



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:47 AM BST

PDB ID : 6NNF
Title : Crystal Structure of HIV-1 BG505 SOSIP.664 Prefusion Env Trimer Bound to VRC01 FR3-03 scFv in Complex with Crystallization Chaperones 3H109L Fab and 35O22 scFv at 3.5 Angstrom
Authors : Lai, Y.-T.; Kwong, P.D.
Deposited on : 2019-01-14
Resolution : 2.76 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

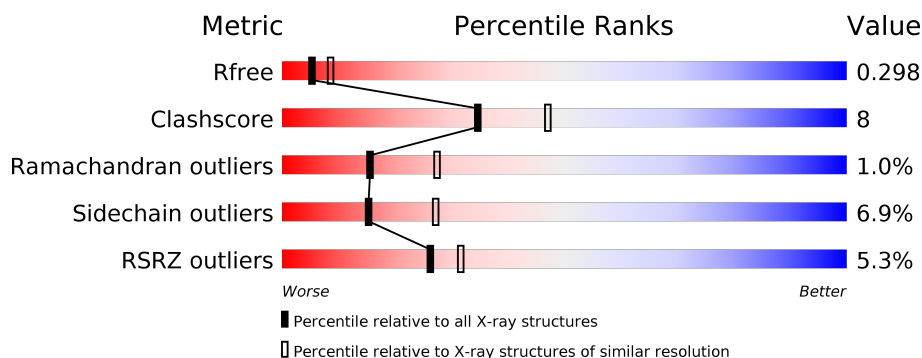
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	B	153	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>22%</div> <div>•</div> <div>15%</div> </div> </div>
2	D	153	<div> <div>12%</div> <div> <div></div> <div>62%</div> <div>20%</div> <div>•</div> <div>16%</div> </div> </div>
3	E	130	<div> <div>7%</div> <div> <div></div> <div>63%</div> <div>23%</div> <div>14%</div> </div> </div>
4	G	481	<div> <div></div> <div> <div></div> <div>61%</div> <div>25%</div> <div>•</div> <div>10%</div> </div> </div>
5	H	244	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>•</div> <div>7%</div> </div> </div>
6	L	217	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>•</div> <div>•</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	U	142	
8	V	115	
9	A	6	
10	C	2	
10	I	2	
10	K	2	
10	M	2	
10	N	2	
10	P	2	
10	Q	2	
11	F	5	
12	J	4	
13	O	10	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 11926 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 Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	130	Total	C	N	O	S	0	0	0
			1030	655	177	192	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called 35O22 scFv heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	128	Total	C	N	O	S	0	0	0
			994	628	169	192	5			

- Molecule 3 is a protein called 35O22 scFv light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	112	Total	C	N	O	S	0	0	0
			851	533	141	171	6			

- Molecule 4 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	431	Total	C	N	O	S	0	0	0
			3400	2140	601	632	27			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	137	ALA	ASN	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 5 is a protein called 3H109L Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	227	Total	C	N	O	S	0	0	0
			1721	1096	279	340	6			

- Molecule 6 is a protein called 3H109L Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	211	Total	C	N	O	S	0	0	0
			1604	1009	276	312	7			

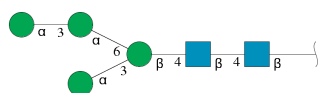
- Molecule 7 is a protein called VRC01 FR3-03 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	U	126	Total	C	N	O	S	0	0	0
			1010	636	183	183	8			

- Molecule 8 is a protein called VRC01 FR3-03 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	V	97	Total	C	N	O	S	0	0	0
			751	474	129	146	2			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



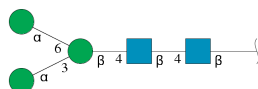
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	A	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



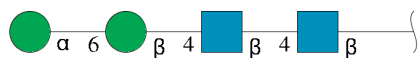
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 11 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.



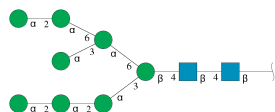
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



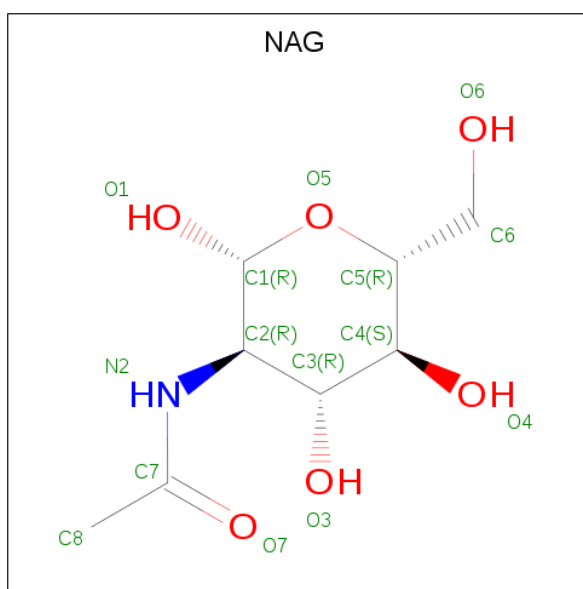
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	O	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

Continued on next page...

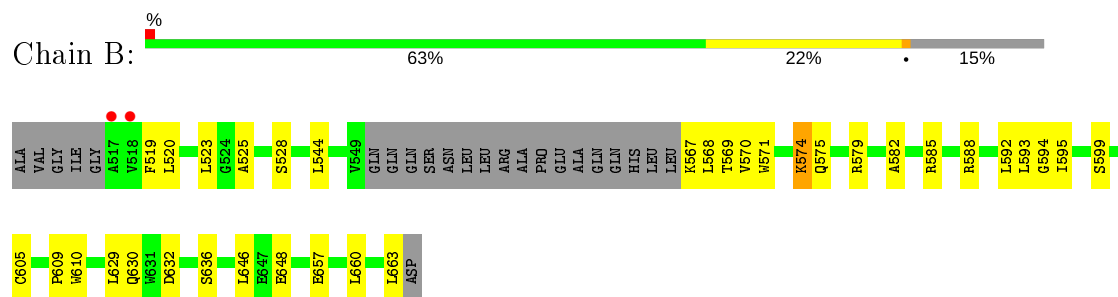
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		

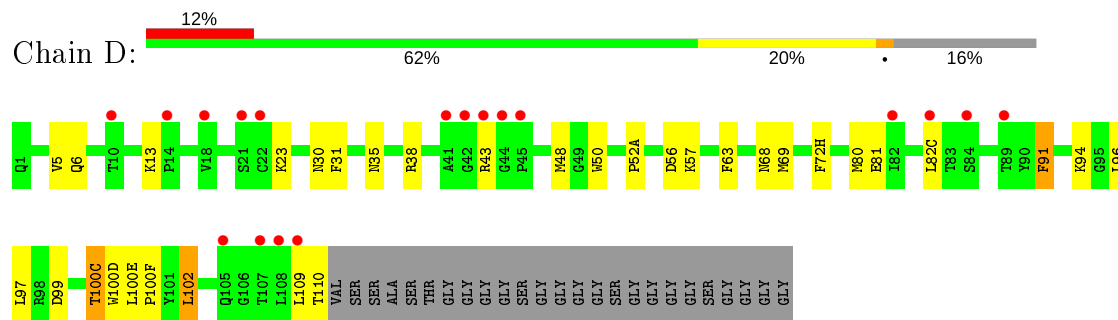
3 Residue-property plots

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

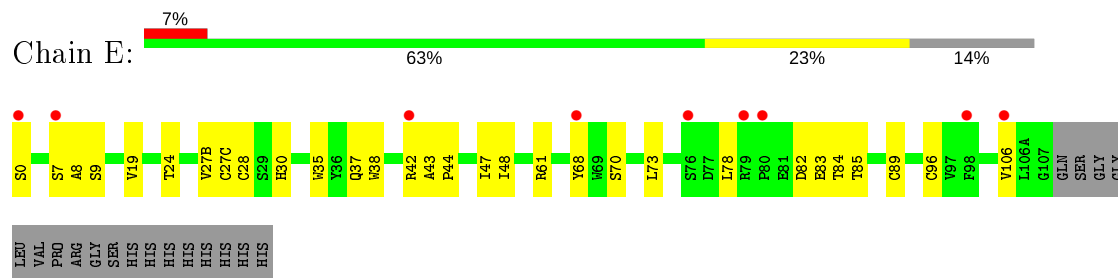
- Molecule 1: Envelope glycoprotein gp41



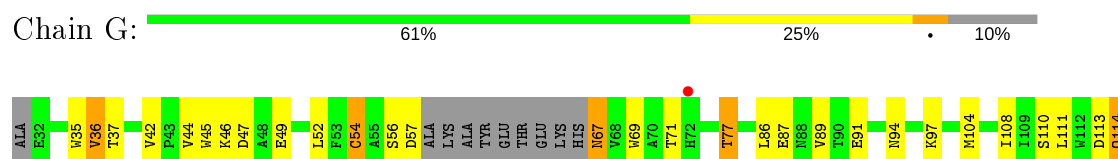
- Molecule 2: 35O22 scFv heavy chain



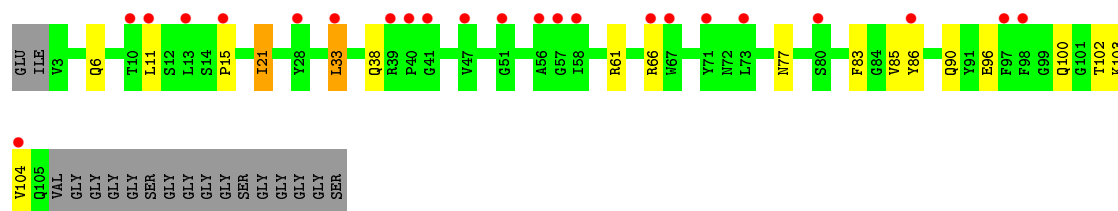
- Molecule 3: 35O22 scFv light chain



- Molecule 4: Envelope glycoprotein gp120







- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 17% 33% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

UAG1
UAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

UAG1
UAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  50% 50%

UAG1
UAG2

- Molecule 11: 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 F:  60% 40%

UAG1
UAG2
BMA3
MAN4
MAN5

- Molecule 12: 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 J:  50% 50%

UAG1
UAG2
BMA3
MAN4

- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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 O:  20% 50% 30%

UAG1
UAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	130.87Å 130.87Å 315.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.84 – 2.76 42.84 – 2.67	Depositor EDS
% Data completeness (in resolution range)	34.8 (42.84-2.76) 31.5 (42.84-2.67)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.242 , 0.298 0.242 , 0.298	Depositor DCC
R_{free} test set	1381 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 8.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.089 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	11926	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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 [i](#)

5.1 Standard geometry [i](#)

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	B	0.22	0/1048	0.40	0/1421
2	D	0.24	0/1021	0.46	0/1390
3	E	0.24	0/875	0.41	0/1195
4	G	0.24	0/3469	0.44	0/4707
5	H	0.25	0/1764	0.47	0/2405
6	L	0.24	0/1647	0.44	0/2247
7	U	0.24	0/1038	0.44	0/1408
8	V	0.25	0/771	0.43	0/1048
All	All	0.24	0/11633	0.44	0/15821

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1030	0	1021	21	0
2	D	994	0	953	21	0
3	E	851	0	801	14	0
4	G	3400	0	3349	86	0
5	H	1721	0	1690	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	1604	0	1553	25	0
7	U	1010	0	973	14	0
8	V	751	0	711	12	0
9	A	72	0	61	8	0
10	C	28	0	25	0	0
10	I	28	0	25	0	0
10	K	28	0	25	1	0
10	M	28	0	25	0	0
10	N	28	0	25	0	0
10	P	28	0	25	0	0
10	Q	28	0	25	0	0
11	F	61	0	52	0	0
12	J	50	0	43	0	0
13	O	116	0	97	3	0
14	B	28	0	26	0	0
14	G	42	0	39	1	0
All	All	11926	0	11544	195	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 8.

