



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 10:37 AM BST

PDB ID : 6V49
Title : The crystal structure of hemagglutinin from A/wedge-tailed shearwater/Western Australia/2576/1979 (H15N9)
Authors : Yang, H.; Stevens, J.
Deposited on : 2019-11-27
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

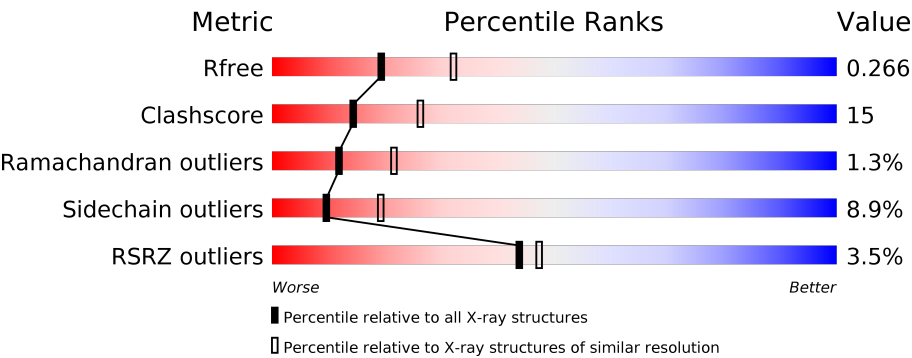
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



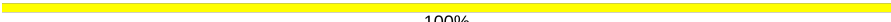
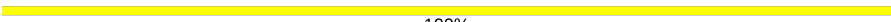
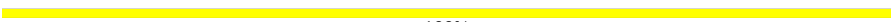
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	332	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>70%26% . .</div></div>
1	C	332	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>70%24% . .</div></div>
1	E	332	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>69%25%5% .</div></div>
2	B	174	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>73%18%5% . .</div></div>
2	D	174	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>75%16% . . .</div></div>
2	F	174	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>76%13%6% . .</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	2	 100%
3	H	2	 100%
3	I	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	301	X	-	-	-
4	NAG	D	301	X	-	-	-
4	NAG	F	301	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11781 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2516	1566	446	490	14			
1	C	329	Total	C	N	O	S	0	0	0
			2516	1566	446	490	14			
1	E	329	Total	C	N	O	S	0	0	0
			2516	1566	446	490	14			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q20ND8
A	132	SER	THR	conflict	UNP Q20ND8
A	133	SER	VAL	conflict	UNP Q20ND8
C	0	GLY	-	expression tag	UNP Q20ND8
C	132	SER	THR	conflict	UNP Q20ND8
C	133	SER	VAL	conflict	UNP Q20ND8
E	0	GLY	-	expression tag	UNP Q20ND8
E	132	SER	THR	conflict	UNP Q20ND8
E	133	SER	VAL	conflict	UNP Q20ND8

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1369	843	245	275	6			
2	D	167	Total	C	N	O	S	0	0	0
			1369	843	245	275	6			
2	F	167	Total	C	N	O	S	0	0	0
			1369	843	245	275	6			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

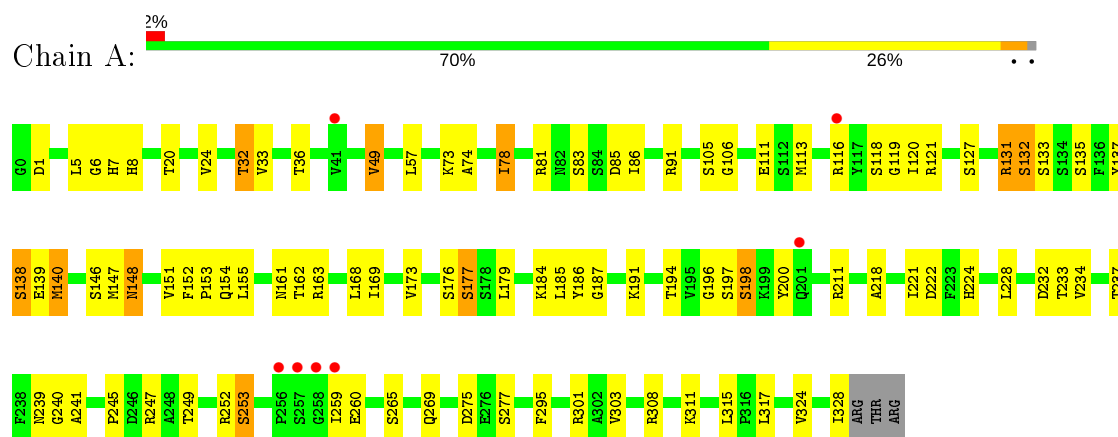


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

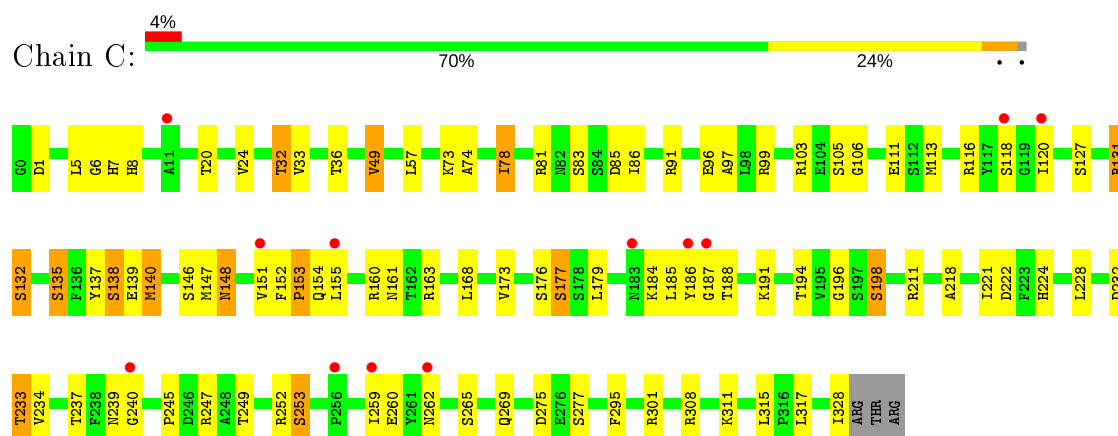
3 Residue-property plots [i](#)

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.

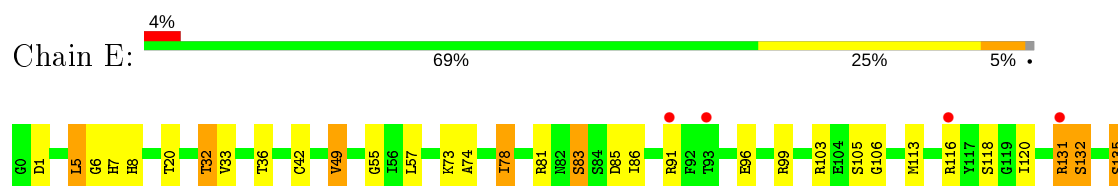
- Molecule 1: Hemagglutinin HA1 chain

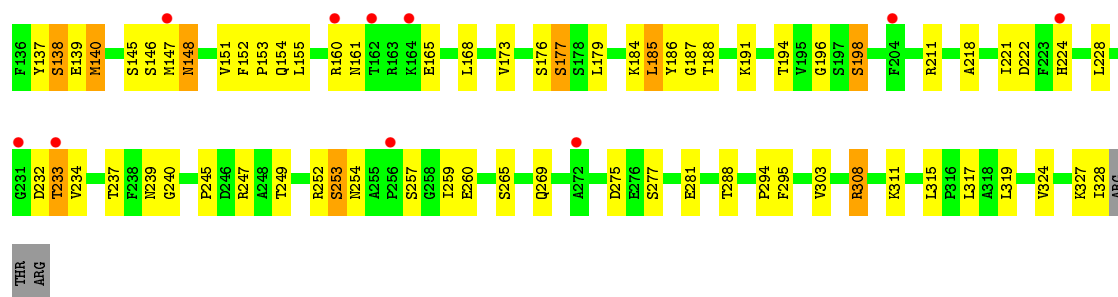


- Molecule 1: Hemagglutinin HA1 chain

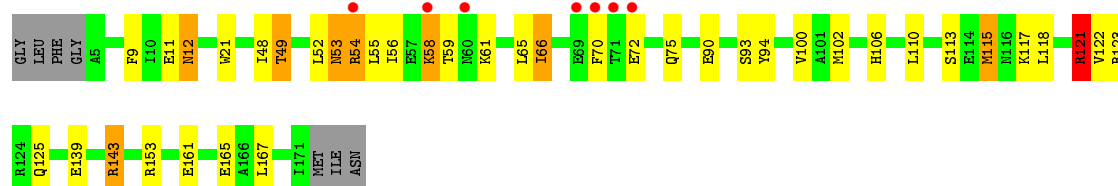


- Molecule 1: Hemagglutinin HA1 chain

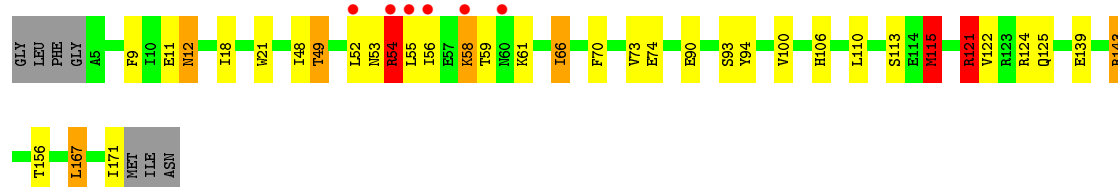
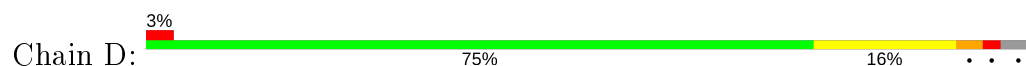




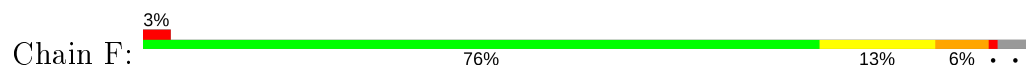
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



