAG	P	2	14/15	0.27	0.13	128,142,146,147	0
6	MAN	Q	4	11/12	0.31	0.13	134,139,142,143	0
4	BMA	G	3	11/12	0.38	0.11	115,127,135,136	0
6	MAN	L	5	11/12	0.41	0.10	91,115,122,136	0
6	BMA	Q	3	11/12	0.42	0.13	124,131,134,143	0
4	MAN	M	4	11/12	0.43	0.12	119,125,134,139	0
4	MAN	G	4	11/12	0.44	0.11	121,132,140,142	0
5	NAG	J	1	14/15	0.45	0.11	106,130,137,141	0
5	NAG	I	2	14/15	0.50	0.12	96,107,111,111	0
5	NAG	P	1	14/15	0.51	0.10	133,141,146,152	0
5	NAG	J	2	14/15	0.52	0.11	123,138,144,145	0
4	BMA	R	3	11/12	0.55	0.14	89,100,107,107	0
6	MAN	K	4	11/12	0.59	0.09	106,117,125,129	0
6	BMA	L	3	11/12	0.59	0.11	104,109,118,122	0
4	MAN	R	4	11/12	0.62	0.10	95,112,127,127	0
6	MAN	L	4	11/12	0.63	0.11	113,118,120,122	0
5	NAG	O	2	14/15	0.64	0.12	109,116,122,127	0
4	BMA	M	3	11/12	0.67	0.08	104,116,123,128	0
6	BMA	K	3	11/12	0.69	0.10	113,120,124,126	0
4	NAG	G	2	14/15	0.70	0.11	94,108,120,124	0
5	NAG	N	2	14/15	0.76	0.09	106,114,121,122	0
5	NAG	H	2	14/15	0.77	0.10	100,120,128,134	0
4	NAG	R	2	14/15	0.79	0.13	76,86,96,101	0
6	NAG	Q	2	14/15	0.80	0.10	99,108,117,126	0
4	NAG	M	2	14/15	0.80	0.09	91,99,102,109	0
6	NAG	K	1	14/15	0.82	0.12	95,100,102,107	0
6	NAG	Q	1	14/15	0.83	0.14	79,98,103,105	0
5	NAG	N	1	14/15	0.84	0.10	87,99,108,112	0
6	NAG	L	2	14/15	0.84	0.10	81,92,95,104	0
4	NAG	R	1	14/15	0.85	0.11	70,77,84,85	0

Continued on next page...

Continued from previous page...

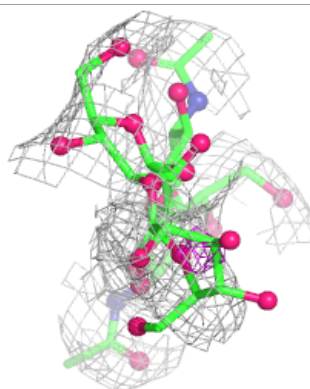
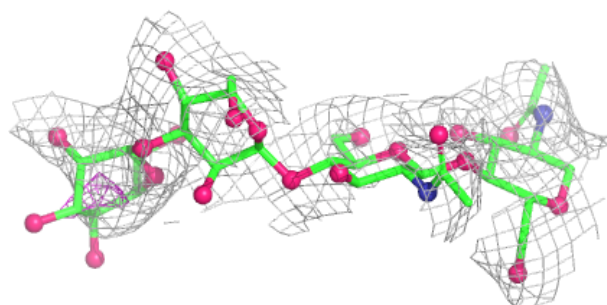
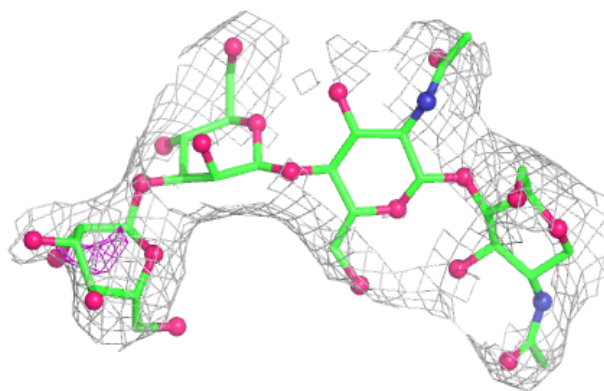
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	K	2	14/15	0.85	0.09	98,104,117,117	0
6	NAG	L	1	14/15	0.86	0.10	74,79,86,93	0
5	NAG	H	1	14/15	0.86	0.10	88,94,100,106	0
5	NAG	O	1	14/15	0.87	0.07	94,98,105,111	0
4	NAG	G	1	14/15	0.89	0.12	74,86,94,95	0
5	NAG	I	1	14/15	0.89	0.09	79,83,93,95	0
4	NAG	M	1	14/15	0.94	0.07	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.

