



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:35 AM UTC

PDB ID : 3D12 / pdb_00003d12
Title : Crystal Structures of Nipah Virus G Attachment Glycoprotein in Complex with its Receptor Ephrin-B3
Authors : Xu, K.; Rajashankar, K.R.; Chan, Y.P.; Himanen, P.; Broder, C.C.; Nikolov, D.B.
Deposited on : 2008-05-02
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

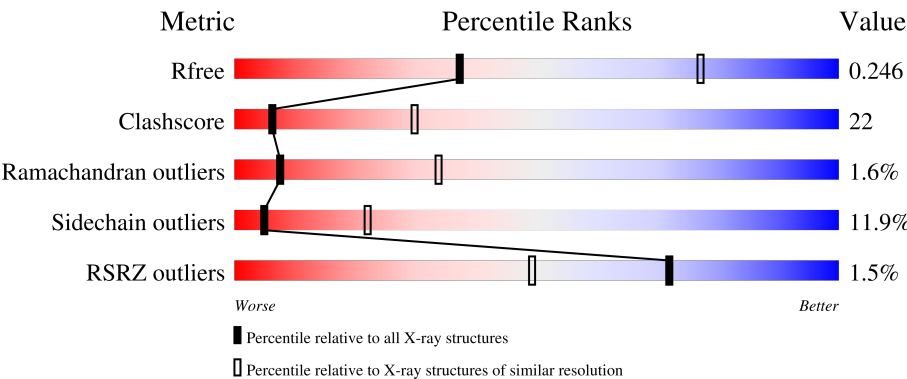
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	428	% 56% 37% 7%
1	D	428	2% 56% 36% 7%
2	B	141	2% 55% 40% 5%
2	E	141	% 50% 38% 11%
3	C	5	60% 40%

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Mol	Chain	Length	Quality of chain
4	F	7	
5	G	2	
5	J	2	
6	H	5	
7	I	7	

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	NGA	F	2	X	-	-	-
4	GL0	F	3	X	-	-	-
4	GLC	F	5	X	-	-	-
4	BGC	F	6	X	-	-	-
4	GLC	F	7	X	-	-	-
5	NAG	G	1	X	-	-	-
5	NAG	G	2	X	-	-	-
5	NAG	J	1	X	-	-	-
5	NAG	J	2	X	-	-	-
7	NGZ	I	2	X	-	-	-
7	GL0	I	3	X	-	-	-
7	GLC	I	5	X	-	-	-
7	BGC	I	6	X	-	-	-
7	GXL	I	7	X	-	-	-
8	NAG	D	1310	X	-	-	-
9	SO4	A	1368	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 9598 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-neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3370	2146	568	635	21			
1	D	428	Total	C	N	O	S	0	0	0
			3370	2146	568	635	21			

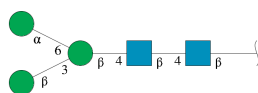
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	603	ALA	-	expression tag	UNP Q9IH62
D	603	ALA	-	expression tag	UNP Q9IH62

- Molecule 2 is a protein called Ephrin-B3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	141	Total	C	N	O	S	0	0	0
			1132	720	201	206	5			
2	E	141	Total	C	N	O	S	0	0	0
			1132	720	201	206	5			

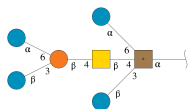
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

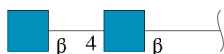
- Molecule 4 is an oligosaccharide called beta-D-glucopyranose-(1-3)-[alpha-D-glucopyranose-

(1-6)]beta-D-gulopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[beta-D-glucopyranose-(1-3)][alpha-D-glucopyranose-(1-6)]2-acetamido-2-deoxy-alpha-D-idopyranos e.



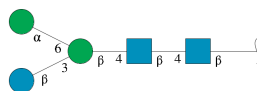
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



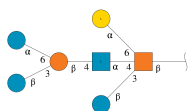
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



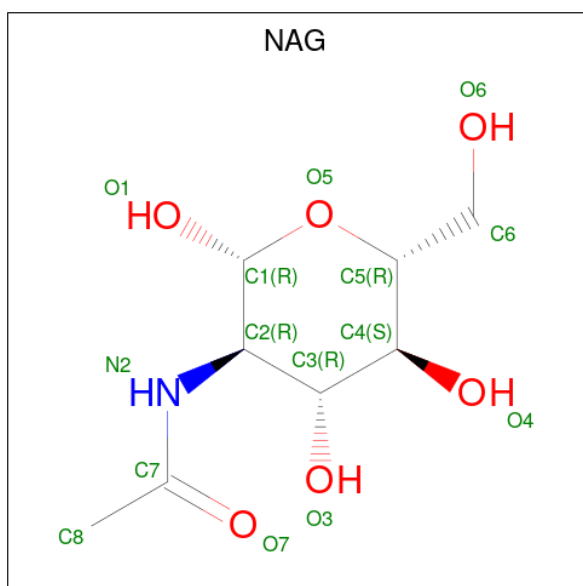
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is an oligosaccharide called beta-D-glucopyranose-(1-3)-[alpha-D-glucopyranose-(1-6)]beta-D-gulopyranose-(1-4)-2-acetamido-2-deoxy-alpha-L-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-3)][alpha-L-galactopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-gulopyranose.