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




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

Chain H:  100%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.67Å 101.38Å 163.27Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	44.09 – 2.50 44.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.09-2.50) 99.5 (44.05-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.230 , 0.265 0.231 , 0.266	Depositor DCC
R_{free} test set	3096 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11781	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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

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	0.48	0/2565	0.89	2/3464 (0.1%)
1	C	0.51	0/2565	0.90	2/3464 (0.1%)
1	E	0.48	0/2565	0.86	2/3464 (0.1%)
2	B	0.68	2/1392 (0.1%)	1.11	10/1879 (0.5%)
2	D	0.74	3/1392 (0.2%)	1.11	7/1879 (0.4%)
2	F	0.63	1/1392 (0.1%)	1.07	8/1879 (0.4%)
All	All	0.57	6/11871 (0.1%)	0.96	31/16029 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	74	GLU	CD-OE1	7.02	1.33	1.25
2	D	139	GLU	CD-OE1	6.65	1.32	1.25
2	B	139	GLU	CD-OE1	6.06	1.32	1.25
2	D	139	GLU	CD-OE2	6.05	1.32	1.25
2	F	131	GLU	CD-OE2	5.22	1.31	1.25
2	B	165	GLU	CD-OE2	5.14	1.31	1.25

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	121	ARG	NE-CZ-NH1	10.21	125.41	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	121	ARG	CG-CD-NE	9.83	132.44	111.80
2	B	121	ARG	CB-CG-CD	8.34	133.28	111.60
2	F	121	ARG	NE-CZ-NH1	7.73	124.16	120.30
2	D	121	ARG	CG-CD-NE	7.67	127.92	111.80
2	B	121	ARG	CG-CD-NE	7.51	127.58	111.80
2	D	121	ARG	CB-CG-CD	7.23	130.39	111.60
2	B	121	ARG	NE-CZ-NH1	6.92	123.76	120.30
2	B	121	ARG	NE-CZ-NH2	-6.79	116.90	120.30
2	F	121	ARG	CB-CG-CD	6.68	128.98	111.60
2	B	123	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	E	91	ARG	CB-CA-C	-6.53	97.34	110.40
2	F	121	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	A	91	ARG	CB-CA-C	-6.34	97.73	110.40
1	C	91	ARG	CB-CA-C	-6.27	97.86	110.40
2	B	153	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	E	308	ARG	CG-CD-NE	-6.13	98.92	111.80
2	F	115	MET	CG-SD-CE	-6.05	90.52	100.20
2	B	115	MET	CG-SD-CE	-5.88	90.79	100.20
2	D	124	ARG	NE-CZ-NH1	-5.74	117.43	120.30
2	B	161	GLU	CB-CA-C	5.57	121.55	110.40
2	D	156	THR	CA-CB-OG1	-5.47	97.52	109.00
1	C	5	LEU	CB-CG-CD1	5.40	120.18	111.00
2	B	143	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	F	107	THR	CA-CB-OG1	-5.26	97.95	109.00
2	D	115	MET	CG-SD-CE	-5.25	91.80	100.20
2	F	53	ASN	CB-CA-C	5.21	120.81	110.40
2	D	54	ARG	CB-CG-CD	-5.21	98.07	111.60
2	B	53	ASN	CB-CA-C	5.14	120.67	110.40
2	F	116	ASN	CB-CA-C	5.06	120.53	110.40
1	A	121	ARG	CD-NE-CZ	5.04	130.66	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	GLY	Peptide

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	2516	0	2471	87	3
1	C	2516	0	2471	88	0
1	E	2516	0	2471	91	3
2	B	1369	0	1275	59	0
2	D	1369	0	1275	53	0
2	F	1369	0	1275	57	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
4	B	14	0	13	2	0
4	D	14	0	13	1	0
4	F	14	0	13	0	0
All	All	11781	0	11352	358	3

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 15.