All (195) 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)
8:V:33:LEU:HD12	8:V:90:GLN:HB2	1.66	0.78
4:G:230:ASP:HB3	4:G:233:PHE:HB2	1.70	0.73
8:V:11:LEU:HB3	8:V:104:VAL:HG12	1.72	0.72
5:H:142:ASP:HB3	5:H:173:LEU:HD22	1.72	0.72
5:H:24:VAL:HG22	5:H:76:ASN:HB3	1.72	0.70
4:G:335:LYS:HB3	4:G:412:ASP:HB3	1.73	0.69
4:G:292:VAL:HG13	4:G:449:ILE:HG23	1.75	0.69
4:G:274:SER:HB2	4:G:284:ILE:HA	1.75	0.68
4:G:465:THR:O	7:U:61:ARG:NH2	2.26	0.68
4:G:67:ASN:HA	4:G:209:SER:H	1.61	0.66
2:D:57:LYS:NZ	2:D:69:MET:O	2.29	0.66
4:G:259:LEU:HD23	4:G:449:ILE:HD12	1.76	0.65
4:G:467:THR:HG23	7:U:61:ARG:HH21	1.63	0.65
4:G:94:ASN:HB3	4:G:97:LYS:HG2	1.80	0.64
1:B:632:ASP:OD2	4:G:46:LYS:NZ	2.31	0.63
4:G:205:CYS:HB3	4:G:207:LYS:HD2	1.81	0.62
4:G:439:ILE:HB	4:G:443:ILE:HD11	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:CYS:HA	4:G:37:THR:HG22	1.79	0.62
8:V:6:GLN:O	8:V:100:GLN:NE2	2.32	0.62
5:H:94:ARG:NH2	5:H:100(Q):ASP:OD2	2.28	0.62
6:L:8:VAL:HA	6:L:101:ALA:HB3	1.81	0.62
5:H:151:SER:HB2	5:H:195:ASN:HB2	1.81	0.61
6:L:50:ASN:O	6:L:52:GLN:N	2.34	0.60
4:G:374:HIS:HB3	4:G:385:CYS:HB2	1.83	0.60
4:G:350:ARG:NH2	4:G:357:THR:O	2.34	0.60
1:B:594:GLY:HA2	1:B:599:SER:HB3	1.83	0.60
6:L:34:GLN:HB2	6:L:89:HIS:HB3	1.84	0.60
7:U:76(C):ASP:O	7:U:76(F):TRP:NE1	2.35	0.59
5:H:100(O):TYR:HB3	6:L:34:GLN:HE21	1.68	0.59
4:G:258:GLN:NE2	4:G:371:VAL:O	2.32	0.58
4:G:270:VAL:HG11	4:G:344:LYS:HB3	1.86	0.58
2:D:56:ASP:OD2	9:A:4:MAN:O4	2.23	0.57
6:L:122:SER:HB3	6:L:125:GLU:HG2	1.87	0.57
2:D:30:ASN:HA	2:D:52(A):PRO:HB2	1.86	0.57
5:H:6:GLU:N	5:H:6:GLU:OE1	2.37	0.57
2:D:31:PHE:HA	9:A:1:NAG:H62	1.86	0.57
3:E:78:LEU:HD13	3:E:106:VAL:HG23	1.85	0.57
9:A:2:NAG:H83	9:A:2:NAG:H3	1.87	0.56
4:G:260:LEU:HD12	4:G:451:GLY:HA3	1.88	0.56
8:V:83:PHE:HA	8:V:104:VAL:HG23	1.86	0.56
4:G:358:ILE:HB	4:G:465:THR:HG23	1.87	0.56
3:E:47:ILE:HG22	3:E:48:ILE:HG13	1.86	0.56
1:B:657:GLU:HA	1:B:660:LEU:HB2	1.88	0.55
3:E:37:GLN:HG3	3:E:84:THR:HG21	1.87	0.55
6:L:135:CYS:HB3	6:L:177:SER:HB3	1.87	0.55
6:L:59:PRO:HB2	6:L:61:ARG:HG2	1.89	0.55
4:G:69:TRP:HE1	4:G:108:ILE:HD12	1.70	0.55
1:B:528:SER:OG	9:A:1:NAG:O7	2.21	0.55
7:U:20:ILE:HD11	7:U:80:LEU:HD23	1.88	0.55
1:B:610:TRP:HE3	4:G:36:VAL:HG12	1.72	0.54
4:G:456:ARG:NH1	4:G:466:GLU:OE2	2.40	0.54
4:G:257:THR:HG22	4:G:258:GLN:HG3	1.90	0.54
4:G:360:ARG:HB3	4:G:467:THR:HG22	1.90	0.54
5:H:161:VAL:HA	5:H:180:VAL:HG22	1.90	0.54
5:H:117:PRO:HD2	5:H:203:THR:HG21	1.89	0.54
6:L:119:PHE:HB2	6:L:134:VAL:HG23	1.89	0.53
4:G:344:LYS:HA	4:G:347:LYS:HD2	1.90	0.53
5:H:157:LEU:HD21	5:H:180:VAL:HG11	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:164:GLU:OE2	4:G:308:ARG:NH1	2.35	0.53
5:H:39:GLN:HB2	5:H:45:LEU:HD23	1.90	0.52
4:G:256:SER:OG	4:G:259:LEU:O	2.28	0.52
6:L:34:GLN:HG3	6:L:49:TYR:HA	1.91	0.52
2:D:6:GLN:HE22	2:D:91:PHE:HA	1.75	0.52
3:E:24:THR:HB	3:E:70:SER:HB3	1.90	0.52
4:G:456:ARG:O	7:U:58:ASN:ND2	2.43	0.52
1:B:585:ARG:NH2	4:G:491:ILE:O	2.38	0.52
3:E:83:GLU:HG3	3:E:106:VAL:HG12	1.91	0.51
7:U:6:GLN:NE2	7:U:107:THR:OG1	2.42	0.51
7:U:30:ILE:HA	7:U:52(A):PRO:HB2	1.92	0.51
2:D:100(C):THR:HG21	9:A:2:NAG:H3	1.92	0.51
2:D:96:LEU:HG	2:D:97:LEU:HG	1.92	0.51
13:O:1:NAG:H83	13:O:1:NAG:H3	1.91	0.51
4:G:122:LEU:HD13	4:G:125:LEU:HD12	1.93	0.51
4:G:67:ASN:HD21	4:G:71:THR:H	1.58	0.50
3:E:37:GLN:HB2	3:E:47:ILE:HD11	1.93	0.50
7:U:39:LEU:HD21	7:U:45:PRO:HG3	1.94	0.50
2:D:94:LYS:HD3	2:D:102:LEU:HB2	1.93	0.50
3:E:61:ARG:NH2	3:E:82:ASP:OD2	2.45	0.50
4:G:298:ARG:NH2	4:G:441:GLY:O	2.45	0.50
4:G:201:ILE:HD11	4:G:435:TYR:HB2	1.93	0.50
5:H:100:ARG:NH2	13:O:4:MAN:O6	2.45	0.49
4:G:104:MET:O	4:G:108:ILE:HG12	2.12	0.49
2:D:50:TRP:HH2	9:A:4:MAN:H62	1.77	0.49
2:D:43:ARG:HG2	3:E:0:SER:HA	1.94	0.49
4:G:286:VAL:HG13	4:G:452:LEU:HB3	1.95	0.48
7:U:87:THR:HG23	7:U:110:ILE:HA	1.96	0.48
2:D:35:ASN:ND2	2:D:100(D):TRP:O	2.45	0.48
4:G:358:ILE:HG23	4:G:396:ILE:HG23	1.94	0.48
1:B:575:GLN:HG2	1:B:579:ARG:HD3	1.94	0.48
3:E:7:SER:O	3:E:9:SER:N	2.47	0.48
6:L:197:THR:HA	6:L:202:THR:HA	1.95	0.48
8:V:6:GLN:NE2	8:V:86:TYR:O	2.41	0.48
2:D:82(C):LEU:HD11	2:D:110:THR:HG21	1.96	0.47
4:G:156:ASN:HA	4:G:175:LEU:HD12	1.96	0.47
4:G:45:TRP:HB3	4:G:491:ILE:HD13	1.96	0.47
6:L:109:GLN:HB2	6:L:141:TYR:CE2	2.49	0.47
4:G:87:GLU:HG2	9:A:1:NAG:H82	1.97	0.47
1:B:609:PRO:HA	4:G:35:TRP:HA	1.97	0.47
1:B:585:ARG:HG2	1:B:588:ARG:HH11	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:LYS:HD2	4:G:52:LEU:O	2.15	0.47
5:H:165:PRO:HG2	6:L:163:THR:HG21	1.97	0.47
8:V:61:ARG:NH1	8:V:77:ASN:O	2.48	0.47
5:H:27:GLY:O	5:H:76:ASN:ND2	2.47	0.46
6:L:37:GLN:HB2	6:L:47:LEU:HD11	1.95	0.46
4:G:110:SER:O	4:G:114:GLN:HB2	2.16	0.46
6:L:185:GLN:HA	6:L:188:MET:HG2	1.96	0.46
5:H:83:THR:O	5:H:109:VAL:HG21	2.16	0.46
6:L:21:ILE:HG23	6:L:102:THR:HG21	1.98	0.46
4:G:69:TRP:NE1	4:G:108:ILE:HD12	2.30	0.46
6:L:18:THR:HG22	6:L:76:SER:HA	1.98	0.46
8:V:38:GLN:HB3	8:V:85:VAL:HG13	1.96	0.46
5:H:99:LYS:HB3	13:O:9:MAN:H62	1.99	0.46
3:E:38:TRP:CE2	3:E:44:PRO:HG3	2.51	0.45
2:D:5:VAL:HG23	2:D:23:LYS:HE3	1.99	0.45
2:D:68:ASN:HB3	2:D:81:GLU:HB2	1.98	0.45
4:G:246:GLN:HE21	4:G:247:CYS:H	1.64	0.45
4:G:360:ARG:HH11	4:G:467:THR:HG21	1.81	0.45
1:B:571:TRP:CD2	4:G:54:CYS:HB3	2.51	0.45
4:G:499:THR:O	4:G:501:CYS:N	2.49	0.45
4:G:390:LEU:HG	4:G:416:LEU:HD21	1.99	0.45
4:G:353:PHE:CD1	4:G:466:GLU:HG3	2.52	0.45
4:G:494:LEU:HD23	4:G:494:LEU:HA	1.84	0.45
4:G:299:PRO:HG2	4:G:327:ARG:HB2	1.99	0.45
1:B:592:LEU:HD23	1:B:595:ILE:HD11	2.00	0.44
1:B:629:LEU:HD23	4:G:44:VAL:HG23	1.97	0.44
7:U:47:TRP:CG	8:V:96:GLU:HB2	2.53	0.44
3:E:35:TRP:CE2	3:E:73:LEU:HB2	2.52	0.44
4:G:259:LEU:HD22	4:G:374:HIS:HD2	1.81	0.44
6:L:39:ARG:NH1	6:L:81:GLY:O	2.43	0.44
8:V:85:VAL:HA	8:V:103:LYS:HA	1.99	0.44
1:B:630:GLN:HG2	2:D:72(H):PHE:CE1	2.53	0.44
4:G:42:VAL:HG23	4:G:44:VAL:HG12	1.98	0.44
2:D:99:ASP:OD1	9:A:6:MAN:O6	2.29	0.44
3:E:27(C):CYS:HA	3:E:28:CYS:HA	1.66	0.44
4:G:333:VAL:HG21	4:G:390:LEU:HD21	1.98	0.44
4:G:113:ASP:OD2	4:G:429:ARG:NH2	2.51	0.44
6:L:151:ALA:O	6:L:153:SER:N	2.50	0.44
6:L:22:SER:HA	6:L:72:THR:HG22	1.99	0.44
4:G:246:GLN:HE21	4:G:247:CYS:N	2.16	0.43
5:H:11:LEU:HD12	5:H:145:PRO:HD3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:12:SER:HB3	6:L:107:LEU:HD11	2.01	0.43
2:D:109:LEU:HG	2:D:110:THR:H	1.83	0.43
8:V:66:ARG:HH12	10:K:2:NAG:H83	1.83	0.43
3:E:42:ARG:HB3	3:E:43:ALA:H	1.66	0.43
4:G:123:THR:N	4:G:124:PRO:HD2	2.34	0.43
5:H:144:PHE:HA	5:H:145:PRO:HA	1.82	0.43
4:G:466:GLU:HA	7:U:61:ARG:HH22	1.83	0.43
4:G:476:ARG:HA	4:G:479:TRP:CD1	2.54	0.43
5:H:72:ASP:OD2	5:H:74:SER:OG	2.30	0.43
4:G:45:TRP:NE1	4:G:91:GLU:OE2	2.46	0.43
7:U:5:VAL:HG13	7:U:105:ARG:HH22	1.84	0.43
4:G:342:LEU:HA	4:G:342:LEU:HD23	1.91	0.43
8:V:15:PRO:HG3	8:V:83:PHE:HE2	1.84	0.43
2:D:100(E):LEU:HD12	2:D:100(F):PRO:HD2	2.00	0.43
1:B:544:LEU:HD12	4:G:222:GLY:HA2	2.01	0.43
4:G:179:LEU:HD21	4:G:419:ARG:CZ	2.49	0.43
4:G:317:PHE:CE2	4:G:319:ALA:HB2	2.54	0.43
1:B:523:LEU:HD11	4:G:491:ILE:HD11	2.01	0.42
4:G:86:LEU:HB3	4:G:89:VAL:HG21	2.01	0.42
7:U:47:TRP:CZ2	7:U:49:GLY:HA2	2.53	0.42
1:B:610:TRP:CD2	4:G:498:PRO:HB3	2.54	0.42
1:B:582:ALA:HB1	4:G:221:ALA:HB3	2.01	0.42
4:G:69:TRP:HA	4:G:111:LEU:HD13	2.00	0.42
4:G:192:ARG:NH2	4:G:197:ASN:OD1	2.53	0.42
4:G:457:ASP:OD2	7:U:64:GLN:NE2	2.52	0.42
1:B:525:ALA:HB1	1:B:528:SER:HB2	2.02	0.42
4:G:120:VAL:HG13	4:G:203:GLN:HB3	2.02	0.42
6:L:36:TYR:HE1	6:L:46:LEU:HD13	1.85	0.42
2:D:23:LYS:HE3	2:D:23:LYS:HB2	1.93	0.42
5:H:103:LYS:HD2	5:H:103:LYS:N	2.35	0.42
4:G:212:PRO:HG2	4:G:254:VAL:HG22	2.01	0.42
2:D:6:GLN:NE2	2:D:91:PHE:HA	2.35	0.41
4:G:335:LYS:HG3	4:G:414:ILE:HD11	2.01	0.41
6:L:125:GLU:HA	6:L:128:ALA:HB3	2.02	0.41
6:L:32:ALA:HA	6:L:51:ASN:ND2	2.35	0.41
3:E:84:THR:OG1	3:E:85:THR:N	2.53	0.41
4:G:257:THR:HG21	4:G:370:GLU:O	2.20	0.41
4:G:257:THR:O	4:G:259:LEU:N	2.44	0.41
4:G:478:ASN:O	4:G:481:SER:OG	2.35	0.41
5:H:18:LEU:N	5:H:82:LEU:O	2.37	0.41
4:G:260:LEU:HD21	4:G:453:ILE:HD11	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:415:THR:HG21	5:H:100(D):MET:HE3	2.02	0.41
4:G:452:LEU:HD12	4:G:452:LEU:HA	1.97	0.41
2:D:48:MET:HG2	2:D:63:PHE:CE2	2.55	0.41
5:H:124:PRO:HD3	5:H:136:LEU:HB3	2.03	0.41
5:H:92:CYS:O	5:H:102:GLY:N	2.53	0.41
1:B:632:ASP:O	1:B:636:SER:OG	2.31	0.41
6:L:50:ASN:O	6:L:53:ASP:N	2.46	0.41
8:V:21:ILE:HD12	8:V:102:THR:HB	2.03	0.41
4:G:136:ASN:HB3	4:G:137:ALA:H	1.71	0.41
4:G:171:LYS:HE2	14:G:614:NAG:H83	2.02	0.41
4:G:56:SER:O	4:G:77:THR:N	2.36	0.40
4:G:270:VAL:HG23	4:G:287:GLN:O	2.21	0.40
4:G:203:GLN:HE22	4:G:318:TYR:HD2	1.69	0.40
6:L:21:ILE:HB	6:L:73:LEU:HB3	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	B	126/153 (82%)	111 (88%)	14 (11%)	1 (1%)	19	34
2	D	126/153 (82%)	107 (85%)	19 (15%)	0	100	100
3	E	110/130 (85%)	89 (81%)	20 (18%)	1 (1%)	17	31
4	G	419/481 (87%)	374 (89%)	39 (9%)	6 (1%)	11	19
5	H	223/244 (91%)	199 (89%)	22 (10%)	2 (1%)	17	31
6	L	209/217 (96%)	186 (89%)	18 (9%)	5 (2%)	6	9
7	U	124/142 (87%)	115 (93%)	9 (7%)	0	100	100
8	V	95/115 (83%)	89 (94%)	6 (6%)	0	100	100
All	All	1432/1635 (88%)	1270 (89%)	147 (10%)	15 (1%)	15	27