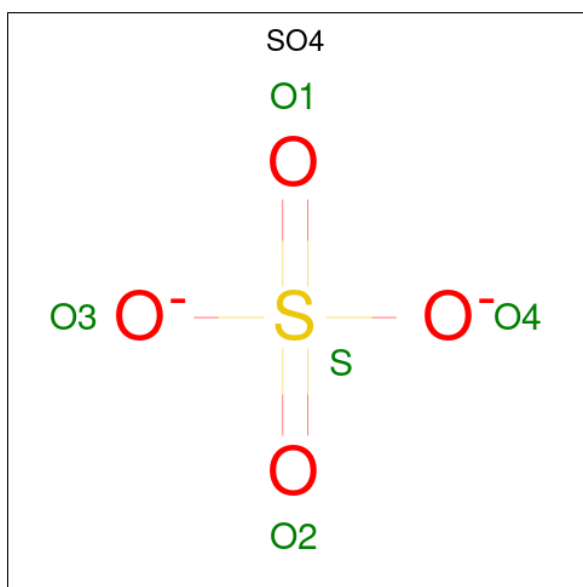
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	I	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		

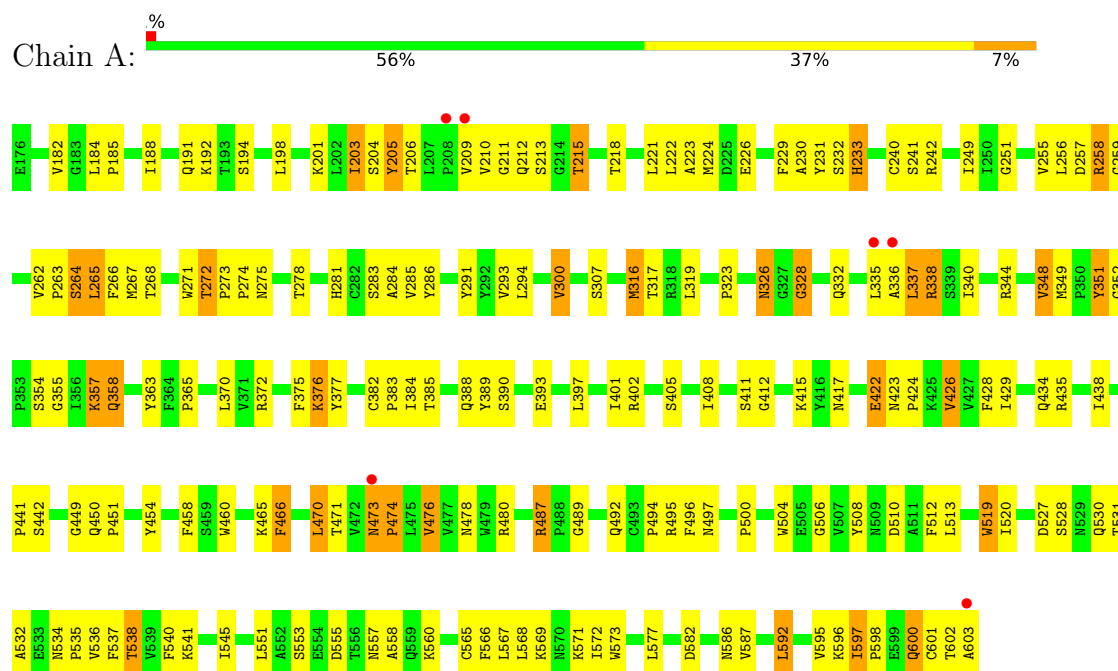
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	46	Total	O	0	0
			46	46		
10	B	9	Total	O	0	0
			9	9		
10	D	44	Total	O	0	0
			44	44		
10	E	13	Total	O	0	0
			13	13		