All (358) 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:C:317:LEU:HD13	2:D:54:ARG:NH2	1.23	1.52
1:A:317:LEU:HD13	2:B:54:ARG:NH2	1.38	1.33
1:E:317:LEU:HD13	2:F:54:ARG:NH2	1.42	1.32
1:C:317:LEU:CD1	2:D:54:ARG:HH21	1.54	1.20
1:C:186:TYR:HB2	1:C:191:LYS:NZ	1.60	1.17
1:A:186:TYR:HB2	1:A:191:LYS:NZ	1.59	1.17
1:E:186:TYR:HB2	1:E:191:LYS:NZ	1.60	1.14
1:C:186:TYR:HB2	1:C:191:LYS:HZ3	0.96	1.08
1:E:186:TYR:CB	1:E:191:LYS:HZ3	1.67	1.07
2:B:9:PHE:HB3	2:B:115:MET:HE3	1.34	1.06
1:A:186:TYR:CB	1:A:191:LYS:HZ3	1.68	1.06
1:A:186:TYR:HB2	1:A:191:LYS:HZ3	0.90	1.06
1:C:317:LEU:CD1	2:D:54:ARG:NH2	2.15	1.05
2:F:9:PHE:HB3	2:F:115:MET:HE3	1.39	1.04
1:A:317:LEU:CD1	2:B:54:ARG:HH21	1.69	1.03
1:E:186:TYR:HB2	1:E:191:LYS:HZ3	0.90	1.02
1:C:186:TYR:CB	1:C:191:LYS:HZ3	1.73	1.01
2:F:54:ARG:CZ	2:F:100:VAL:HG22	1.91	1.00
1:A:269:GLN:HB3	2:B:70:PHE:CE2	1.96	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:MET:CE	1:A:245:PRO:HB2	1.92	0.99
2:D:54:ARG:CZ	2:D:100:VAL:HG22	1.91	0.99
2:B:54:ARG:CZ	2:B:100:VAL:HG22	1.93	0.98
2:D:54:ARG:NH1	2:D:100:VAL:HG22	1.80	0.97
1:E:113:MET:CE	1:E:245:PRO:HB2	1.94	0.96
2:F:54:ARG:NH1	2:F:100:VAL:HG22	1.80	0.95
1:E:317:LEU:CD1	2:F:54:ARG:HH21	1.79	0.95
1:A:317:LEU:CD1	2:B:54:ARG:NH2	2.28	0.95
1:A:113:MET:HE1	1:A:245:PRO:HB2	1.46	0.94
2:B:54:ARG:NH1	2:B:100:VAL:HG22	1.83	0.94
1:C:113:MET:CE	1:C:245:PRO:HB2	1.98	0.93
2:D:54:ARG:NH1	2:D:100:VAL:CG2	2.33	0.92
2:B:72:GLU:OE1	4:B:301:NAG:H61	1.70	0.91
1:A:317:LEU:HD13	2:B:54:ARG:HH21	0.92	0.90
2:F:54:ARG:NH1	2:F:100:VAL:CG2	2.35	0.90
2:B:54:ARG:NH1	2:B:100:VAL:CG2	2.35	0.89
1:E:317:LEU:CD1	2:F:54:ARG:NH2	2.33	0.89
1:C:113:MET:HE1	1:C:245:PRO:HB2	1.56	0.88
2:F:52:LEU:HA	2:F:55:LEU:HB3	1.55	0.88
2:D:52:LEU:HA	2:D:55:LEU:HB3	1.56	0.87
1:E:113:MET:HE1	1:E:245:PRO:HB2	1.57	0.86
1:A:275:ASP:OD1	1:A:277:SER:HB3	1.76	0.86
2:F:9:PHE:HB3	2:F:115:MET:CE	2.06	0.86
2:B:90:GLU:OE1	2:D:59:THR:HG22	1.77	0.85
1:E:317:LEU:HD13	2:F:54:ARG:HH21	1.02	0.85
1:A:7:HIS:HD2	2:B:115:MET:HE2	1.42	0.85
2:D:54:ARG:HH12	2:D:100:VAL:CG2	1.90	0.84
2:B:52:LEU:HA	2:B:55:LEU:HB3	1.57	0.84
2:D:9:PHE:HB3	2:D:115:MET:HE3	1.61	0.82
2:B:9:PHE:HB3	2:B:115:MET:CE	2.09	0.82
2:B:54:ARG:HH12	2:B:100:VAL:CG2	1.93	0.82
1:A:20:THR:HB	2:D:106:HIS:CE1	2.14	0.81
2:F:121:ARG:HH11	2:F:125:GLN:NE2	1.77	0.81
2:D:9:PHE:HB3	2:D:115:MET:CE	2.10	0.81
1:C:275:ASP:OD1	1:C:277:SER:HB3	1.81	0.80
2:B:54:ARG:NH2	2:B:100:VAL:HG22	1.96	0.79
1:C:177:SER:HB3	1:C:218:ALA:HB3	1.62	0.79
2:B:106:HIS:CE1	1:E:20:THR:HB	2.17	0.79
2:D:54:ARG:NH2	2:D:100:VAL:HG22	1.96	0.79
1:A:148:ASN:O	1:A:184:LYS:O	2.01	0.78
2:F:54:ARG:HH12	2:F:100:VAL:CG2	1.93	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:54:ARG:NH2	2:F:100:VAL:HG22	1.98	0.77
2:B:121:ARG:HH11	2:B:125:GLN:NE2	1.82	0.77
2:D:121:ARG:HH11	2:D:125:GLN:NE2	1.81	0.77
1:E:177:SER:HB3	1:E:218:ALA:HB3	1.66	0.77
1:E:148:ASN:O	1:E:184:LYS:O	2.02	0.77
1:A:49:VAL:HG12	1:A:74:ALA:HB2	1.67	0.77
1:E:49:VAL:HG12	1:E:74:ALA:HB2	1.65	0.77
1:C:148:ASN:O	1:C:184:LYS:O	2.03	0.75
1:A:177:SER:HB3	1:A:218:ALA:HB3	1.68	0.75
1:E:275:ASP:OD1	1:E:277:SER:HB3	1.87	0.74
2:B:90:GLU:OE1	2:D:59:THR:CG2	2.37	0.73
1:E:198:SER:HB2	1:E:232:ASP:OD1	1.89	0.72
1:C:198:SER:HB2	1:C:232:ASP:OD1	1.89	0.72
1:E:269:GLN:HB3	2:F:70:PHE:CE2	2.25	0.71
1:A:269:GLN:HB3	2:B:70:PHE:CZ	2.25	0.71
1:C:151:VAL:HA	1:C:187:GLY:HA2	1.71	0.71
1:E:151:VAL:HA	1:E:187:GLY:HA2	1.73	0.71
1:A:198:SER:HB2	1:A:232:ASP:OD1	1.89	0.70
1:C:49:VAL:HG12	1:C:74:ALA:HB2	1.74	0.70
2:F:121:ARG:HH11	2:F:125:GLN:HE22	1.40	0.69
1:C:111:GLU:HB2	1:C:163:ARG:HH21	1.56	0.68
1:C:20:THR:HB	2:F:106:HIS:CE1	2.30	0.67
1:A:151:VAL:HA	1:A:187:GLY:HA2	1.74	0.67
1:C:6:GLY:HA2	2:D:115:MET:HE3	1.77	0.67
1:E:5:LEU:CD2	2:F:118:LEU:HG	2.25	0.66
1:C:32:THR:HG23	1:C:295:PHE:CD2	2.29	0.66
1:A:7:HIS:HD2	2:B:115:MET:CE	2.07	0.66
1:A:154:GLN:NE2	1:A:239:ASN:HB3	2.11	0.65
1:C:154:GLN:NE2	1:C:239:ASN:HB3	2.12	0.65
1:E:113:MET:HE3	1:E:245:PRO:HB2	1.77	0.65
2:F:121:ARG:NH1	2:F:125:GLN:HE22	1.94	0.65
1:A:32:THR:HG23	1:A:295:PHE:CD2	2.32	0.65
2:D:54:ARG:NH1	2:D:100:VAL:HG23	2.10	0.65
1:E:154:GLN:NE2	1:E:239:ASN:HB3	2.12	0.64
2:B:54:ARG:NH1	2:B:100:VAL:HG23	2.12	0.64
1:C:301:ARG:HD2	4:D:301:NAG:O7	1.97	0.64
1:E:7:HIS:HD2	2:F:115:MET:HE2	1.62	0.64
1:A:57:LEU:HB2	1:A:85:ASP:CG	2.19	0.63
1:A:20:THR:HB	2:D:106:HIS:HE1	1.62	0.63
1:C:57:LEU:HB2	1:C:85:ASP:CG	2.19	0.63
2:B:59:THR:HG22	2:F:90:GLU:OE1	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:MET:HE1	1:A:245:PRO:CB	2.26	0.62
1:A:116:ARG:CZ	1:A:116:ARG:HB2	2.29	0.62
1:A:301:ARG:HD2	4:B:301:NAG:O7	1.98	0.62
1:C:6:GLY:CA	2:D:115:MET:HE3	2.30	0.62
1:E:32:THR:HG23	1:E:295:PHE:CD2	2.33	0.62
2:B:12:ASN:HD22	2:B:12:ASN:N	1.97	0.62
1:A:7:HIS:CD2	2:B:115:MET:HE2	2.30	0.62
1:C:32:THR:HG23	1:C:295:PHE:HD2	1.65	0.62
2:D:9:PHE:CB	2:D:115:MET:HE2	2.30	0.61
1:A:7:HIS:CD2	2:B:115:MET:CE	2.83	0.61
1:E:57:LEU:HB2	1:E:85:ASP:CG	2.21	0.61
2:D:121:ARG:HH11	2:D:125:GLN:HE22	1.48	0.61
1:C:187:GLY:H	1:C:191:LYS:HE2	1.66	0.60
1:E:311:LYS:HG2	2:F:93:SER:OG	2.01	0.60
2:B:121:ARG:HH11	2:B:125:GLN:HE22	1.48	0.60
1:C:269:GLN:HB3	2:D:70:PHE:CE2	2.37	0.60
1:A:49:VAL:HG12	1:A:74:ALA:CB	2.31	0.60
2:F:12:ASN:N	2:F:12:ASN:HD22	1.99	0.60
1:A:49:VAL:CG1	1:A:74:ALA:HB2	2.31	0.60
2:F:9:PHE:CB	2:F:115:MET:CE	2.79	0.60
1:A:116:ARG:HB2	1:A:116:ARG:NH1	2.17	0.59
1:E:303:VAL:HG11	2:F:65:LEU:HG	1.85	0.59
2:D:121:ARG:NH1	2:D:125:GLN:HE22	1.99	0.59
2:D:12:ASN:N	2:D:12:ASN:HD22	1.99	0.59
1:E:49:VAL:HG12	1:E:74:ALA:CB	2.32	0.59
1:A:303:VAL:HG11	2:B:65:LEU:HG	1.83	0.59
1:E:105:SER:O	1:E:253:SER:HB3	2.03	0.58
1:A:317:LEU:HD13	2:B:54:ARG:CZ	2.28	0.58
1:A:187:GLY:H	1:A:191:LYS:HE2	1.68	0.58
1:C:151:VAL:HA	1:C:187:GLY:CA	2.34	0.58
2:F:54:ARG:NH1	2:F:100:VAL:HG23	2.16	0.58
2:B:9:PHE:CB	2:B:115:MET:HE3	2.21	0.58
1:E:187:GLY:H	1:E:191:LYS:HE2	1.67	0.58
1:E:151:VAL:HA	1:E:187:GLY:CA	2.34	0.58
1:C:317:LEU:HD13	2:D:54:ARG:CZ	2.20	0.58
1:E:327:LYS:NZ	2:F:11:GLU:HG2	2.18	0.57
2:D:54:ARG:HH12	2:D:100:VAL:HG23	1.67	0.57
1:C:186:TYR:CB	1:C:191:LYS:NZ	2.48	0.57
2:D:9:PHE:HB3	2:D:115:MET:HE2	1.87	0.57
1:C:105:SER:O	1:C:253:SER:HB3	2.05	0.56
1:C:275:ASP:OD1	1:C:277:SER:CB	2.51	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:VAL:CG1	1:E:74:ALA:HB2	2.33	0.56
1:A:198:SER:HB2	1:A:232:ASP:CG	2.27	0.56
1:A:78:ILE:N	1:A:78:ILE:HD13	2.21	0.56
1:C:78:ILE:HD13	1:C:78:ILE:N	2.21	0.55
1:E:198:SER:HB2	1:E:232:ASP:CG	2.27	0.55
2:B:9:PHE:CB	2:B:115:MET:CE	2.81	0.55
1:A:105:SER:O	1:A:253:SER:HB3	2.06	0.55
1:A:151:VAL:HA	1:A:187:GLY:CA	2.35	0.55
1:A:32:THR:HG23	1:A:295:PHE:HD2	1.70	0.55
1:C:317:LEU:HD13	2:D:54:ARG:HH21	0.73	0.55
2:D:90:GLU:OE1	2:F:59:THR:HG22	2.07	0.55
2:B:121:ARG:NH1	2:B:125:GLN:HE22	2.04	0.54
1:E:32:THR:HG23	1:E:295:PHE:HD2	1.72	0.54
1:A:32:THR:HG22	1:A:315:LEU:HB2	1.89	0.54
1:C:198:SER:HB2	1:C:232:ASP:CG	2.27	0.54
2:B:106:HIS:HE1	1:E:20:THR:HB	1.66	0.54
1:E:275:ASP:OD1	1:E:277:SER:CB	2.55	0.54
1:C:139:GLU:OE1	1:C:247:ARG:HD3	2.07	0.54
1:C:252:ARG:NH1	1:C:260:GLU:HB3	2.22	0.54
1:C:49:VAL:CG1	1:C:74:ALA:HB2	2.37	0.54
2:B:54:ARG:HH12	2:B:100:VAL:HG23	1.69	0.53
1:E:161:ASN:HB2	1:E:228:LEU:HD23	1.90	0.53
1:A:113:MET:HE3	1:A:245:PRO:HB2	1.88	0.53
1:C:131:ARG:HH12	1:C:138:SER:HB2	1.73	0.53
2:D:48:ILE:O	2:D:49:THR:HG23	2.09	0.53
1:E:32:THR:HG22	1:E:315:LEU:HB2	1.90	0.53
1:E:5:LEU:HD21	2:F:118:LEU:HG	1.90	0.53
1:E:78:ILE:N	1:E:78:ILE:HD13	2.24	0.53
1:A:275:ASP:OD1	1:A:277:SER:CB	2.53	0.52
1:A:196:GLY:HA3	1:E:211:ARG:HG2	1.91	0.52
1:A:161:ASN:HB2	1:A:228:LEU:HD23	1.90	0.52
1:E:252:ARG:NH1	1:E:260:GLU:HB3	2.24	0.52
1:C:154:GLN:HE22	1:C:239:ASN:HB3	1.73	0.52
1:A:131:ARG:HH12	1:A:138:SER:HB2	1.74	0.52
1:C:161:ASN:HB2	1:C:228:LEU:HD23	1.91	0.52
1:A:153:PRO:HB2	1:A:155:LEU:HG	1.92	0.52
1:A:154:GLN:HE22	1:A:239:ASN:HB3	1.72	0.52
1:A:7:HIS:HB3	2:B:115:MET:HE1	1.92	0.52