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	428	GLN
6	L	51	ASN
3	E	8	ALA
5	H	48	ILE
4	G	274	SER
6	L	152	ASP
1	B	569	THR
4	G	136	ASN
4	G	500	ARG
5	H	142	ASP
4	G	413	SER
6	L	100	GLY
6	L	95(A)	GLY
4	G	321	GLY
6	L	165	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	B	111/129 (86%)	101 (91%)	10 (9%)	9	16
2	D	107/115 (93%)	101 (94%)	6 (6%)	21	36
3	E	98/113 (87%)	92 (94%)	6 (6%)	18	33
4	G	386/427 (90%)	351 (91%)	35 (9%)	9	16
5	H	197/212 (93%)	183 (93%)	14 (7%)	14	26
6	L	175/181 (97%)	167 (95%)	8 (5%)	27	46
7	U	107/120 (89%)	101 (94%)	6 (6%)	21	36
8	V	80/86 (93%)	78 (98%)	2 (2%)	47	67
All	All	1261/1383 (91%)	1174 (93%)	87 (7%)	15	27

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	519	PHE
1	B	520	LEU
1	B	567	LYS
1	B	568	LEU
1	B	570	VAL
1	B	574	LYS
1	B	593	LEU
1	B	646	LEU
1	B	648	GLU
1	B	663	LEU
2	D	13	LYS
2	D	38	ARG
2	D	80	MET
2	D	91	PHE
2	D	100(C)	THR
2	D	102	LEU
3	E	19	VAL
3	E	27(B)	VAL
3	E	30	HIS
3	E	68	TYR
3	E	89	CYS
3	E	96	CYS
4	G	36	VAL
4	G	47	ASP
4	G	49	GLU
4	G	54	CYS
4	G	57	ASP
4	G	67	ASN
4	G	77	THR
4	G	114	GLN
4	G	120	VAL
4	G	151	ARG
4	G	153	GLU
4	G	154	LEU
4	G	175	LEU
4	G	192	ARG
4	G	201	ILE
4	G	207	LYS
4	G	234	ASN
4	G	236	THR
4	G	246	GLN
4	G	270	VAL
4	G	272	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	G	273	ARG
4	G	276	ASN
4	G	286	VAL
4	G	290	THR
4	G	292	VAL
4	G	328	GLN
4	G	365	SER
4	G	424	ILE
4	G	428	GLN
4	G	444	ARG
4	G	449	ILE
4	G	464	THR
4	G	479	TRP
4	G	488	VAL
5	H	20	LEU
5	H	21	THR
5	H	24	VAL
5	H	46	GLU
5	H	51	ILE
5	H	55	GLU
5	H	57	THR
5	H	75	LYS
5	H	78	LEU
5	H	100(P)	MET
5	H	115	LYS
5	H	191	THR
5	H	207	LYS
5	H	209	VAL
6	L	11	LEU
6	L	25	ARG
6	L	134	VAL
6	L	190	LYS
6	L	197	THR
6	L	201	SER
6	L	202	THR
6	L	209	PRO
7	U	32	CYS
7	U	71	ARG
7	U	72	GLN
7	U	73	LEU
7	U	76(B)	ASP
7	U	76(F)	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	V	21	ILE
8	V	33	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	30	ASN
5	H	162	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	$\# Z > 2$
9	NAG	A	1	9,4	14,14,15	0.32	0	17,19,21	0.47	0
9	NAG	A	2	9	14,14,15	0.41	0	17,19,21	1.27	1 (5%)
9	BMA	A	3	9	11,11,12	0.59	0	15,15,17	0.68	0
9	MAN	A	4	9	11,11,12	1.07	1 (9%)	15,15,17	1.09	1 (6%)
9	MAN	A	5	9	11,11,12	1.62	2 (18%)	15,15,17	1.97	4 (26%)
9	MAN	A	6	9	11,11,12	0.63	0	15,15,17	0.98	2 (13%)
10	NAG	C	1	10,4	14,14,15	0.23	0	17,19,21	0.45	0
10	NAG	C	2	10	14,14,15	0.25	0	17,19,21	0.43	0
11	NAG	F	1	11,4	14,14,15	0.25	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	F	2	11	14,14,15	0.20	0	17,19,21	0.38	0
11	BMA	F	3	11	11,11,12	0.61	0	15,15,17	0.73	0
11	MAN	F	4	11	11,11,12	0.76	1 (9%)	15,15,17	1.13	2 (13%)
11	MAN	F	5	11	11,11,12	0.69	0	15,15,17	1.04	2 (13%)
10	NAG	I	1	10,4	14,14,15	0.33	0	17,19,21	0.46	0
10	NAG	I	2	10	14,14,15	0.23	0	17,19,21	0.39	0
12	NAG	J	1	12,4	14,14,15	0.23	0	17,19,21	0.46	0
12	NAG	J	2	12	14,14,15	0.25	0	17,19,21	0.50	0
12	BMA	J	3	12	11,11,12	1.11	2 (18%)	15,15,17	1.18	1 (6%)
12	MAN	J	4	12	11,11,12	0.63	0	15,15,17	1.04	2 (13%)
10	NAG	K	1	10,4	14,14,15	0.27	0	17,19,21	0.39	0
10	NAG	K	2	10	14,14,15	0.21	0	17,19,21	0.46	0
10	NAG	M	1	10,4	14,14,15	0.23	0	17,19,21	0.44	0
10	NAG	M	2	10	14,14,15	0.24	0	17,19,21	0.41	0
10	NAG	N	1	10,4	14,14,15	0.28	0	17,19,21	0.44	0
10	NAG	N	2	10	14,14,15	0.22	0	17,19,21	0.50	0
13	NAG	O	1	13,4	14,14,15	0.43	0	17,19,21	1.41	2 (11%)
13	MAN	O	10	13	11,11,12	1.06	0	15,15,17	1.17	2 (13%)
13	NAG	O	2	13	14,14,15	0.24	0	17,19,21	0.44	0
13	BMA	O	3	13	11,11,12	0.92	0	15,15,17	0.92	0
13	MAN	O	4	13	11,11,12	0.82	1 (9%)	15,15,17	1.40	2 (13%)
13	MAN	O	5	13	11,11,12	0.73	0	15,15,17	0.93	1 (6%)
13	MAN	O	6	13	11,11,12	0.65	0	15,15,17	0.88	1 (6%)
13	MAN	O	7	13	11,11,12	0.70	0	15,15,17	1.06	2 (13%)
13	MAN	O	8	13	11,11,12	0.74	0	15,15,17	1.00	1 (6%)
13	MAN	O	9	13	11,11,12	0.82	1 (9%)	15,15,17	1.34	2 (13%)
10	NAG	P	1	10,4	14,14,15	0.33	0	17,19,21	0.46	0
10	NAG	P	2	10	14,14,15	0.25	0	17,19,21	0.50	0
10	NAG	Q	1	10,4	14,14,15	0.96	1 (7%)	17,19,21	1.60	1 (5%)
10	NAG	Q	2	10	14,14,15	0.22	0	17,19,21	0.42	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
9	NAG	A	1	9,4	-	0/6/23/26	0/1/1/1
9	NAG	A	2	9	-	5/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	A	3	9	-	2/2/19/22	0/1/1/1
9	MAN	A	4	9	-	2/2/19/22	0/1/1/1
9	MAN	A	5	9	-	1/2/19/22	0/1/1/1
9	MAN	A	6	9	-	0/2/19/22	0/1/1/1
10	NAG	C	1	10,4	-	0/6/23/26	0/1/1/1
10	NAG	C	2	10	-	2/6/23/26	0/1/1/1
11	NAG	F	1	11,4	-	1/6/23/26	0/1/1/1
11	NAG	F	2	11	-	0/6/23/26	0/1/1/1
11	BMA	F	3	11	-	2/2/19/22	0/1/1/1
11	MAN	F	4	11	-	0/2/19/22	0/1/1/1
11	MAN	F	5	11	-	2/2/19/22	0/1/1/1
10	NAG	I	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	I	2	10	-	2/6/23/26	0/1/1/1
12	NAG	J	1	12,4	-	2/6/23/26	0/1/1/1
12	NAG	J	2	12	-	2/6/23/26	0/1/1/1
12	BMA	J	3	12	-	0/2/19/22	0/1/1/1
12	MAN	J	4	12	-	2/2/19/22	0/1/1/1
10	NAG	K	1	10,4	-	1/6/23/26	0/1/1/1
10	NAG	K	2	10	-	0/6/23/26	0/1/1/1
10	NAG	M	1	10,4	-	0/6/23/26	0/1/1/1
10	NAG	M	2	10	-	0/6/23/26	0/1/1/1
10	NAG	N	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	N	2	10	-	2/6/23/26	0/1/1/1
13	NAG	O	1	13,4	-	3/6/23/26	0/1/1/1
13	MAN	O	10	13	-	2/2/19/22	0/1/1/1
13	NAG	O	2	13	-	2/6/23/26	0/1/1/1
13	BMA	O	3	13	-	0/2/19/22	0/1/1/1
13	MAN	O	4	13	-	2/2/19/22	0/1/1/1
13	MAN	O	5	13	-	2/2/19/22	0/1/1/1
13	MAN	O	6	13	-	0/2/19/22	0/1/1/1
13	MAN	O	7	13	-	0/2/19/22	0/1/1/1
13	MAN	O	8	13	-	0/2/19/22	0/1/1/1
13	MAN	O	9	13	-	2/2/19/22	0/1/1/1
10	NAG	P	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	P	2	10	-	0/6/23/26	0/1/1/1
10	NAG	Q	1	10,4	-	4/6/23/26	0/1/1/1
10	NAG	Q	2	10	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	5	MAN	C1-C2	4.60	1.62	1.52
10	Q	1	NAG	O5-C1	3.45	1.49	1.43
13	O	4	MAN	C1-C2	2.52	1.58	1.52
13	O	9	MAN	C1-C2	2.35	1.57	1.52
9	A	4	MAN	O5-C1	-2.26	1.40	1.43
9	A	5	MAN	O5-C1	2.12	1.47	1.43
11	F	4	MAN	C1-C2	2.11	1.57	1.52
12	J	3	BMA	C4-C3	2.08	1.57	1.52
12	J	3	BMA	C2-C3	2.00	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	1	NAG	C1-O5-C5	6.23	120.63	112.19
13	O	1	NAG	C2-N2-C7	4.51	129.32	122.90
9	A	5	MAN	C1-O5-C5	4.48	118.26	112.19
9	A	5	MAN	C1-C2-C3	4.36	115.03	109.67
9	A	2	NAG	C2-N2-C7	4.33	129.07	122.90
13	O	9	MAN	C1-O5-C5	3.80	117.34	112.19
13	O	4	MAN	C1-O5-C5	3.62	117.09	112.19
13	O	8	MAN	C1-O5-C5	2.70	115.85	112.19
12	J	3	BMA	C2-C3-C4	2.69	115.56	110.89
9	A	5	MAN	O5-C1-C2	2.64	114.84	110.77
11	F	4	MAN	C1-O5-C5	2.62	115.74	112.19
13	O	4	MAN	O2-C2-C3	-2.52	105.09	110.14
12	J	4	MAN	C1-O5-C5	2.51	115.59	112.19
13	O	7	MAN	C1-O5-C5	2.51	115.59	112.19
9	A	6	MAN	C1-O5-C5	2.45	115.52	112.19
11	F	5	MAN	C1-O5-C5	2.45	115.51	112.19
13	O	10	MAN	O2-C2-C3	-2.36	105.42	110.14
13	O	1	NAG	C1-C2-N2	2.31	114.44	110.49
13	O	5	MAN	O2-C2-C3	-2.30	105.53	110.14
13	O	7	MAN	O2-C2-C3	-2.26	105.61	110.14
9	A	5	MAN	O2-C2-C3	-2.24	105.65	110.14
12	J	4	MAN	O2-C2-C3	-2.23	105.67	110.14
13	O	9	MAN	O2-C2-C3	-2.21	105.70	110.14
9	A	4	MAN	O2-C2-C3	-2.21	105.71	110.14
9	A	6	MAN	O2-C2-C3	-2.19	105.75	110.14
11	F	5	MAN	O2-C2-C3	-2.18	105.77	110.14
13	O	6	MAN	O2-C2-C3	-2.14	105.85	110.14
11	F	4	MAN	O2-C2-C3	-2.13	105.88	110.14
13	O	10	MAN	C1-C2-C3	2.08	112.22	109.67