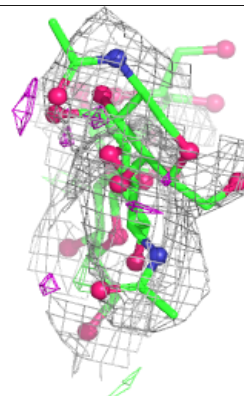
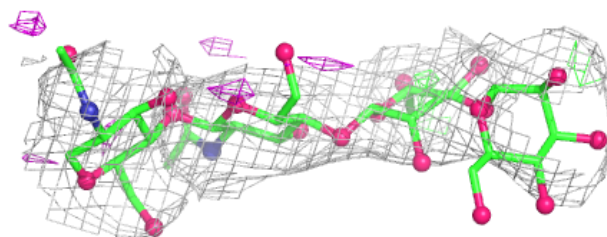
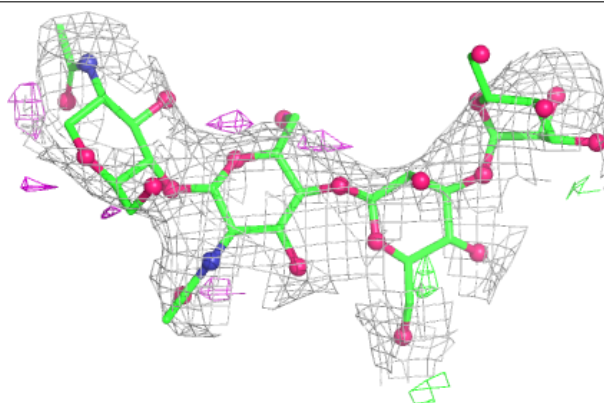


Electron density around Chain M:

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

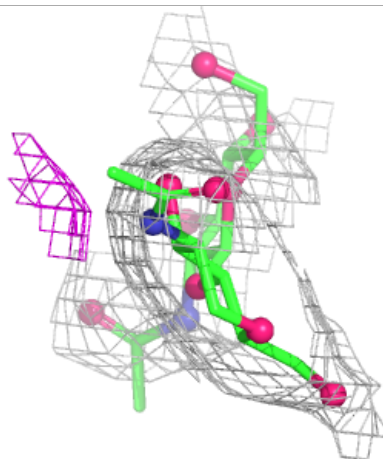
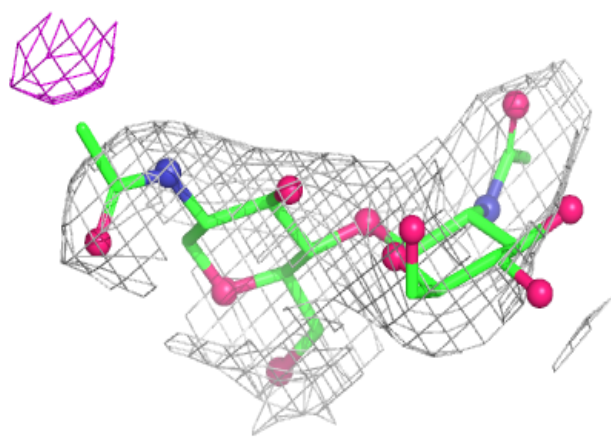
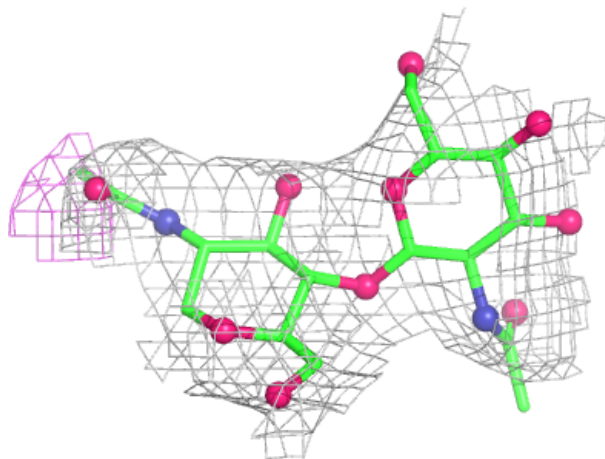
**Electron density around Chain R:**

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



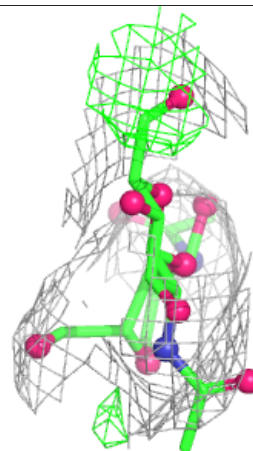
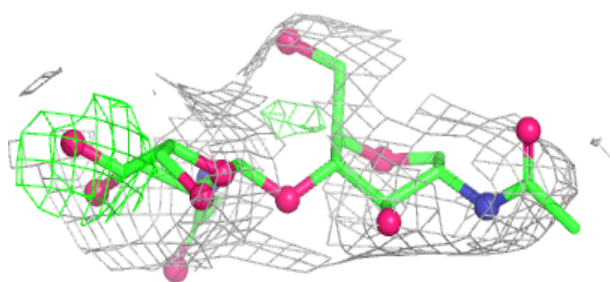
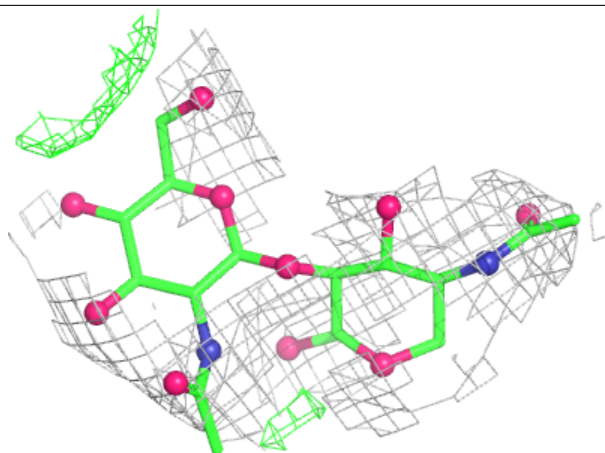
Electron density around Chain H:

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



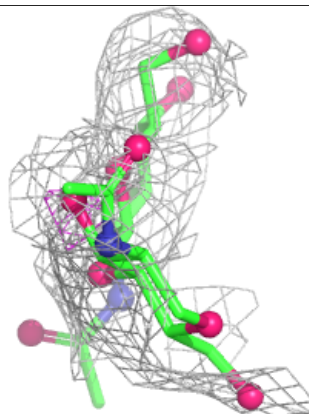
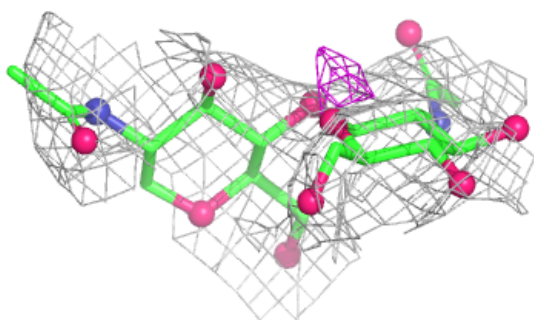
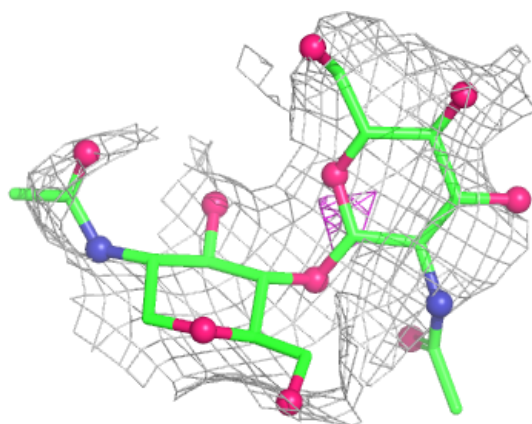
Electron density around Chain I:

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

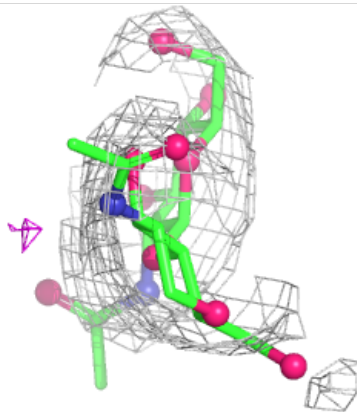
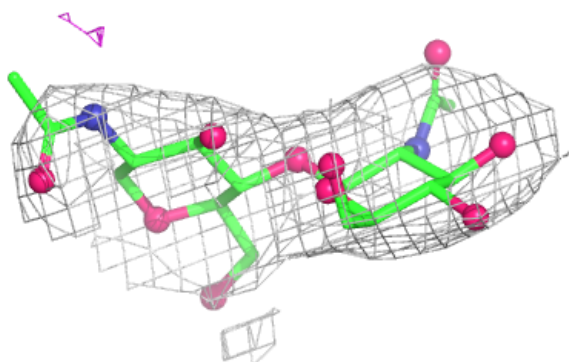
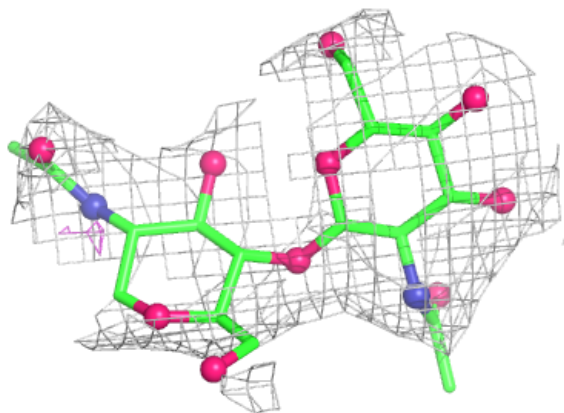


Electron density around Chain J:

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

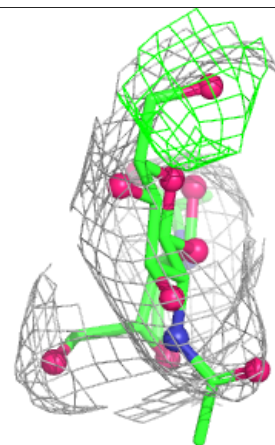
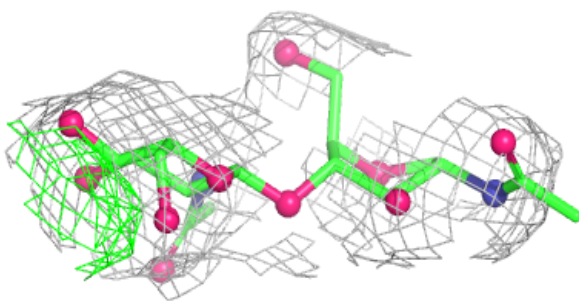
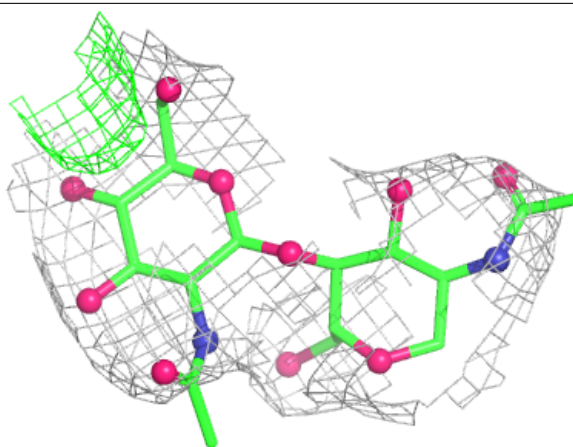
**Electron density around Chain N:**

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



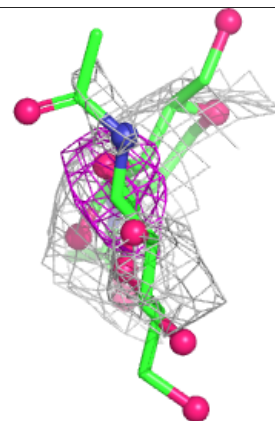
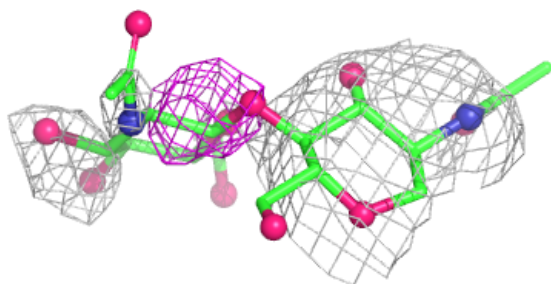
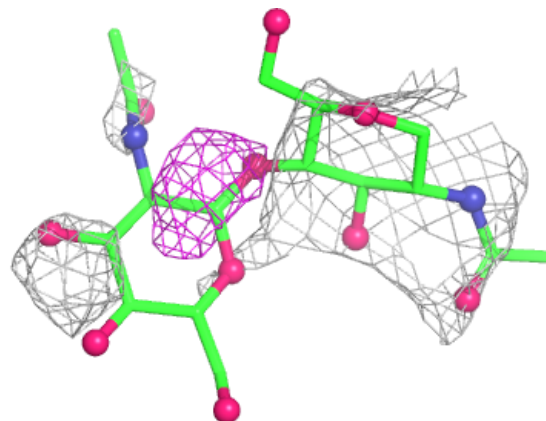
Electron density around Chain O:

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



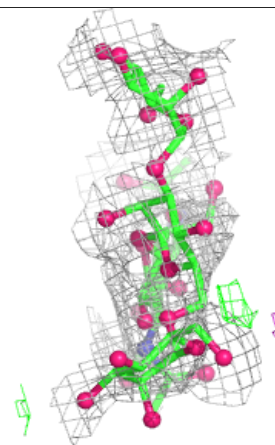
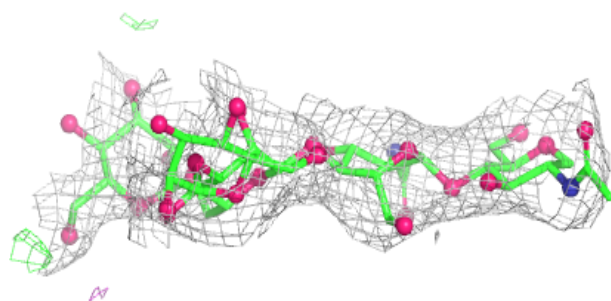
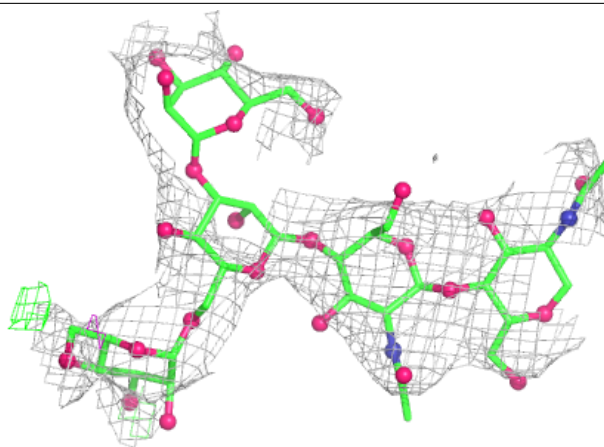
Electron density around Chain P:

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



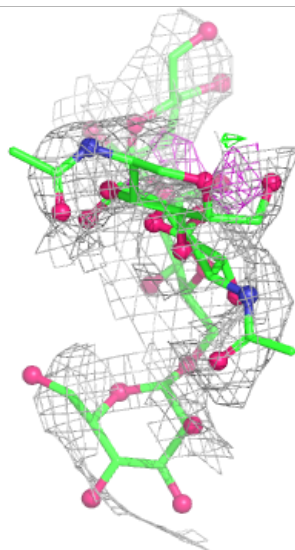
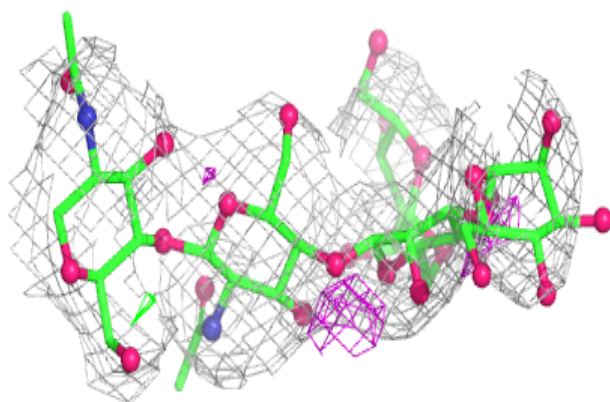
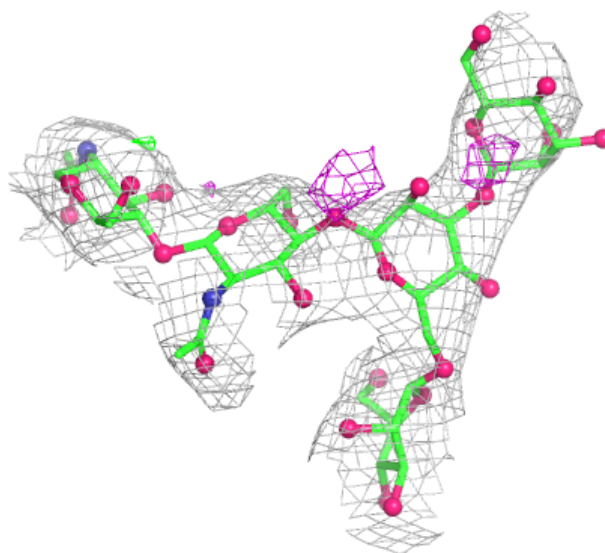
Electron density around Chain K:

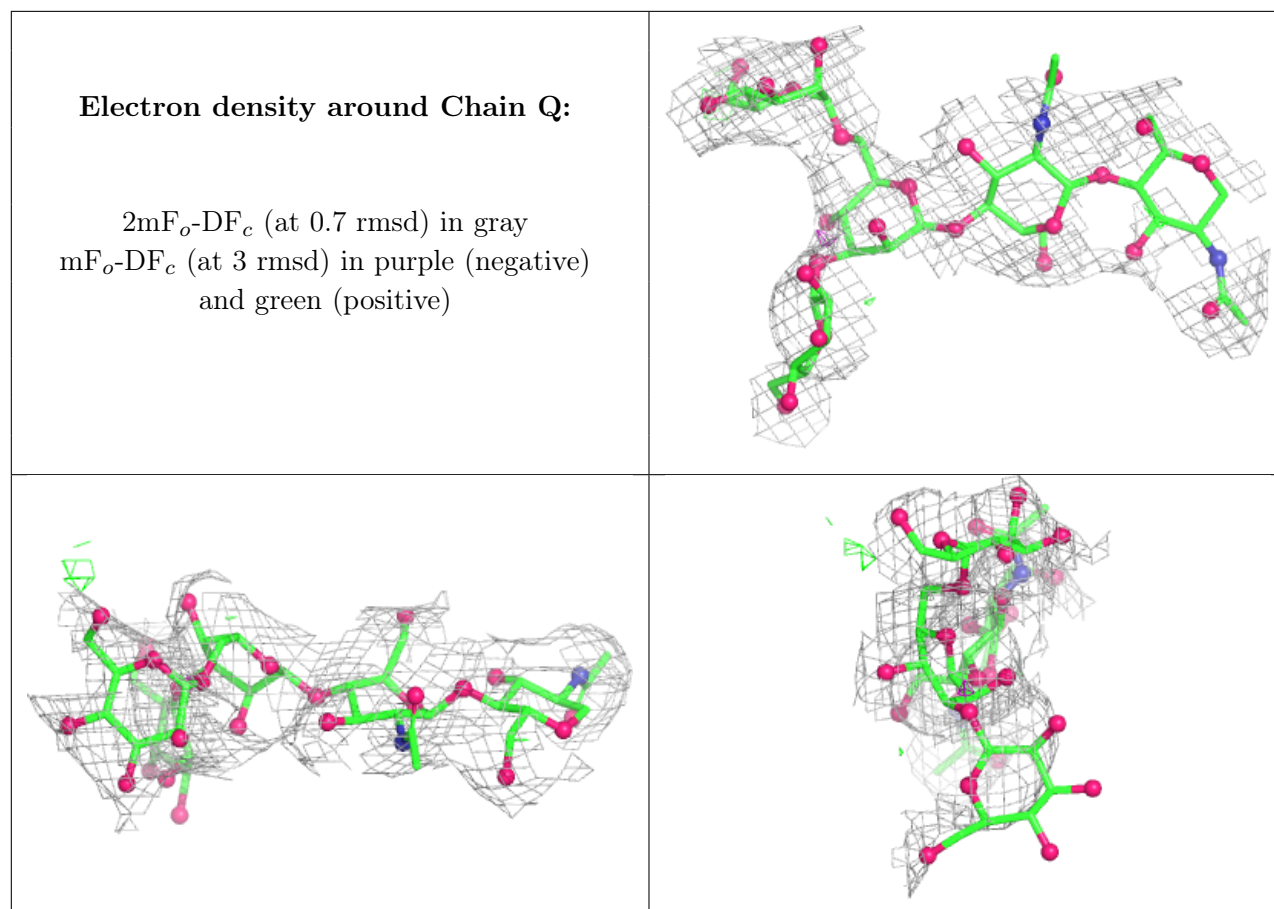
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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($\text{\AA}^2$)	Q<0.9
7	NAG	C	507	14/15	0.79	0.11	108,114,122,123	0
7	NAG	F	507	14/15	0.87	0.07	112,117,122,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.