1:C:186:TYR:HB2	1:C:191:LYS:HZ2	1.66	0.52
2:D:59:THR:HB	2:D:61:LYS:H	1.76	0.51
1:E:113:MET:HE1	1:E:245:PRO:CB	2.37	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:THR:HB	2:F:106:HIS:HE1	1.73	0.51
1:E:139:GLU:OE1	1:E:247:ARG:HD3	2.09	0.51
1:A:252:ARG:NH1	1:A:260:GLU:HB3	2.25	0.51
1:C:113:MET:HE3	1:C:245:PRO:HB2	1.89	0.51
1:C:32:THR:HG22	1:C:315:LEU:HB2	1.92	0.51
2:F:54:ARG:HH12	2:F:100:VAL:CA	2.23	0.51
1:E:120:ILE:HA	1:E:146:SER:HB2	1.93	0.51
1:E:252:ARG:HH11	1:E:260:GLU:HB3	1.76	0.50
1:E:7:HIS:HD2	2:F:115:MET:CE	2.22	0.50
1:A:311:LYS:HG2	2:B:93:SER:OG	2.11	0.50
2:F:48:ILE:O	2:F:49:THR:HG23	2.10	0.50
1:A:86:ILE:C	1:A:86:ILE:HD12	2.30	0.50
2:B:48:ILE:O	2:B:49:THR:HG23	2.11	0.50
1:E:187:GLY:O	1:E:191:LYS:NZ	2.44	0.50
2:B:54:ARG:HH12	2:B:100:VAL:CA	2.24	0.50
2:D:54:ARG:HH12	2:D:100:VAL:CA	2.25	0.50
1:C:6:GLY:C	2:D:115:MET:HE1	2.31	0.50
1:A:187:GLY:O	1:A:191:LYS:NZ	2.44	0.49
1:E:153:PRO:HB2	1:E:155:LEU:HG	1.94	0.49
1:A:6:GLY:C	2:B:115:MET:HE1	2.33	0.49
1:A:5:LEU:CD2	2:B:118:LEU:HG	2.42	0.49
1:C:49:VAL:HG12	1:C:74:ALA:CB	2.43	0.49
2:F:121:ARG:NH1	2:F:125:GLN:NE2	2.52	0.49
1:A:194:THR:HB	1:A:237:THR:HG23	1.94	0.49
1:E:154:GLN:HE22	1:E:239:ASN:HB3	1.75	0.49
2:B:54:ARG:HH12	2:B:100:VAL:HA	1.77	0.49
1:E:131:ARG:HG3	1:E:135:SER:OG	2.13	0.49
1:A:211:ARG:HG2	1:C:196:GLY:HA3	1.93	0.49
2:B:59:THR:CG2	2:F:90:GLU:OE1	2.60	0.48
1:C:168:LEU:HB3	1:C:249:THR:HB	1.95	0.48
1:E:86:ILE:HD12	1:E:86:ILE:C	2.33	0.48
1:A:196:GLY:O	1:A:234:VAL:HA	2.14	0.48
1:C:6:GLY:C	2:D:115:MET:CE	2.82	0.48
1:A:120:ILE:HA	1:A:146:SER:HB2	1.96	0.48
1:C:252:ARG:HH11	1:C:260:GLU:HB3	1.79	0.48
1:C:153:PRO:HB2	1:C:155:LEU:HG	1.96	0.48
1:A:168:LEU:HB3	1:A:249:THR:HB	1.96	0.47
1:C:187:GLY:H	1:C:191:LYS:CE	2.27	0.47
2:D:9:PHE:CB	2:D:115:MET:CE	2.83	0.47
1:E:131:ARG:HH12	1:E:138:SER:HB2	1.78	0.47
2:B:21:TRP:HH2	2:B:48:ILE:HD12	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:GLY:O	1:E:234:VAL:HA	2.14	0.47
1:A:308:ARG:HE	1:A:308:ARG:HB2	1.49	0.47
1:C:86:ILE:C	1:C:86:ILE:HD12	2.34	0.47
1:E:186:TYR:CB	1:E:191:LYS:NZ	2.47	0.47
1:E:191:LYS:HD3	1:E:240:GLY:HA3	1.96	0.47
1:A:7:HIS:CB	2:B:115:MET:HE1	2.45	0.47
1:C:120:ILE:HA	1:C:146:SER:HB2	1.96	0.47
1:E:168:LEU:HB3	1:E:249:THR:HB	1.96	0.47
2:F:54:ARG:HH12	2:F:100:VAL:HA	1.79	0.47
1:C:187:GLY:N	1:C:191:LYS:HZ3	2.12	0.47
1:C:187:GLY:O	1:C:191:LYS:NZ	2.45	0.46
1:A:252:ARG:HH11	1:A:260:GLU:HB3	1.80	0.46
2:D:54:ARG:HH12	2:D:100:VAL:HA	1.80	0.46
1:E:7:HIS:CD2	2:F:115:MET:CE	2.98	0.46
2:F:9:PHE:CB	2:F:115:MET:HE2	2.45	0.46
1:A:137:TYR:HB2	1:A:140:MET:HG3	1.97	0.46
1:C:211:ARG:HG2	1:E:196:GLY:HA3	1.96	0.46
1:A:317:LEU:HB2	2:B:54:ARG:HH21	1.81	0.46
1:E:222:ASP:HB3	1:E:224:HIS:NE2	2.30	0.46
1:C:194:THR:HB	1:C:237:THR:HG23	1.98	0.46
1:C:196:GLY:O	1:C:234:VAL:HA	2.15	0.46
1:E:327:LYS:HZ1	2:F:11:GLU:HG2	1.81	0.46
1:C:191:LYS:HD3	1:C:240:GLY:HA3	1.97	0.45
1:A:139:GLU:OE1	1:A:247:ARG:HD3	2.17	0.45
1:A:5:LEU:HD22	2:B:118:LEU:HG	1.99	0.45
2:B:110:LEU:HG	2:B:110:LEU:O	2.16	0.45
1:A:173:VAL:O	1:A:221:ILE:HA	2.16	0.45
1:E:96:GLU:HG2	2:F:73:VAL:HG12	1.97	0.45
1:A:191:LYS:HD3	1:A:240:GLY:HA3	1.97	0.45
1:C:131:ARG:HG3	1:C:135:SER:OG	2.16	0.45
1:C:7:HIS:HB3	2:D:115:MET:HE1	1.98	0.45
1:E:7:HIS:HB3	2:F:115:MET:HE1	1.99	0.45
1:A:187:GLY:H	1:A:191:LYS:CE	2.28	0.44
2:B:121:ARG:NH1	2:B:125:GLN:NE2	2.58	0.44
1:A:7:HIS:N	2:B:115:MET:HE1	2.32	0.44
1:A:211:ARG:NH2	1:C:194:THR:HG21	2.32	0.44
2:F:59:THR:HB	2:F:61:LYS:H	1.82	0.44
1:A:111:GLU:HB2	1:A:163:ARG:HH21	1.83	0.44
2:B:59:THR:HB	2:B:61:LYS:H	1.82	0.44
2:B:75:GLN:HB3	1:C:97:ALA:HB1	2.00	0.44
1:C:116:ARG:HB2	1:C:116:ARG:CZ	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:167:LEU:HD12	2:D:167:LEU:HA	1.82	0.44
1:E:173:VAL:O	1:E:221:ILE:HA	2.18	0.44
1:E:187:GLY:H	1:E:191:LYS:CE	2.28	0.44
1:E:259:ILE:O	1:E:260:GLU:HB2	2.18	0.44
2:F:12:ASN:ND2	2:F:12:ASN:N	2.65	0.44
2:F:54:ARG:HH12	2:F:100:VAL:HG23	1.73	0.44
1:C:222:ASP:HB3	1:C:224:HIS:NE2	2.33	0.44
1:E:275:ASP:C	1:E:277:SER:H	2.21	0.44
1:A:106:GLY:HA2	1:A:265:SER:HB3	1.98	0.44
1:A:275:ASP:C	1:A:277:SER:H	2.21	0.44
1:E:106:GLY:HA2	1:E:265:SER:HB3	2.00	0.44
1:A:222:ASP:HB3	1:A:224:HIS:NE2	2.32	0.44
2:B:12:ASN:ND2	2:B:12:ASN:N	2.64	0.44
1:A:7:HIS:HA	2:B:21:TRP:O	2.18	0.44
1:C:191:LYS:HA	1:C:239:ASN:HD21	1.82	0.44
2:D:21:TRP:HH2	2:D:48:ILE:HD12	1.83	0.44
1:A:259:ILE:O	1:A:260:GLU:HB2	2.17	0.44
1:E:294:PRO:HG3	2:F:54:ARG:HD2	2.00	0.44
1:C:259:ILE:O	1:C:260:GLU:HB2	2.18	0.43
1:C:32:THR:HG22	1:C:33:VAL:HG23	2.00	0.43
1:E:99:ARG:O	1:E:103:ARG:HG3	2.17	0.43
2:D:121:ARG:NH1	2:D:125:GLN:NE2	2.54	0.43
1:C:151:VAL:HG23	1:C:188:THR:H	1.83	0.43
1:C:137:TYR:HB2	1:C:140:MET:HG3	2.00	0.43
2:D:54:ARG:HH22	2:D:100:VAL:HA	1.83	0.43
2:F:55:LEU:HD22	2:F:58:LYS:CB	2.49	0.43
2:D:12:ASN:N	2:D:12:ASN:ND2	2.64	0.43
1:E:32:THR:HG22	1:E:33:VAL:HG23	2.00	0.43
1:E:194:THR:HB	1:E:237:THR:HG23	1.99	0.43
1:C:317:LEU:CG	2:D:54:ARG:HH21	2.25	0.43
1:E:327:LYS:HZ3	2:F:11:GLU:HG2	1.83	0.43
1:A:152:PHE:HA	1:A:153:PRO:HD2	1.82	0.42
1:A:197:SER:HB3	1:A:200:TYR:HB3	2.01	0.42
1:C:173:VAL:O	1:C:221:ILE:HA	2.18	0.42
1:C:275:ASP:C	1:C:277:SER:H	2.21	0.42
1:C:7:HIS:HD2	2:D:115:MET:HE2	1.84	0.42
1:E:191:LYS:HA	1:E:239:ASN:HD21	1.83	0.42
1:E:165:GLU:HG2	1:E:254:ASN:O	2.19	0.42
1:A:169:ILE:HD13	1:A:234:VAL:HG11	2.01	0.42
1:A:191:LYS:HA	1:A:239:ASN:HD21	1.84	0.42
1:C:308:ARG:HB2	1:C:308:ARG:HE	1.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ALA:O	1:C:262:ASN:ND2	2.52	0.42
2:D:55:LEU:HD22	2:D:58:LYS:CB	2.50	0.42
2:B:54:ARG:HH22	2:B:100:VAL:HG22	1.79	0.42
1:E:137:TYR:HB2	1:E:140:MET:HG3	2.00	0.42
2:B:122:VAL:HA	2:B:125:GLN:NE2	2.34	0.42
2:B:66:ILE:HA	2:B:66:ILE:HD13	1.72	0.42
1:E:55:GLY:HA2	1:E:83:SER:HB3	2.01	0.42
1:E:6:GLY:C	2:F:115:MET:HE1	2.39	0.42
1:A:57:LEU:HB2	1:A:85:ASP:OD2	2.19	0.42
1:C:99:ARG:O	1:C:103:ARG:HG3	2.19	0.42
1:E:308:ARG:HB2	1:E:308:ARG:HE	1.49	0.42
1:E:317:LEU:HD13	2:F:54:ARG:CZ	2.34	0.42
1:E:317:LEU:CG	2:F:54:ARG:HH21	2.32	0.42
1:C:160:ARG:HG3	1:C:233:THR:HB	2.00	0.42
2:D:66:ILE:HD13	2:D:66:ILE:HA	1.72	0.42
1:C:96:GLU:HG2	2:D:73:VAL:HG12	2.01	0.42
1:A:32:THR:HG22	1:A:33:VAL:HG23	2.02	0.41
2:B:55:LEU:HD22	2:B:58:LYS:CB	2.50	0.41
1:C:57:LEU:HB2	1:C:85:ASP:OD2	2.20	0.41
2:D:52:LEU:CA	2:D:55:LEU:HB3	2.40	0.41
1:E:42:CYS:HB2	1:E:288:THR:HG21	2.02	0.41
2:F:66:ILE:HA	2:F:66:ILE:HD13	1.71	0.41
1:C:187:GLY:N	1:C:191:LYS:NZ	2.69	0.41
1:C:259:ILE:O	1:C:260:GLU:CB	2.68	0.41
1:E:160:ARG:HG3	1:E:233:THR:HB	2.02	0.41
1:E:317:LEU:HB2	2:F:54:ARG:HH21	1.86	0.41
1:E:151:VAL:HG23	1:E:188:THR:H	1.85	0.41
2:B:54:ARG:HH22	2:B:100:VAL:HA	1.85	0.41
2:F:110:LEU:HG	2:F:110:LEU:O	2.19	0.41
1:A:187:GLY:N	1:A:191:LYS:HZ3	2.19	0.41
2:D:122:VAL:HA	2:D:125:GLN:NE2	2.35	0.41
1:E:319:LEU:O	2:F:48:ILE:HD13	2.20	0.41
2:D:110:LEU:O	2:D:110:LEU:HG	2.18	0.41
1:C:7:HIS:N	2:D:115:MET:HE1	2.35	0.41
1:E:32:THR:CG2	1:E:315:LEU:HB2	2.51	0.41
2:B:102:MET:HE2	2:B:102:MET:HB3	1.78	0.41
1:C:106:GLY:HA2	1:C:265:SER:HB3	2.02	0.41
1:C:311:LYS:HG2	2:D:93:SER:OG	2.21	0.41
1:C:32:THR:CG2	1:C:315:LEU:HB2	2.52	0.41
2:F:55:LEU:HD22	2:F:58:LYS:HB3	2.02	0.41
1:C:152:PHE:HA	1:C:153:PRO:HD2	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:GLN:HB3	2:F:70:PHE:CZ	2.55	0.40
1:E:152:PHE:HB3	1:E:239:ASN:O	2.21	0.40
2:F:167:LEU:HD12	2:F:167:LEU:HA	1.82	0.40
2:F:52:LEU:CA	2:F:55:LEU:HB3	2.39	0.40
1:E:32:THR:HB	1:E:315:LEU:O	2.21	0.40
1:A:152:PHE:HB3	1:A:239:ASN:O	2.21	0.40
1:C:152:PHE:HB3	1:C:239:ASN:O	2.22	0.40
1:E:57:LEU:HB2	1:E:85:ASP:OD2	2.21	0.40
1:A:186:TYR:CZ	1:A:241:ALA:HA	2.57	0.40
2:D:143:ARG:HD2	2:D:143:ARG:HA	1.84	0.40
1:E:145:SER:OG	1:E:185:LEU:O	2.39	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:THR:OG1	1:E:116:ARG:NH1[4_446]	1.81	0.39
1:A:133:SER:CB	1:E:281:GLU:OE2[3_445]	2.05	0.15
1:A:116:ARG:NH1	1:E:247:ARG:NH2[4_446]	2.08	0.12