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	O	2	NAG	O5-C5-C6-O6
9	A	3	BMA	O5-C5-C6-O6
11	F	3	BMA	C4-C5-C6-O6
10	Q	1	NAG	O5-C5-C6-O6
10	I	2	NAG	O5-C5-C6-O6
12	J	2	NAG	O5-C5-C6-O6
13	O	2	NAG	C4-C5-C6-O6
9	A	3	BMA	C4-C5-C6-O6
13	O	9	MAN	C4-C5-C6-O6
10	I	2	NAG	C4-C5-C6-O6
12	J	1	NAG	O5-C5-C6-O6
10	I	1	NAG	O5-C5-C6-O6
12	J	4	MAN	C4-C5-C6-O6
11	F	3	BMA	O5-C5-C6-O6
10	C	2	NAG	O5-C5-C6-O6
13	O	9	MAN	O5-C5-C6-O6
12	J	4	MAN	O5-C5-C6-O6
13	O	10	MAN	C4-C5-C6-O6
10	C	2	NAG	C4-C5-C6-O6
9	A	2	NAG	C8-C7-N2-C2
9	A	2	NAG	O7-C7-N2-C2
13	O	1	NAG	C8-C7-N2-C2
13	O	1	NAG	O7-C7-N2-C2
10	Q	1	NAG	C8-C7-N2-C2
10	Q	1	NAG	O7-C7-N2-C2
9	A	2	NAG	O5-C5-C6-O6
13	O	4	MAN	O5-C5-C6-O6
12	J	1	NAG	C4-C5-C6-O6
10	N	2	NAG	C4-C5-C6-O6
12	J	2	NAG	C4-C5-C6-O6
9	A	2	NAG	C4-C5-C6-O6
10	P	1	NAG	O5-C5-C6-O6
13	O	4	MAN	C4-C5-C6-O6
13	O	10	MAN	O5-C5-C6-O6
10	N	1	NAG	O5-C5-C6-O6
9	A	4	MAN	O5-C5-C6-O6
10	N	2	NAG	O5-C5-C6-O6
9	A	4	MAN	C4-C5-C6-O6
10	Q	1	NAG	C4-C5-C6-O6
13	O	5	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

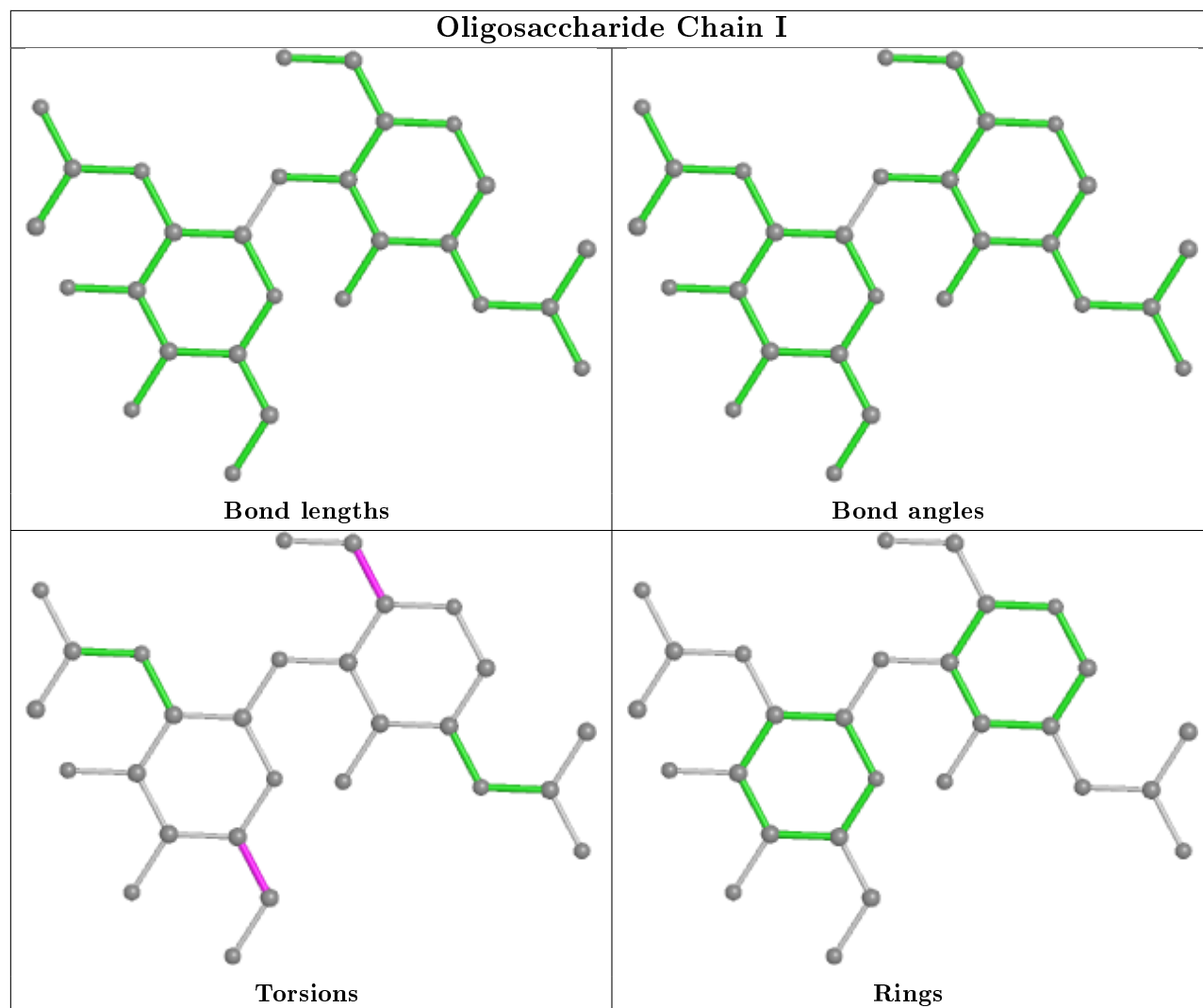
Mol	Chain	Res	Type	Atoms
11	F	5	MAN	C4-C5-C6-O6
13	O	5	MAN	C4-C5-C6-O6
9	A	5	MAN	O5-C5-C6-O6
10	I	1	NAG	C4-C5-C6-O6
11	F	5	MAN	O5-C5-C6-O6
10	P	1	NAG	C4-C5-C6-O6
10	N	1	NAG	C4-C5-C6-O6
10	K	1	NAG	C1-C2-N2-C7
11	F	1	NAG	C4-C5-C6-O6
9	A	2	NAG	C3-C2-N2-C7
13	O	1	NAG	C3-C2-N2-C7