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	327/332 (98%)	297 (91%)	25 (8%)	5 (2%)	10	18
1	C	327/332 (98%)	297 (91%)	25 (8%)	5 (2%)	10	18
1	E	327/332 (98%)	297 (91%)	24 (7%)	6 (2%)	8	14
2	B	165/174 (95%)	158 (96%)	6 (4%)	1 (1%)	25	43
2	D	165/174 (95%)	158 (96%)	6 (4%)	1 (1%)	25	43
2	F	165/174 (95%)	161 (98%)	3 (2%)	1 (1%)	25	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1476/1518 (97%)	1368 (93%)	89 (6%)	19 (1%)	12 21

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	SER
1	A	132	SER
1	C	83	SER
1	E	83	SER
1	A	138	SER
1	C	132	SER
1	C	138	SER
2	D	49	THR
1	E	132	SER
1	E	138	SER
2	B	49	THR
1	C	148	ASN
1	E	148	ASN
1	A	148	ASN
1	C	118	SER
2	F	49	THR
1	A	118	SER
1	E	118	SER
1	E	257	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	278/281 (99%)	254 (91%)	24 (9%)	10 20
1	C	278/281 (99%)	254 (91%)	24 (9%)	10 20
1	E	278/281 (99%)	255 (92%)	23 (8%)	11 22
2	B	144/149 (97%)	131 (91%)	13 (9%)	9 19
2	D	144/149 (97%)	129 (90%)	15 (10%)	7 13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	144/149 (97%)	130 (90%)	14 (10%)	8	16
All	All	1266/1290 (98%)	1153 (91%)	113 (9%)	9	19

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	8	HIS
1	A	24	VAL
1	A	32	THR
1	A	36	THR
1	A	49	VAL
1	A	73	LYS
1	A	78	ILE
1	A	81	ARG
1	A	127	SER
1	A	131	ARG
1	A	132	SER
1	A	135	SER
1	A	140	MET
1	A	147	MET
1	A	176	SER
1	A	177	SER
1	A	179	LEU
1	A	185	LEU
1	A	198	SER
1	A	233	THR
1	A	253	SER
1	A	324	VAL
1	A	328	ILE
2	B	11	GLU
2	B	12	ASN
2	B	53	ASN
2	B	54	ARG
2	B	56	ILE
2	B	58	LYS
2	B	66	ILE
2	B	94	TYR
2	B	113	SER
2	B	117	LYS
2	B	121	ARG
2	B	143	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	167	LEU
1	C	1	ASP
1	C	8	HIS
1	C	24	VAL
1	C	32	THR
1	C	36	THR
1	C	49	VAL
1	C	73	LYS
1	C	78	ILE
1	C	81	ARG
1	C	127	SER
1	C	131	ARG
1	C	132	SER
1	C	135	SER
1	C	140	MET
1	C	147	MET
1	C	153	PRO
1	C	176	SER
1	C	177	SER
1	C	179	LEU
1	C	185	LEU
1	C	198	SER
1	C	233	THR
1	C	253	SER
1	C	328	ILE
2	D	11	GLU
2	D	12	ASN
2	D	18	ILE
2	D	53	ASN
2	D	54	ARG
2	D	56	ILE
2	D	58	LYS
2	D	66	ILE
2	D	94	TYR
2	D	113	SER
2	D	115	MET
2	D	121	ARG
2	D	143	ARG
2	D	167	LEU
2	D	171	ILE
1	E	1	ASP
1	E	5	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	8	HIS
1	E	32	THR
1	E	36	THR
1	E	49	VAL
1	E	73	LYS
1	E	78	ILE
1	E	81	ARG
1	E	131	ARG
1	E	132	SER
1	E	135	SER
1	E	140	MET
1	E	147	MET
1	E	176	SER
1	E	177	SER
1	E	179	LEU
1	E	185	LEU
1	E	198	SER
1	E	233	THR
1	E	253	SER
1	E	324	VAL
1	E	328	ILE
2	F	11	GLU
2	F	12	ASN
2	F	53	ASN
2	F	54	ARG
2	F	56	ILE
2	F	58	LYS
2	F	66	ILE
2	F	94	TYR
2	F	110	LEU
2	F	113	SER
2	F	117	LYS
2	F	121	ARG
2	F	167	LEU
2	F	171	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	154	GLN
2	B	106	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	125	GLN
2	B	164	GLN
1	C	7	HIS
1	C	154	GLN
1	C	262	ASN
2	D	106	HIS
2	D	125	GLN
1	E	7	HIS
1	E	154	GLN
2	F	106	HIS
2	F	125	GLN
2	F	164	GLN

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 ⓘ

6 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	$\# Z > 2$
3	NAG	G	1	1,3	14,14,15	0.55	0	17,19,21	2.44	9 (52%)
3	NAG	G	2	3	14,14,15	1.56	3 (21%)	17,19,21	2.57	7 (41%)
3	NAG	H	1	1,3	14,14,15	0.90	1 (7%)	17,19,21	2.78	8 (47%)
3	NAG	H	2	3	14,14,15	1.23	1 (7%)	17,19,21	2.36	9 (52%)
3	NAG	I	1	1,3	14,14,15	0.67	0	17,19,21	1.94	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	I	2	3	14,14,15	0.65	0	17,19,21	1.70	4 (23%)

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
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2	NAG	C1-C2	3.80	1.58	1.52
3	G	2	NAG	O5-C1	2.51	1.47	1.43
3	H	1	NAG	O7-C7	2.30	1.28	1.23
3	G	2	NAG	C2-N2	2.24	1.50	1.46
3	H	2	NAG	O4-C4	2.02	1.47	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C1-O5-C5	-6.13	103.89	112.19
3	G	1	NAG	C1-O5-C5	-6.07	103.97	112.19
3	G	2	NAG	C1-O5-C5	5.66	119.86	112.19
3	G	2	NAG	O5-C1-C2	5.60	120.13	111.29
3	H	1	NAG	C2-N2-C7	-4.81	116.05	122.90
3	H	2	NAG	O4-C4-C5	4.59	120.70	109.30
3	H	1	NAG	C3-C4-C5	-4.57	102.09	110.24
3	I	2	NAG	O5-C1-C2	3.98	117.58	111.29
3	G	2	NAG	C2-N2-C7	3.89	128.44	122.90
3	H	2	NAG	C3-C4-C5	-3.88	103.31	110.24
3	I	1	NAG	O4-C4-C5	3.53	118.07	109.30
3	H	1	NAG	O5-C5-C6	3.49	112.67	107.20
3	I	1	NAG	O3-C3-C4	-3.34	102.62	110.35
3	I	2	NAG	O5-C5-C4	-3.30	102.79	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C2-N2-C7	-3.09	118.50	122.90
3	G	1	NAG	C1-C2-N2	2.99	115.60	110.49
3	H	2	NAG	O5-C5-C6	2.98	111.87	107.20
3	H	1	NAG	O5-C1-C2	-2.78	106.91	111.29
3	I	1	NAG	C1-C2-N2	2.76	115.20	110.49
3	G	1	NAG	O3-C3-C2	-2.69	103.89	109.47
3	G	1	NAG	C6-C5-C4	2.68	119.27	113.00
3	H	2	NAG	O6-C6-C5	-2.63	102.28	111.29
3	H	1	NAG	C6-C5-C4	2.63	119.15	113.00
3	G	1	NAG	C8-C7-N2	2.58	120.46	116.10
3	I	1	NAG	O5-C5-C4	-2.56	104.61	110.83
3	H	2	NAG	C8-C7-N2	-2.55	111.78	116.10
3	H	2	NAG	O7-C7-N2	2.44	126.44	121.95
3	H	2	NAG	O3-C3-C2	2.39	114.40	109.47
3	I	2	NAG	O4-C4-C5	2.38	115.20	109.30
3	G	2	NAG	C1-C2-N2	2.25	114.33	110.49
3	G	1	NAG	O5-C5-C4	-2.25	105.36	110.83
3	G	1	NAG	O5-C5-C6	2.25	110.72	107.20
3	H	1	NAG	C8-C7-N2	-2.22	112.34	116.10
3	G	2	NAG	O7-C7-C8	-2.21	117.95	122.06
3	G	2	NAG	C3-C4-C5	-2.17	106.36	110.24
3	H	2	NAG	C2-N2-C7	2.10	125.90	122.90
3	I	2	NAG	C1-O5-C5	2.07	114.99	112.19
3	G	1	NAG	O4-C4-C5	2.06	114.40	109.30
3	G	2	NAG	C8-C7-N2	2.05	119.58	116.10
3	H	1	NAG	O4-C4-C5	2.05	114.39	109.30
3	H	2	NAG	C6-C5-C4	2.01	117.72	113.00

There are no chirality outliers.

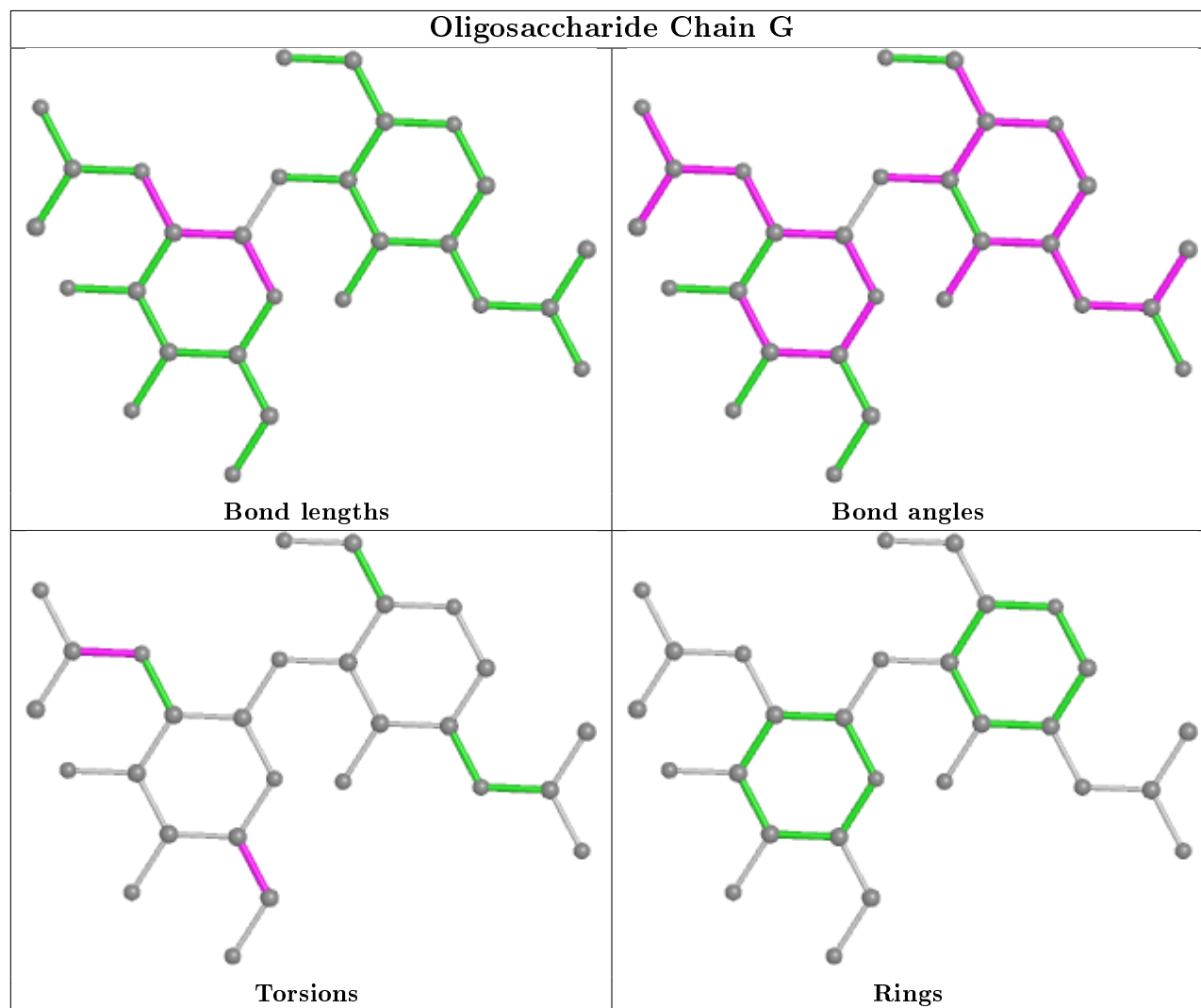
All (9) torsion outliers are listed below:

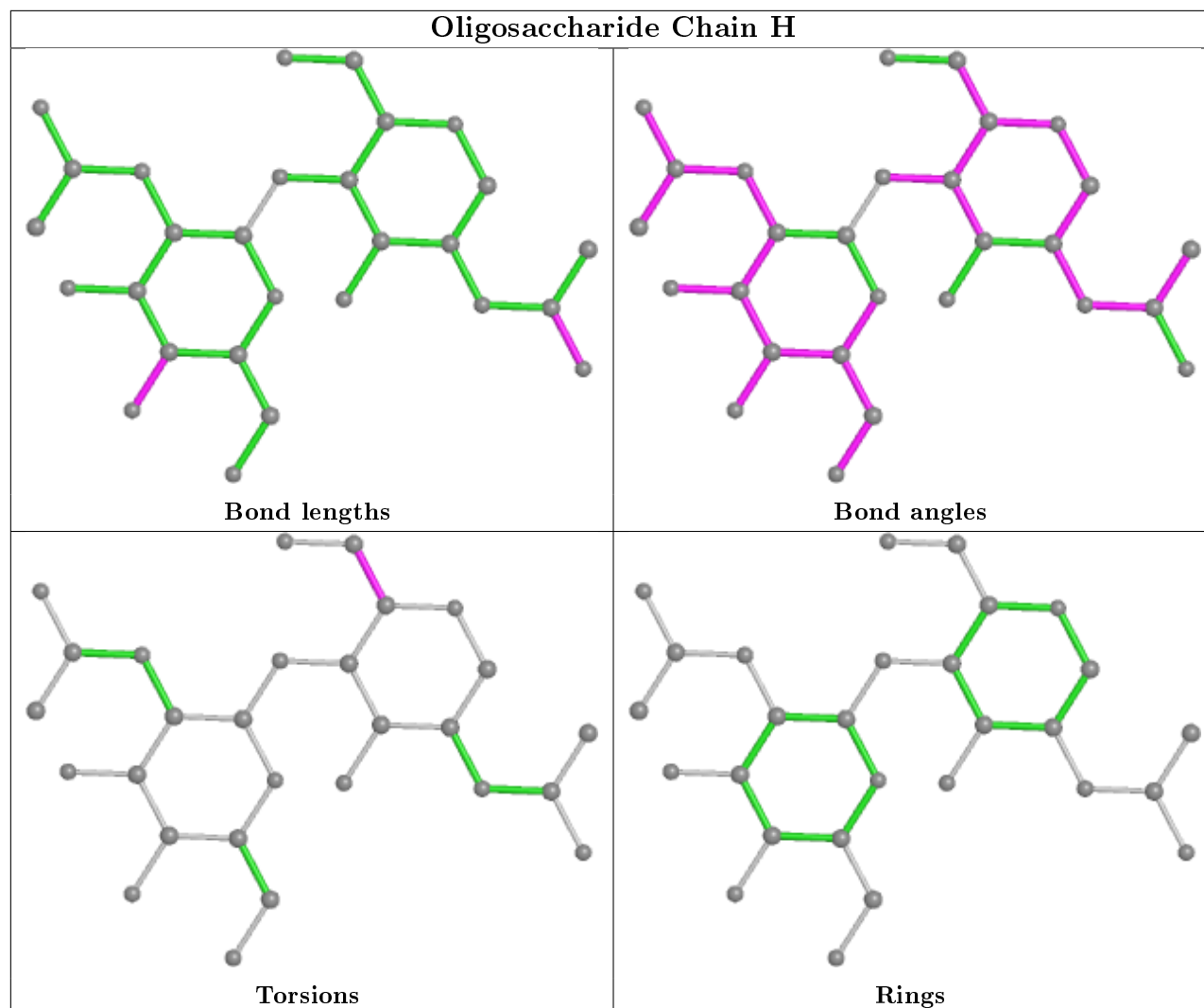
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
3	I	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	G	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C4-C5-C6-O6