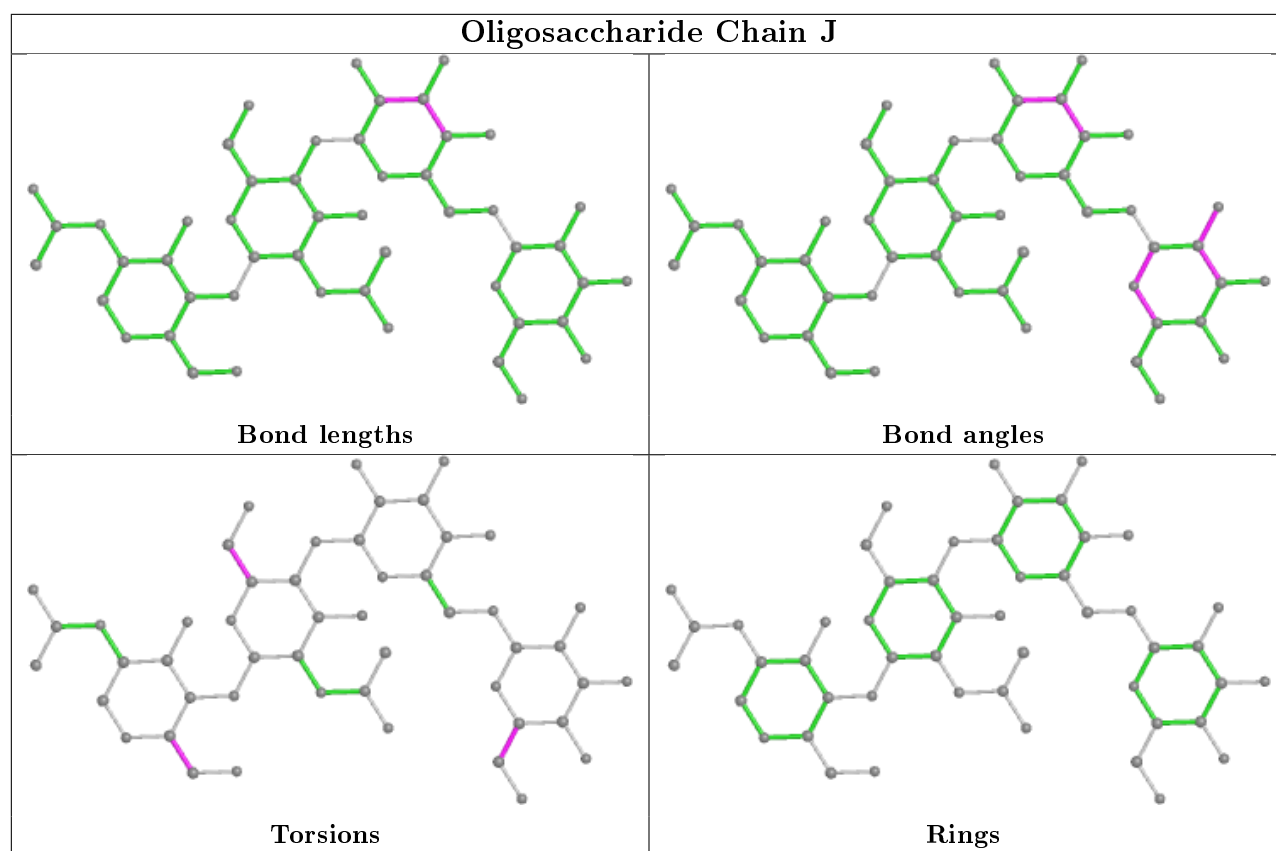
There are no ring outliers.

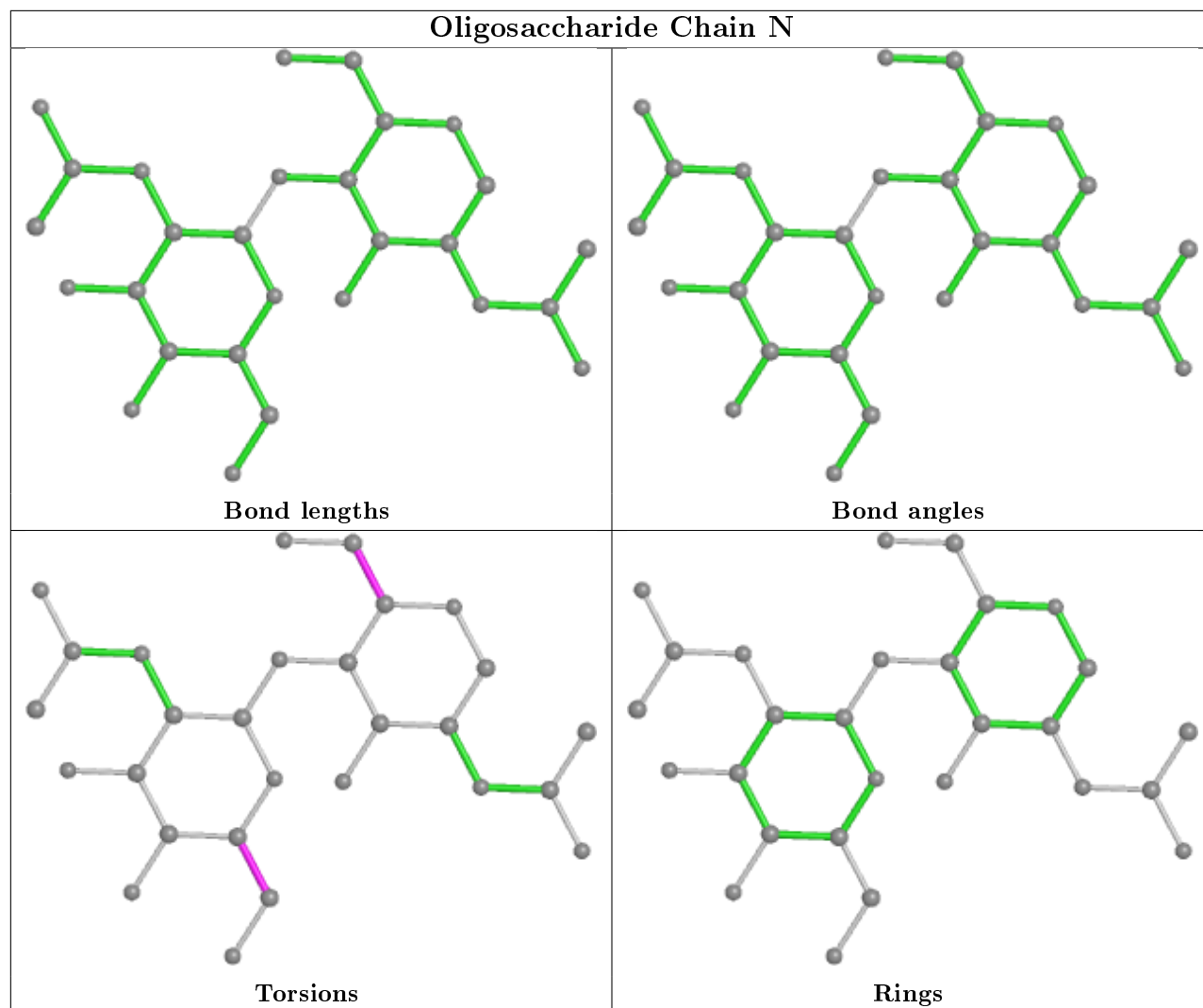
8 monomers are involved in 12 short contacts:

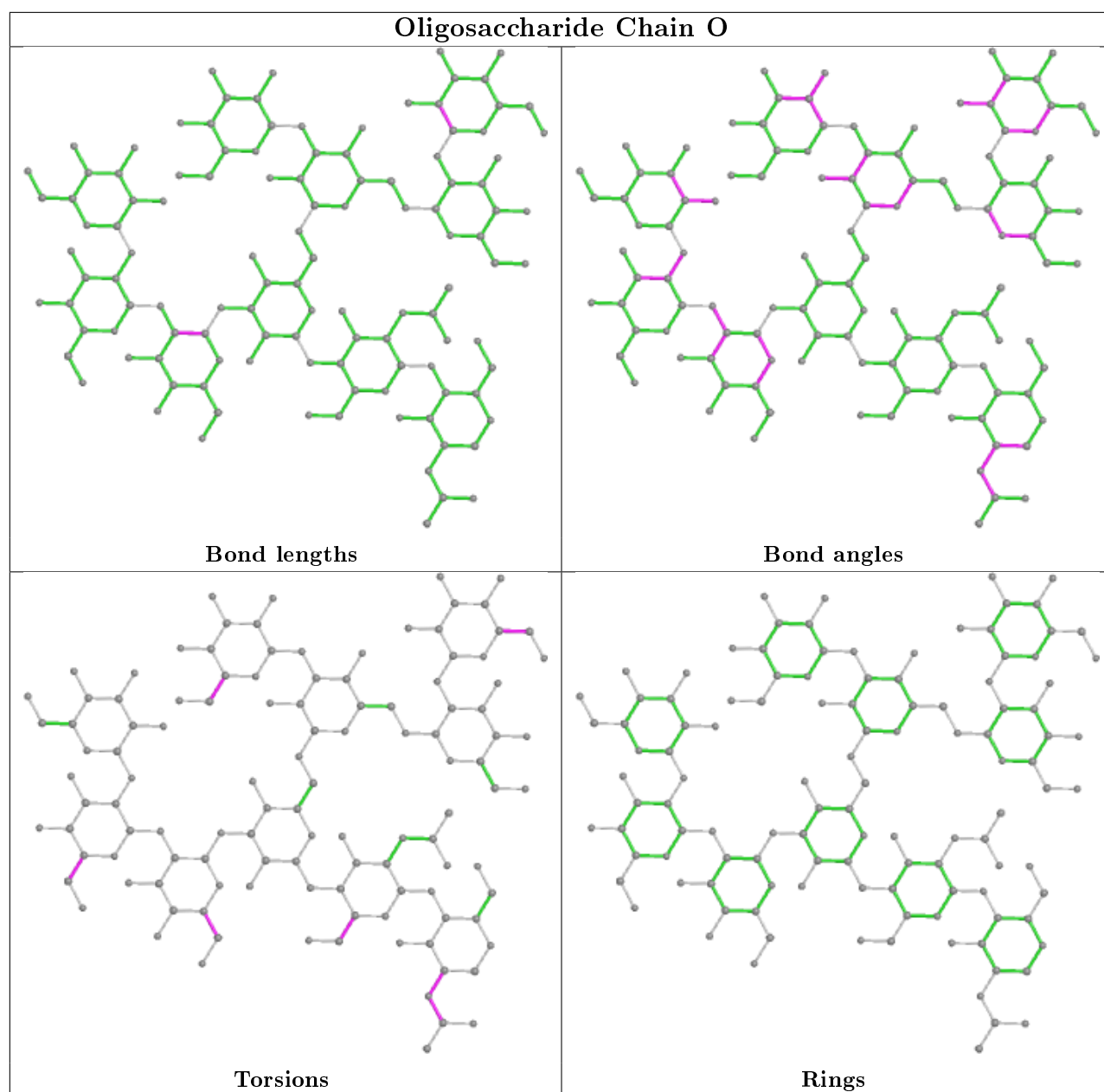
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2	NAG	2	0
9	A	6	MAN	1	0
9	A	1	NAG	3	0
9	A	4	MAN	2	0
13	O	1	NAG	1	0
13	O	9	MAN	1	0
10	K	2	NAG	1	0
13	O	4	MAN	1	0

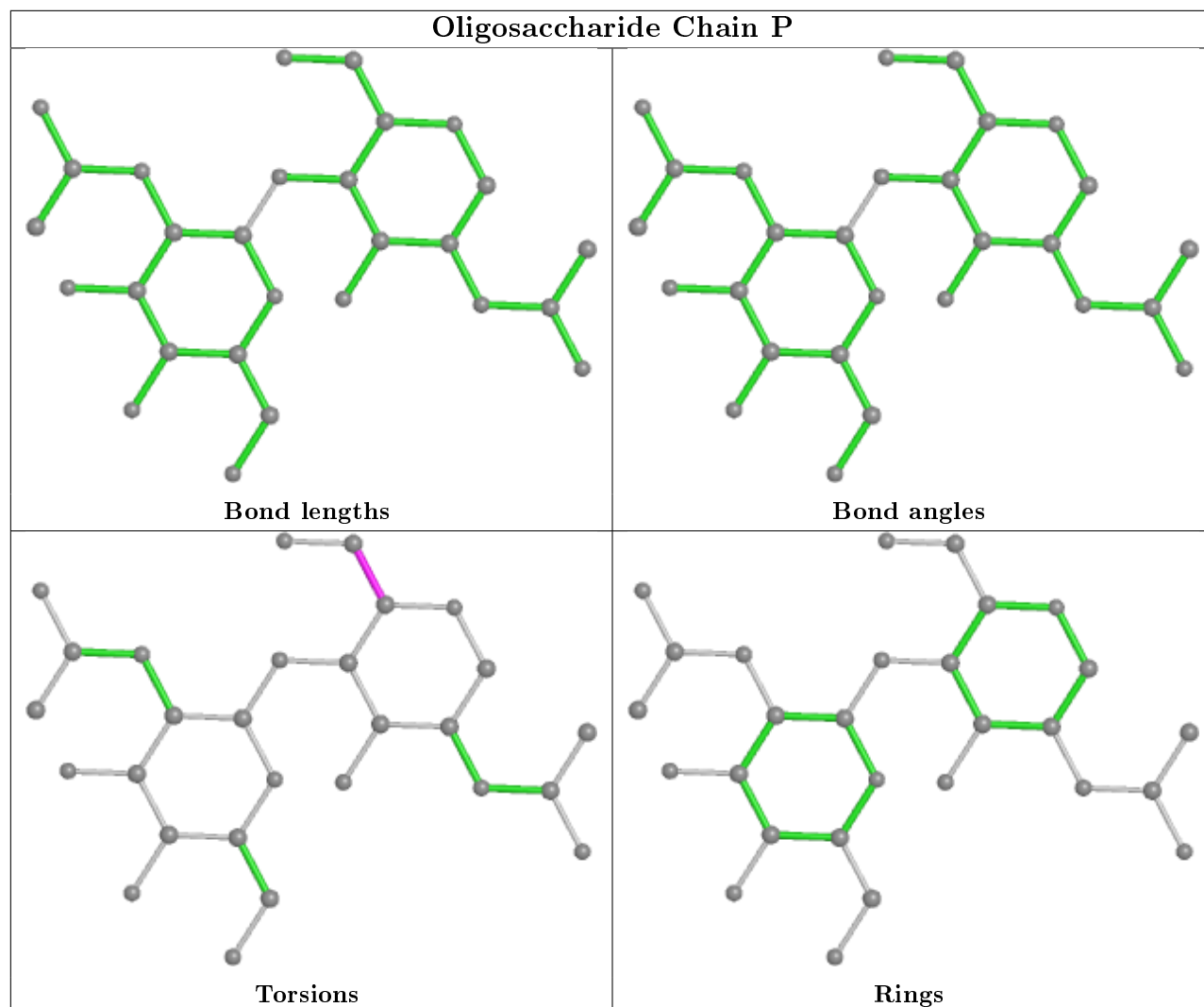
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