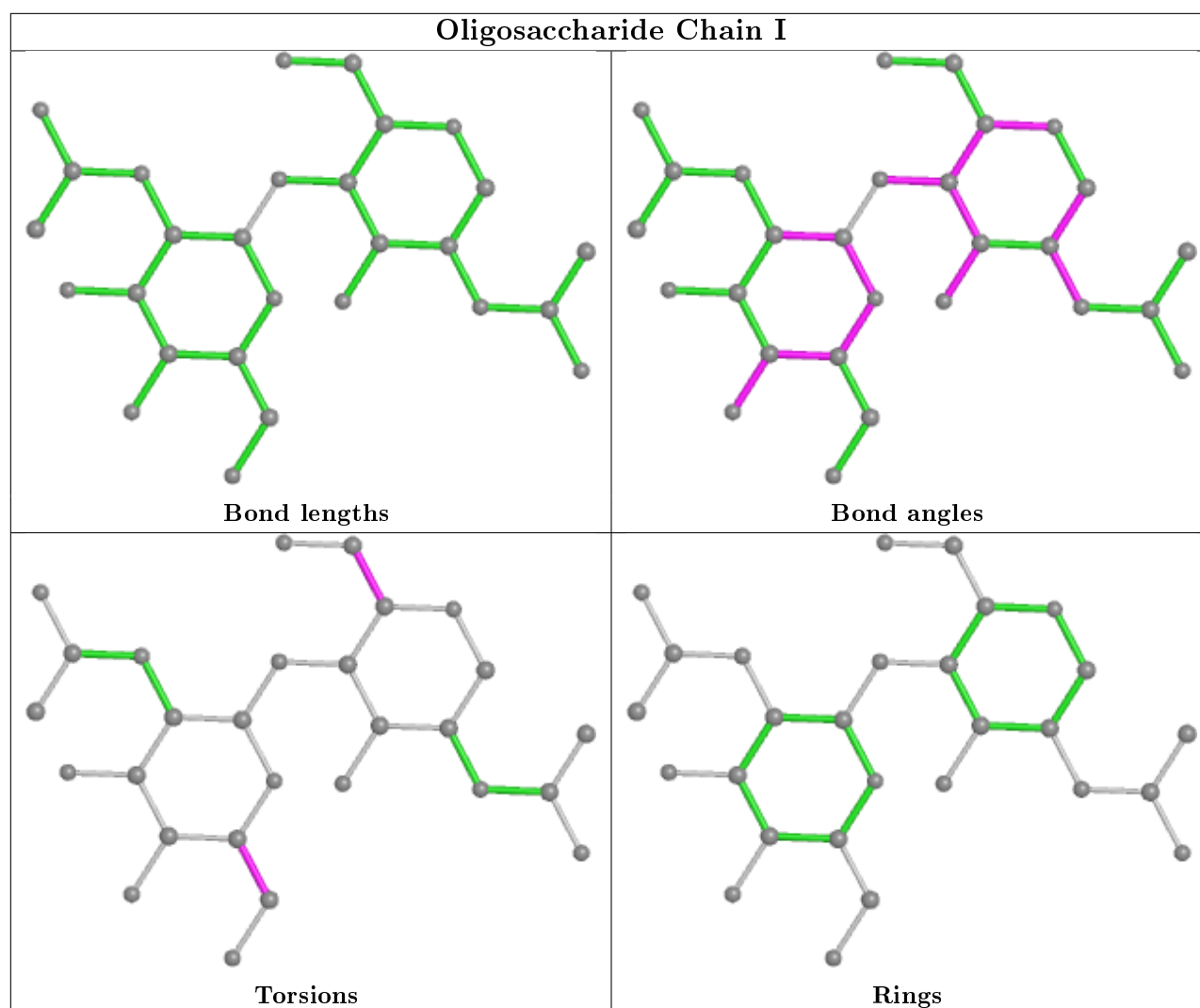
There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

3 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$
4	NAG	F	301	2	14,14,15	0.98	1 (7%)	17,19,21	1.90	6 (35%)
4	NAG	B	301	2	14,14,15	1.32	1 (7%)	17,19,21	2.51	10 (58%)
4	NAG	D	301	2	14,14,15	1.25	2 (14%)	17,19,21	1.83	4 (23%)

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	F	301	2	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	B	301	2	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	D	301	2	1/1/5/7	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	NAG	C1-C2	4.21	1.58	1.52
4	D	301	NAG	C1-C2	3.28	1.57	1.52
4	F	301	NAG	C1-C2	2.55	1.56	1.52
4	D	301	NAG	C3-C2	2.31	1.57	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301	NAG	C4-C3-C2	4.41	117.48	111.02
4	B	301	NAG	C1-O5-C5	4.25	117.96	112.19
4	B	301	NAG	C1-C2-N2	4.18	117.64	110.49
4	F	301	NAG	C4-C3-C2	3.79	116.58	111.02
4	B	301	NAG	O5-C1-C2	3.72	117.17	111.29
4	F	301	NAG	O3-C3-C4	-3.47	102.33	110.35
4	B	301	NAG	O4-C4-C5	3.28	117.44	109.30
4	D	301	NAG	O3-C3-C4	-3.05	103.30	110.35
4	B	301	NAG	O6-C6-C5	-2.99	101.04	111.29
4	F	301	NAG	C6-C5-C4	2.80	119.57	113.00
4	B	301	NAG	O4-C4-C3	-2.76	103.96	110.35
4	F	301	NAG	O4-C4-C5	2.49	115.47	109.30
4	D	301	NAG	C1-C2-N2	2.48	114.72	110.49
4	B	301	NAG	C6-C5-C4	2.45	118.74	113.00
4	F	301	NAG	C2-N2-C7	-2.42	119.46	122.90
4	B	301	NAG	O5-C5-C6	-2.42	103.42	107.20
4	D	301	NAG	O4-C4-C3	-2.37	104.88	110.35
4	B	301	NAG	C3-C4-C5	-2.30	106.14	110.24
4	B	301	NAG	O3-C3-C4	-2.02	105.68	110.35
4	F	301	NAG	O5-C5-C4	-2.00	105.96	110.83

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	301	NAG	C1
4	B	301	NAG	C1
4	D	301	NAG	C1

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	NAG	O5-C5-C6-O6
4	D	301	NAG	C8-C7-N2-C2
4	B	301	NAG	C4-C5-C6-O6
4	D	301	NAG	O7-C7-N2-C2
4	F	301	NAG	C8-C7-N2-C2
4	F	301	NAG	O7-C7-N2-C2
4	F	301	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	NAG	2	0
4	D	301	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	329/332 (99%)	0.12	7 (2%) 63 66	36, 76, 115, 170	0
1	C	329/332 (99%)	0.09	12 (3%) 42 46	32, 70, 112, 153	0
1	E	329/332 (99%)	0.13	14 (4%) 35 38	42, 77, 116, 140	0
2	B	167/174 (95%)	-0.02	7 (4%) 36 39	28, 46, 103, 168	0
2	D	167/174 (95%)	-0.13	6 (3%) 42 46	29, 44, 92, 146	0
2	F	167/174 (95%)	-0.08	6 (3%) 42 46	33, 58, 103, 144	0
All	All	1488/1518 (98%)	0.05	52 (3%) 44 47	28, 67, 114, 170	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	187	GLY	5.7
2	F	60	ASN	5.6
2	D	60	ASN	5.3
2	B	58	LYS	4.7
1	A	257	SER	4.6
2	F	54	ARG	4.5
1	A	258	GLY	4.5
2	B	54	ARG	4.4
2	B	70	PHE	4.3
1	C	155	LEU	3.6
2	F	58	LYS	3.6
1	C	120	ILE	3.6
2	B	60	ASN	3.5
2	D	54	ARG	3.4
1	A	256	PRO	3.4
2	B	71	THR	3.3
2	D	58	LYS	3.3
2	F	38	TYR	3.2
2	D	52	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	56	ILE	3.2
1	C	262	ASN	3.1
1	E	231	GLY	3.0
1	E	256	PRO	2.9
1	C	186	TYR	2.9
1	A	41	VAL	2.9
1	A	259	ILE	2.9
1	E	162	THR	2.8
1	C	183	ASN	2.8
1	E	147	MET	2.7
2	B	72	GLU	2.6
1	E	116	ARG	2.6
2	B	69	GLU	2.6
1	E	272	ALA	2.5
1	C	118	SER	2.5
1	C	259	ILE	2.5
1	E	164	LYS	2.5
1	E	160	ARG	2.4
1	E	233	THR	2.4
1	E	91	ARG	2.4
1	C	11	ALA	2.4
1	A	201	GLN	2.4
1	A	116	ARG	2.3
1	E	204	PHE	2.3
1	C	240	GLY	2.2
1	E	131	ARG	2.2
2	F	143	ARG	2.2
1	E	93	THR	2.2
2	F	49	THR	2.2
1	C	151	VAL	2.1
1	C	256	PRO	2.0
1	E	224	HIS	2.0
2	D	55	LEU	2.0

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

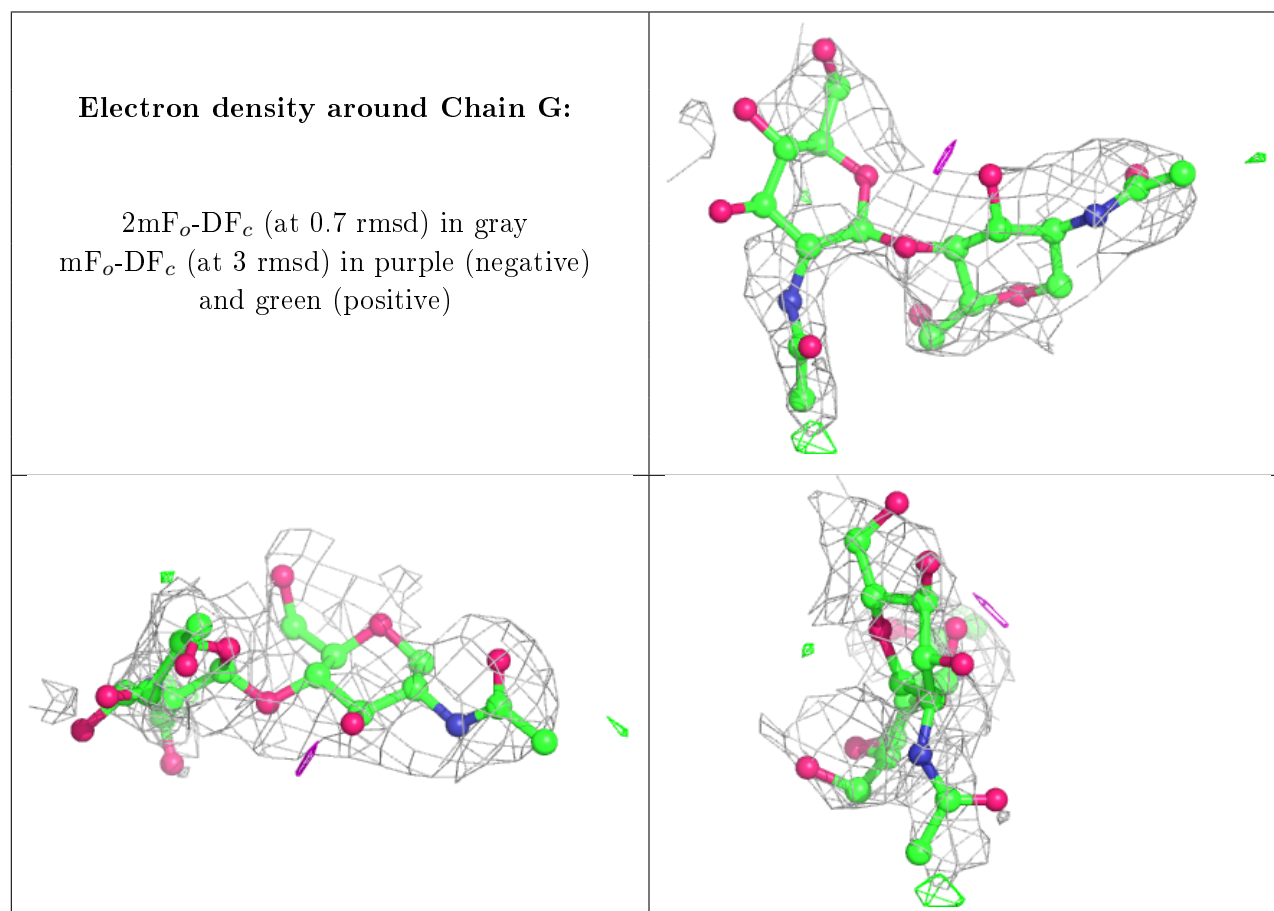
There are no non-standard protein/DNA/RNA residues in this entry.

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.

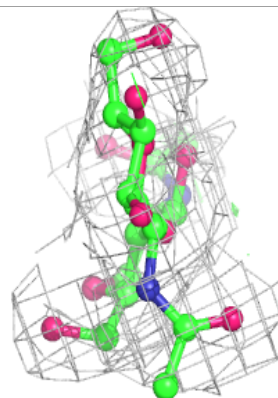
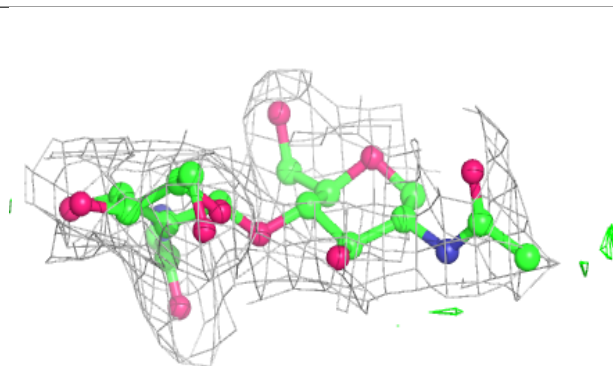
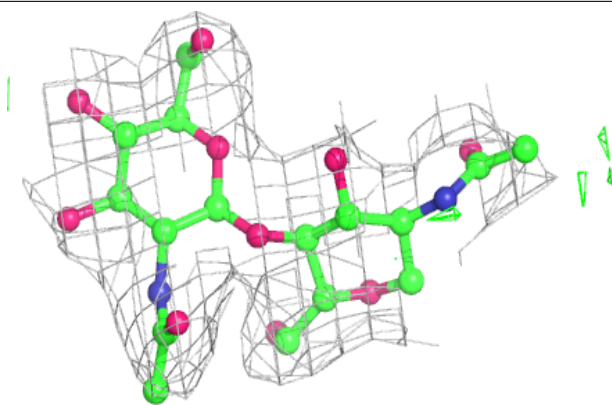
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	G	2	14/15	0.61	0.27	99,126,136,140	0
3	NAG	H	2	14/15	0.82	0.21	74,93,101,102	0
3	NAG	I	2	14/15	0.84	0.22	105,125,130,132	0
3	NAG	H	1	14/15	0.85	0.14	62,78,90,90	0
3	NAG	I	1	14/15	0.86	0.22	92,116,124,135	0
3	NAG	G	1	14/15	0.88	0.16	91,103,123,129	0

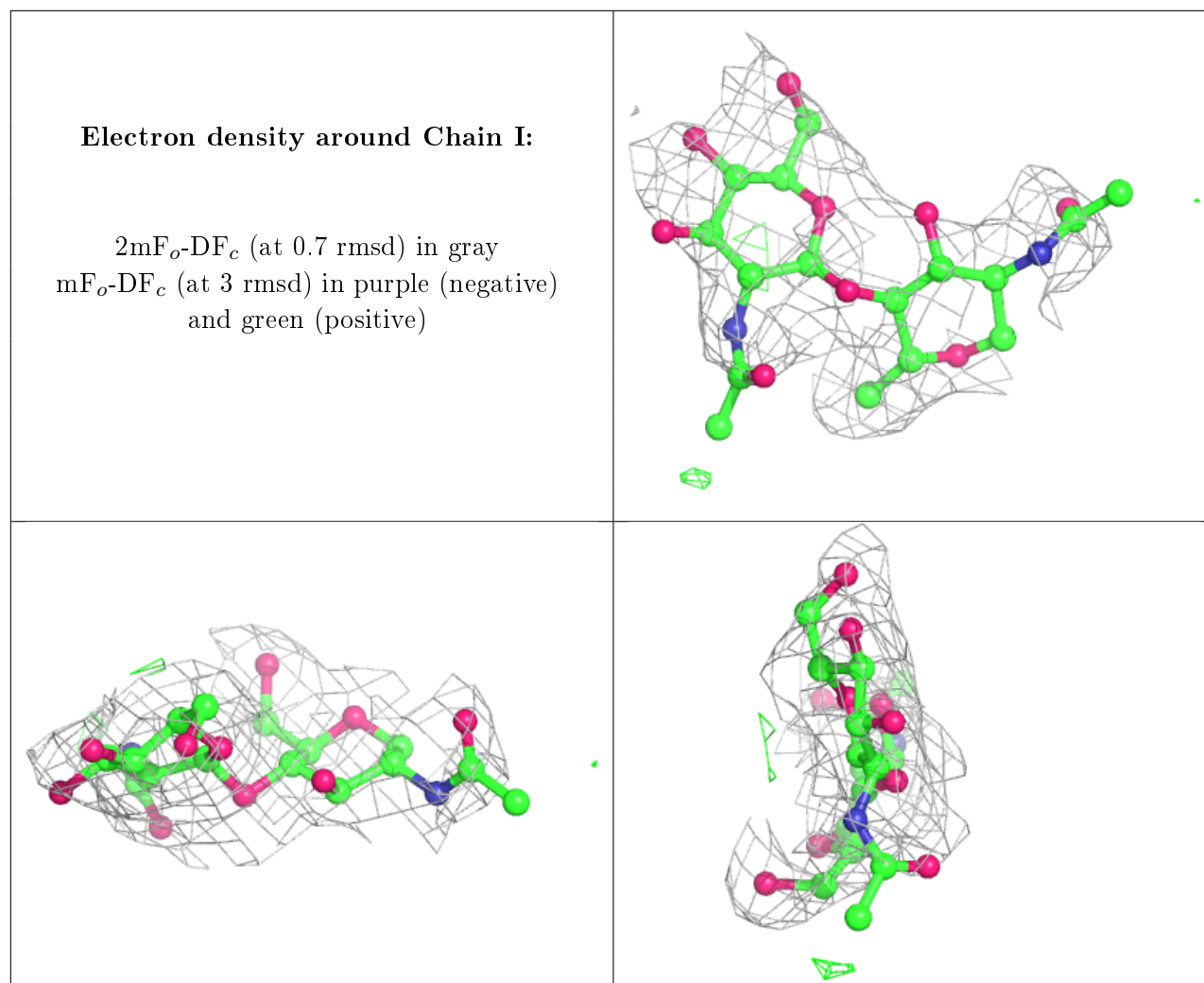
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain H:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	D	301	14/15	0.73	0.31	101,114,146,157	0
4	NAG	F	301	14/15	0.76	0.26	97,118,137,142	0
4	NAG	B	301	14/15	0.79	0.30	97,110,121,124	0

6.5 Other polymers ⓘ

There are no such residues in this entry.