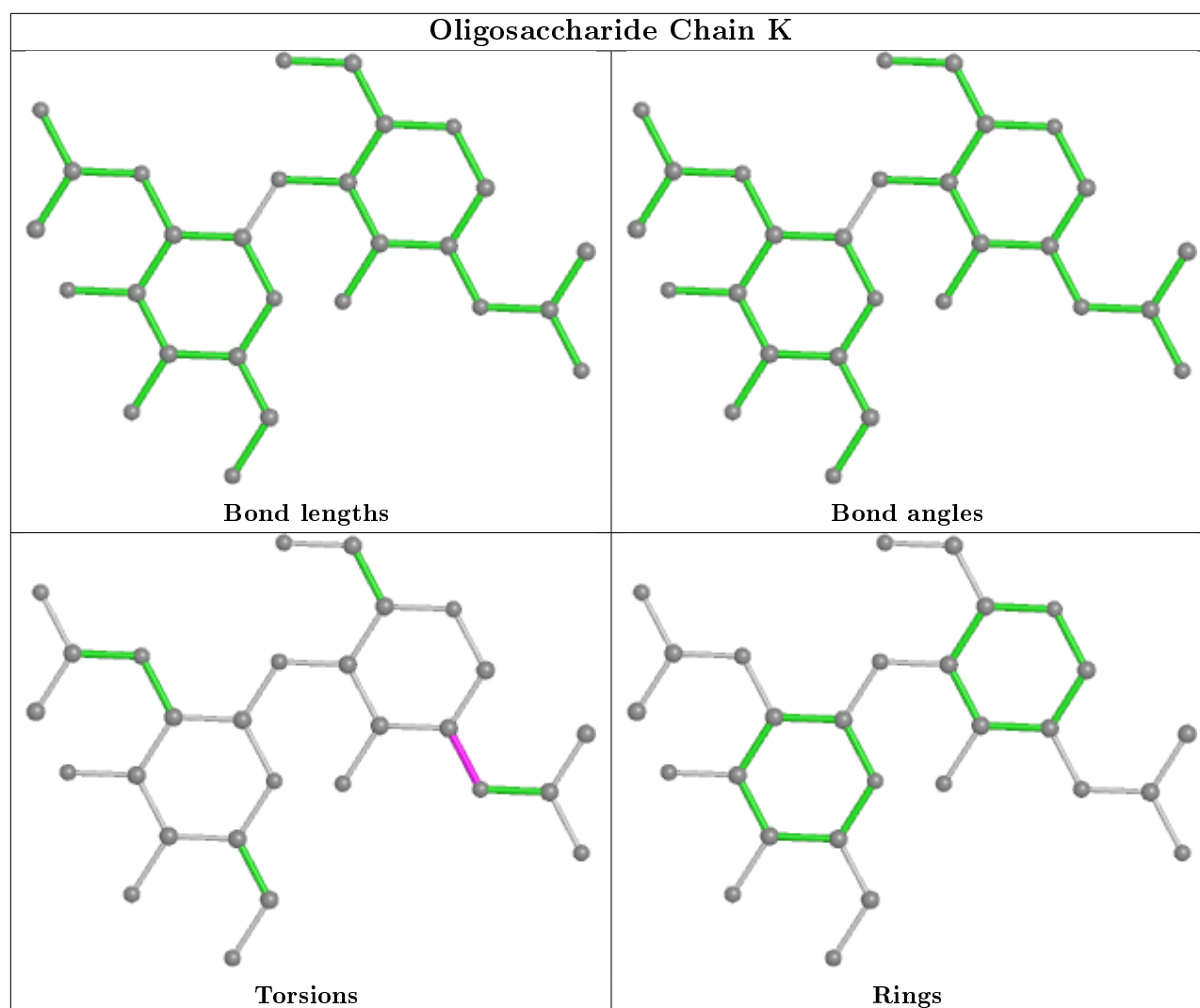


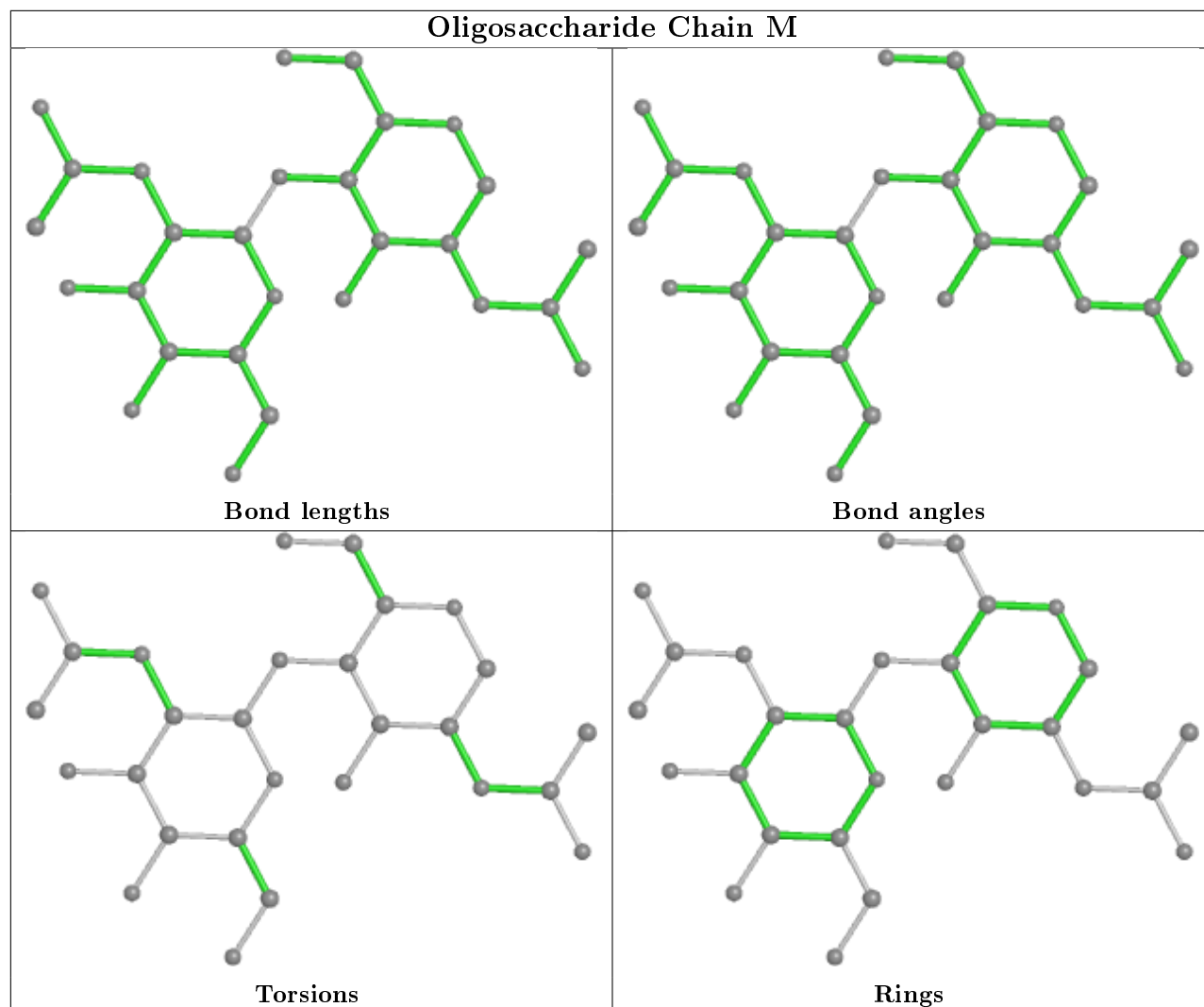


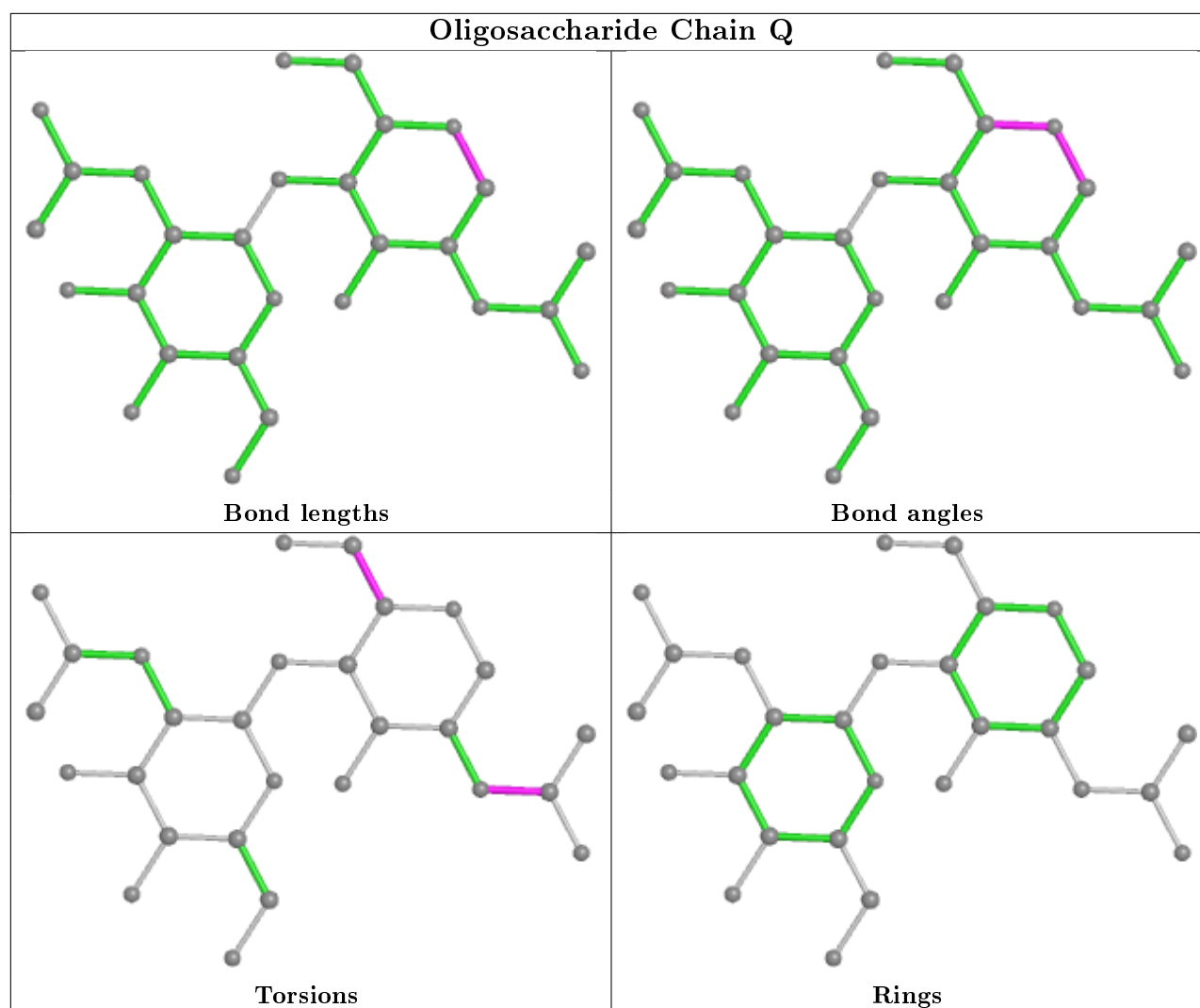












5.6 Ligand geometry ⓘ

5 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	$\# Z > 2$
14	NAG	G	617	4	14,14,15	0.31	0	17,19,21	0.45	0
14	NAG	G	614	4	14,14,15	0.27	0	17,19,21	0.44	0
14	NAG	B	702	1	14,14,15	0.29	0	17,19,21	0.45	0
14	NAG	G	638	4	14,14,15	0.20	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	B	701	1	14,14,15	0.34	0	17,19,21	0.54	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
14	NAG	G	617	4	-	2/6/23/26	0/1/1/1
14	NAG	G	614	4	-	1/6/23/26	0/1/1/1
14	NAG	B	702	1	-	1/6/23/26	0/1/1/1
14	NAG	G	638	4	-	0/6/23/26	0/1/1/1
14	NAG	B	701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	G	617	NAG	O5-C5-C6-O6
14	G	617	NAG	C4-C5-C6-O6
14	B	702	NAG	O5-C5-C6-O6
14	G	614	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
14	G	614	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	B	130/153 (84%)	-0.13	2 (1%) 73 81	20, 44, 85, 120	0
2	D	128/153 (83%)	0.40	18 (14%) 2 3	45, 101, 130, 141	0
3	E	112/130 (86%)	0.08	9 (8%) 12 15	44, 84, 120, 143	0
4	G	431/481 (89%)	-0.30	1 (0%) 95 97	12, 37, 87, 131	0
5	H	227/244 (93%)	-0.34	2 (0%) 84 89	34, 67, 109, 129	0
6	L	211/217 (97%)	-0.37	2 (0%) 84 89	25, 49, 78, 109	0
7	U	126/142 (88%)	0.74	20 (15%) 1 2	60, 117, 150, 155	0
8	V	97/115 (84%)	1.26	23 (23%) 0 0	93, 136, 156, 171	0
All	All	1462/1635 (89%)	-0.02	77 (5%) 26 31	12, 61, 137, 171	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	517	ALA	6.0
8	V	67	TRP	5.9
8	V	40	PRO	5.9
8	V	71	TYR	5.5
3	E	68	TYR	5.3
8	V	28	TYR	4.9
2	D	18	VAL	4.7
7	U	105	ARG	4.7
7	U	10	GLN	4.7
2	D	41	ALA	4.3
8	V	104	VAL	4.2
5	H	126	SER	4.2
8	V	51	GLY	4.2
7	U	39	LEU	4.1
7	U	91	PHE	4.0
7	U	18	MET	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	V	57	GLY	4.0
8	V	98	PHE	4.0
7	U	4	LEU	4.0
8	V	13	LEU	3.9
2	D	44	GLY	3.8
8	V	58	ILE	3.7
7	U	7	SER	3.7
8	V	33	LEU	3.6
7	U	109	VAL	3.5
2	D	14	PRO	3.4
2	D	10	THR	3.4
3	E	106	VAL	3.4
8	V	86	TYR	3.3
8	V	56	ALA	3.3
3	E	7	SER	3.2
8	V	41	GLY	3.2
2	D	42	GLY	3.1
7	U	90	TYR	3.1
7	U	89	VAL	3.0
7	U	23	ARG	2.9
2	D	109	LEU	2.9
7	U	76(B)	ASP	2.9
8	V	80	SER	2.7
3	E	80	PRO	2.7
2	D	21	SER	2.7
1	B	518	VAL	2.7
2	D	84	SER	2.6
2	D	107	THR	2.6
3	E	79	ARG	2.5
2	D	43	ARG	2.5
7	U	82(A)	ARG	2.5
7	U	93	THR	2.5
8	V	47	VAL	2.5
2	D	108	LEU	2.5
2	D	82	ILE	2.4
8	V	11	LEU	2.4
2	D	22	CYS	2.4
3	E	98	PHE	2.4
3	E	42	ARG	2.4
7	U	110	ILE	2.4
6	L	210	THR	2.4
2	D	82(C)	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	89	THR	2.3
2	D	45	PRO	2.3
8	V	66	ARG	2.3
7	U	20	ILE	2.3
7	U	11	MET	2.2
8	V	97	PHE	2.2
8	V	39	ARG	2.2
7	U	29	PHE	2.2
6	L	6	SER	2.2
7	U	75	GLN	2.2
8	V	73	LEU	2.2
8	V	15	PRO	2.2
4	G	72	HIS	2.1
7	U	103	TRP	2.1
3	E	0	SER	2.1
8	V	10	THR	2.1
2	D	105	GLN	2.0
3	E	76	SER	2.0
5	H	73	THR	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
11	MAN	F	4	11/12	0.78	0.15	86,140,151,155	0
12	MAN	J	4	11/12	0.82	0.16	73,103,110,112	0
11	MAN	F	5	11/12	0.84	0.22	125,143,155,155	0
11	BMA	F	3	11/12	0.86	0.18	130,142,153,158	0
12	BMA	J	3	11/12	0.88	0.12	96,109,123,124	0
10	NAG	C	2	14/15	0.88	0.30	102,136,141,148	0
10	NAG	Q	2	14/15	0.88	0.18	96,119,133,134	0
9	MAN	A	5	11/12	0.89	0.14	64,93,112,115	0
10	NAG	P	2	14/15	0.89	0.15	67,85,107,110	0

Continued on next page...

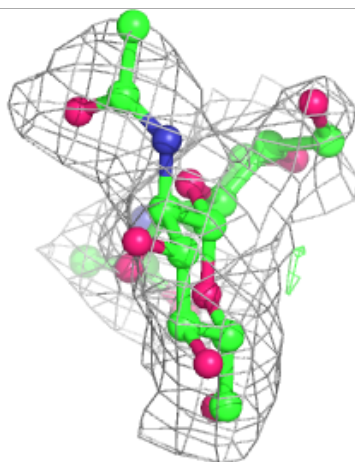
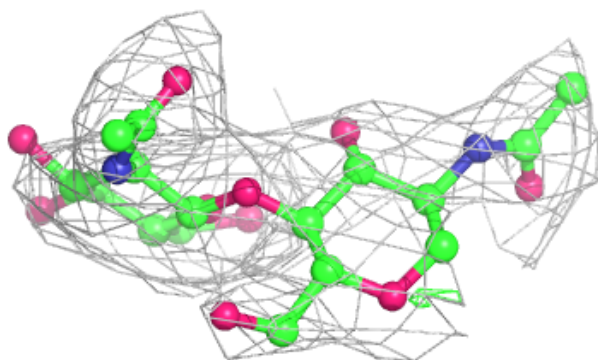
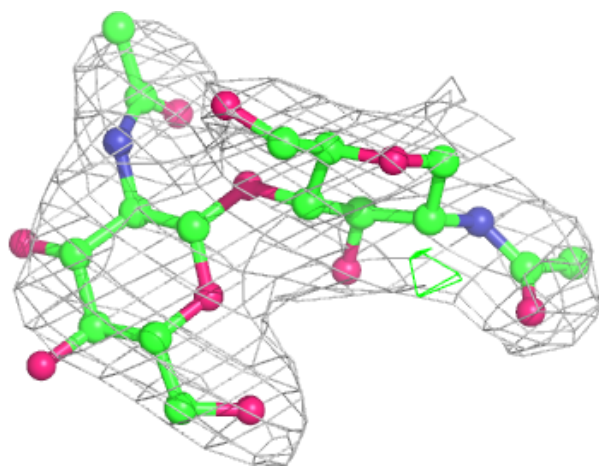
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	NAG	C	1	14/15	0.90	0.18	81,108,132,134	0
9	MAN	A	4	11/12	0.90	0.14	76,91,104,110	0
10	NAG	K	2	14/15	0.91	0.14	83,97,118,119	0
13	MAN	O	10	11/12	0.92	0.17	45,80,104,113	0
10	NAG	K	1	14/15	0.92	0.18	89,106,117,119	0
13	MAN	O	8	11/12	0.93	0.14	41,63,91,94	0
10	NAG	I	1	14/15	0.94	0.15	83,97,111,112	0
12	NAG	J	2	14/15	0.94	0.12	29,60,81,88	0
10	NAG	Q	1	14/15	0.94	0.12	60,72,92,104	0
10	NAG	I	2	14/15	0.94	0.17	72,103,128,141	0
11	NAG	F	2	14/15	0.94	0.15	75,99,112,133	0
13	MAN	O	9	11/12	0.95	0.13	63,78,96,98	0
9	BMA	A	3	11/12	0.95	0.14	45,50,63,77	0
13	NAG	O	1	14/15	0.95	0.15	50,71,84,90	0
10	NAG	M	2	14/15	0.95	0.15	59,90,104,105	0
10	NAG	N	2	14/15	0.95	0.14	75,85,105,112	0
13	BMA	O	3	11/12	0.96	0.11	40,52,59,64	0
10	NAG	P	1	14/15	0.96	0.12	45,68,86,95	0
13	NAG	O	2	14/15	0.96	0.11	50,68,77,80	0
9	MAN	A	6	11/12	0.97	0.12	45,60,72,81	0
10	NAG	N	1	14/15	0.97	0.14	33,41,54,59	0
11	NAG	F	1	14/15	0.97	0.13	23,51,74,78	0
10	NAG	M	1	14/15	0.97	0.12	42,47,64,70	0
13	MAN	O	5	11/12	0.97	0.17	37,45,69,69	0
13	MAN	O	7	11/12	0.97	0.12	47,56,67,74	0
9	NAG	A	2	14/15	0.97	0.12	36,49,58,62	0
13	MAN	O	6	11/12	0.97	0.16	37,60,94,102	0
13	MAN	O	4	11/12	0.97	0.14	28,37,50,74	0
12	NAG	J	1	14/15	0.98	0.13	16,33,51,57	0
9	NAG	A	1	14/15	0.98	0.15	33,41,56,68	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.

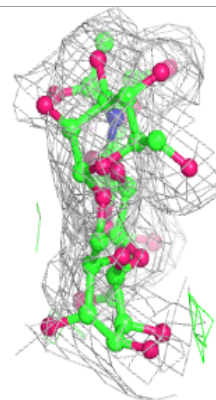
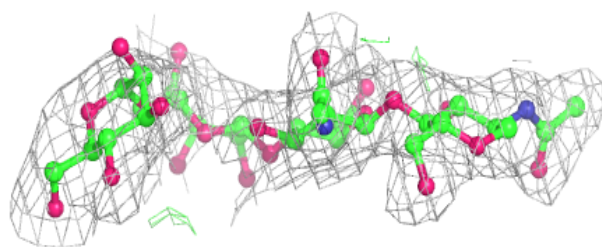
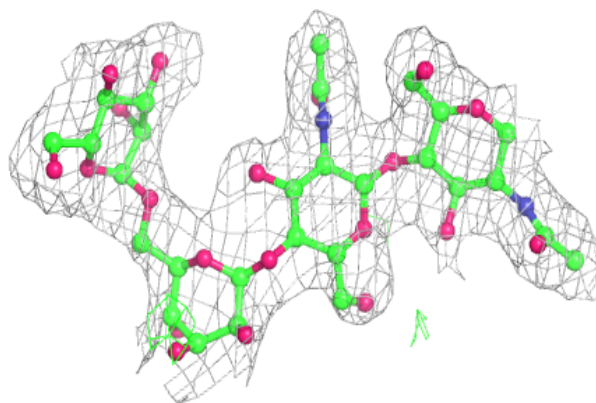
Electron density around Chain I:

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



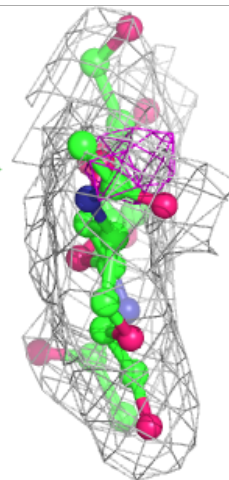
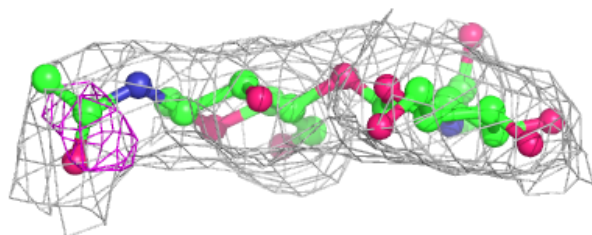
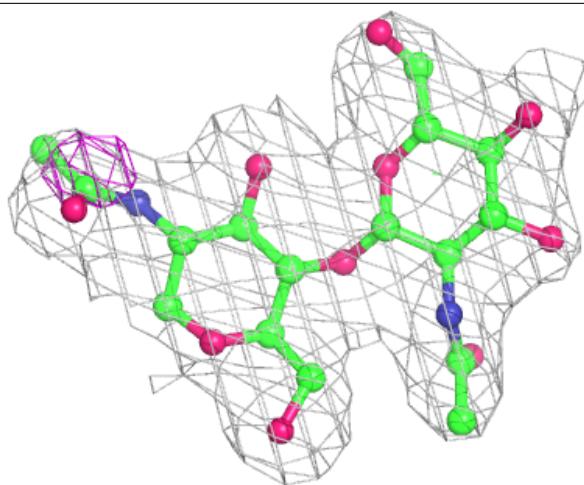
Electron density around Chain J:

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



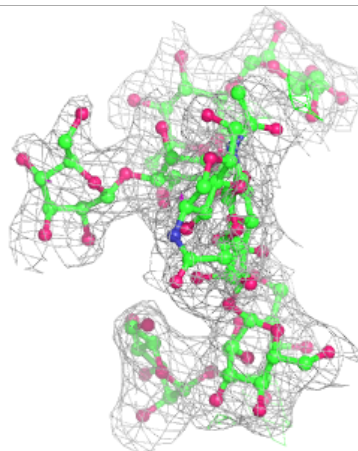
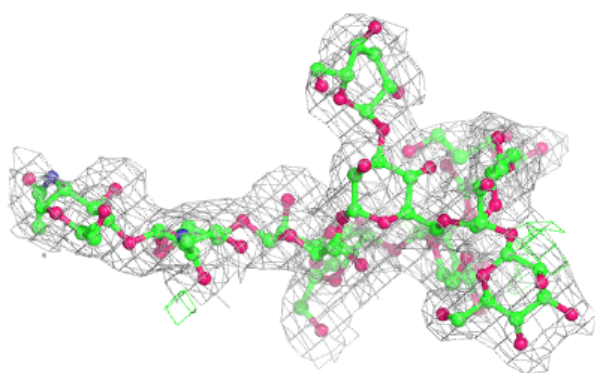
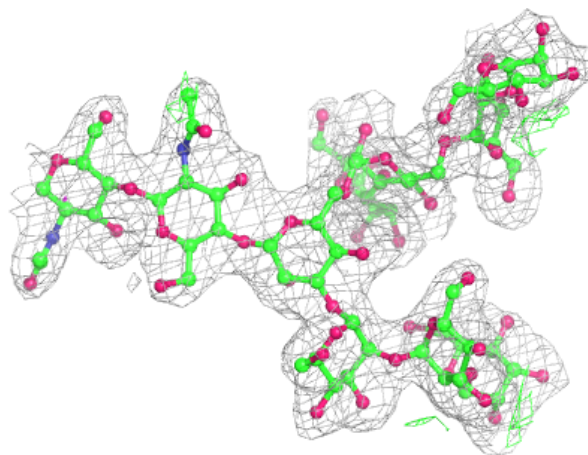
Electron density around Chain N:

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



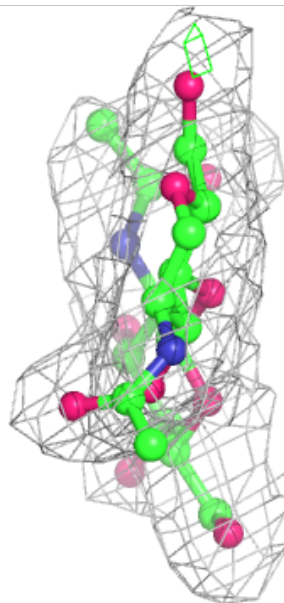
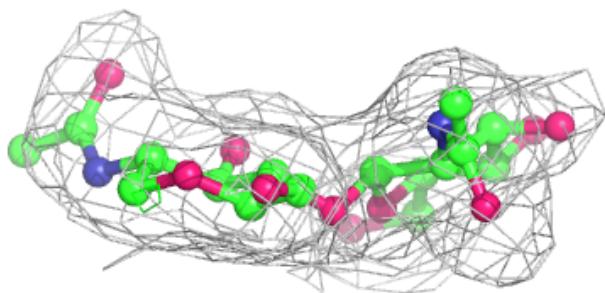
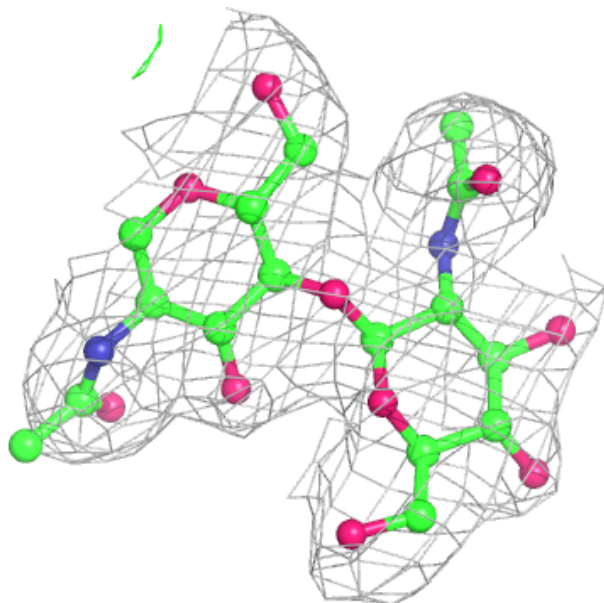
Electron density around Chain O:

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



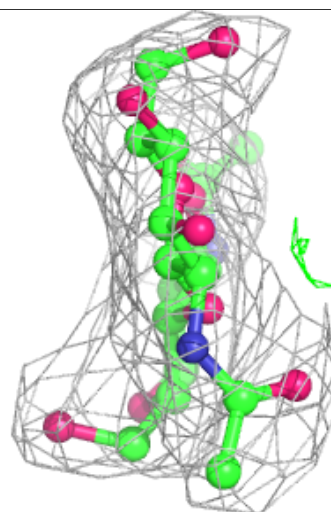
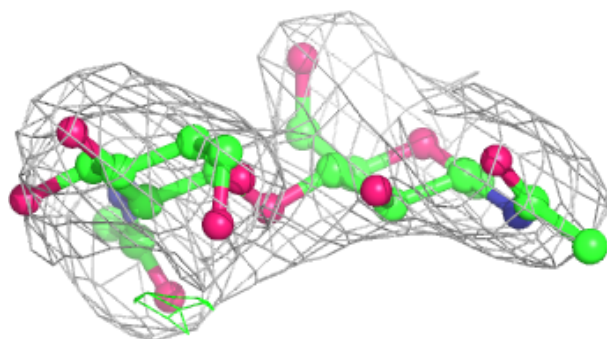
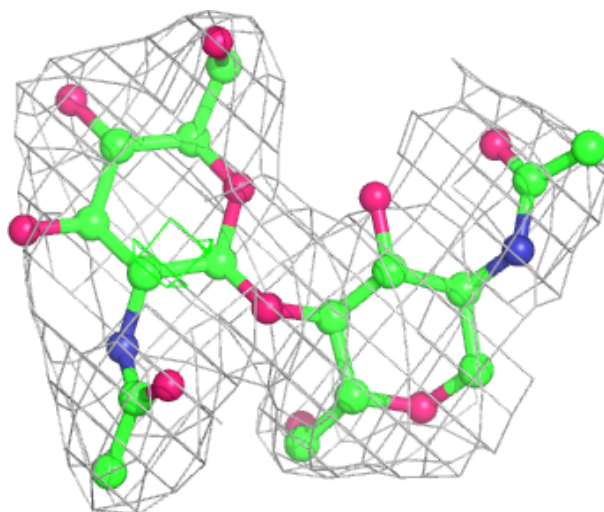
Electron density around Chain P:

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



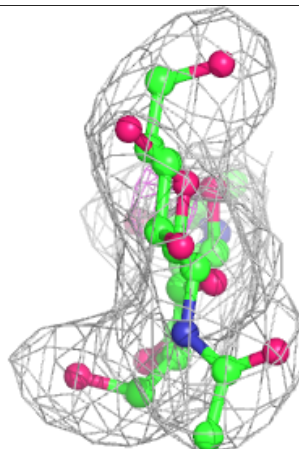
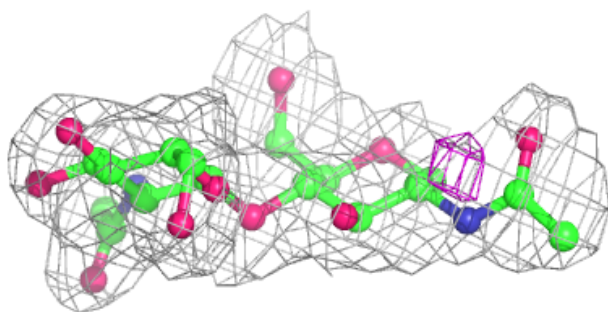
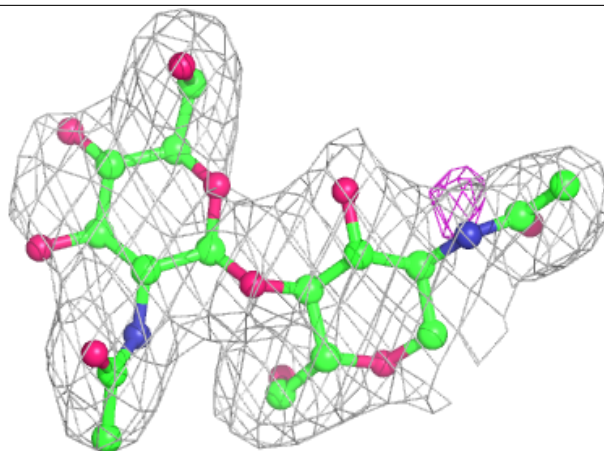
Electron density around Chain K:

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

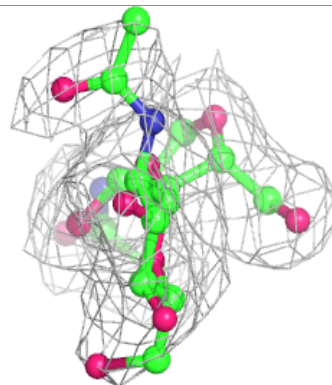
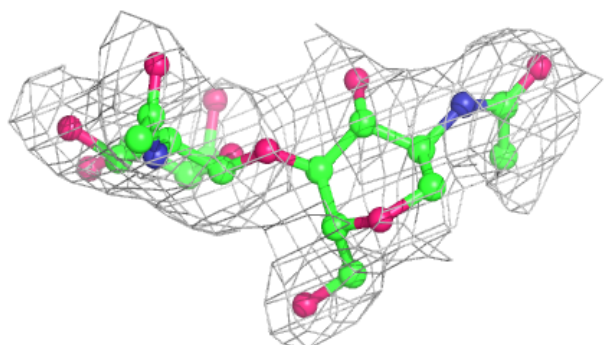
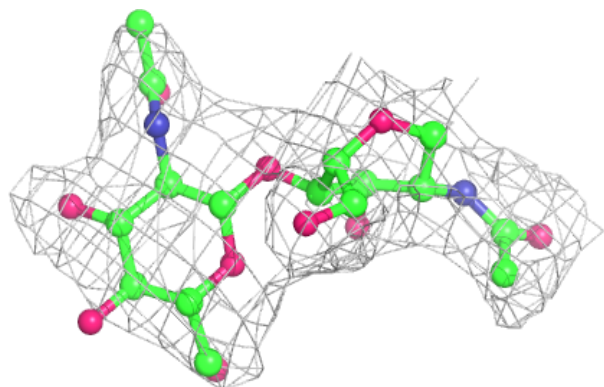


Electron density around Chain M:

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

**Electron density around Chain Q:**

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
14	NAG	B	701	14/15	0.90	0.31	72,106,125,132	0
14	NAG	B	702	14/15	0.93	0.36	103,121,132,156	0
14	NAG	G	617	14/15	0.95	0.19	85,93,111,118	0
14	NAG	G	614	14/15	0.95	0.15	29,63,85,95	0
14	NAG	G	638	14/15	0.98	0.12	52,64,75,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.