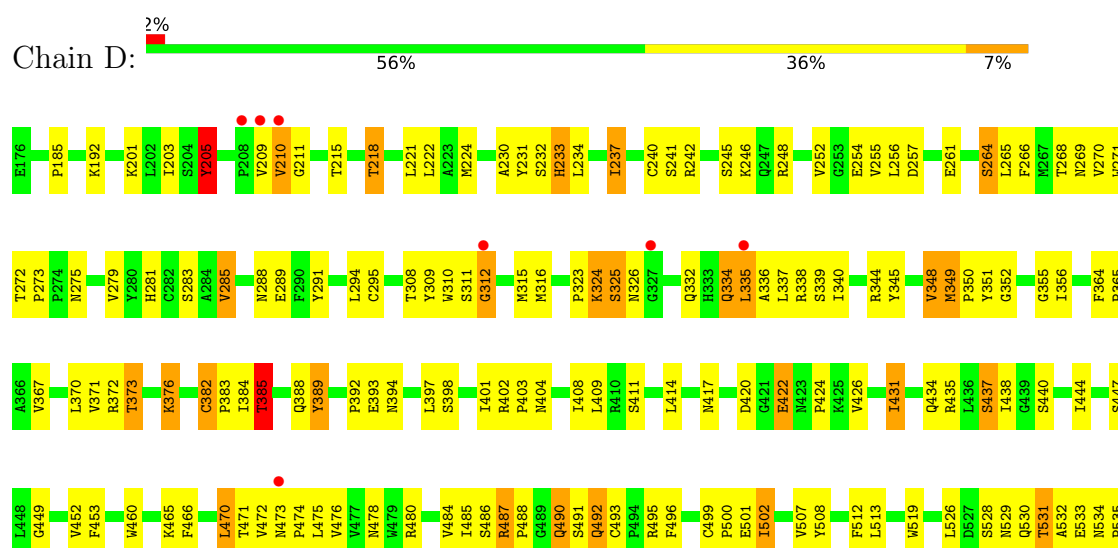
3 Residue-property plots

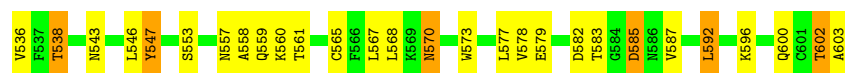
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Hemagglutinin-neuraminidase

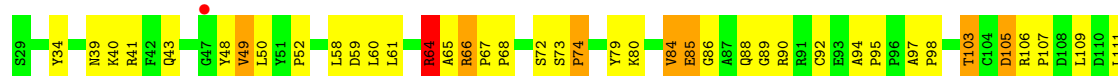




• Molecule 2: Ephrin-B3



• Molecule 2: Ephrin-B3



• Molecule 3: beta-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



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



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



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

Chain J:  100%

MAG1
MAG2

- Molecule 6: beta-D-glucopyranose-(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 H:  40% 60%

MAG1
MAG2
BMA3
BGC4
MAN5

- Molecule 7: beta-D-glucopyranose-(1-3)-[alpha-D-glucopyranose-(1-6)]beta-D-gulopyranose-(1-4)-2-acetamido-2-deoxy-alpha-L-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-3)][alpha-L-galactopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-gulopyranose

Chain I:  43% 57%

LXB1
NGZ2
GLO3
BGC4
GLC5
BGC6
GIL7

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	189.49Å 189.49Å 277.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.34 – 3.00 39.34 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.3 (39.34-3.00) 91.3 (39.34-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.221 , 0.265 0.207 , 0.246	Depositor DCC
R_{free} test set	2911 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9598	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NGA, NGZ, BGC, SO4, LXB, GLC, GL0, NAG, LXZ, GXL, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/3451	0.91	6/4694 (0.1%)
1	D	0.49	0/3451	0.89	11/4694 (0.2%)
2	B	0.40	0/1165	0.87	3/1582 (0.2%)
2	E	0.45	0/1165	0.86	1/1582 (0.1%)
All	All	0.48	0/9232	0.89	21/12552 (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
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	597	ILE	CA-C-N	8.84	129.37	119.83
1	A	597	ILE	C-N-CA	8.84	129.37	119.83
1	D	352	GLY	CA-C-N	8.17	127.46	118.97
1	D	352	GLY	C-N-CA	8.17	127.46	118.97
1	D	349	MET	N-CA-C	7.97	115.39	108.22
2	B	62	CYS	CA-C-N	6.59	126.95	119.83
2	B	62	CYS	C-N-CA	6.59	126.95	119.83
1	D	312	GLY	N-CA-C	-6.31	106.53	115.30
1	D	382	CYS	CA-C-N	6.25	127.66	119.84
1	D	382	CYS	C-N-CA	6.25	127.66	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	THR	CA-C-N	6.06	124.09	119.66
1	A	272	THR	C-N-CA	6.06	124.09	119.66
1	D	394	ASN	N-CA-C	6.01	117.50	111.07
1	D	218	THR	N-CA-C	5.58	115.77	108.07
2	E	85	GLU	N-CA-C	5.44	117.21	111.28
1	A	540	PHE	N-CA-C	5.30	116.89	108.79
2	B	41	ARG	N-CA-C	-5.13	106.13	112.38
1	D	275	ASN	CA-C-N	5.12	126.24	119.84
1	D	275	ASN	C-N-CA	5.12	126.24	119.84
1	D	385	THR	N-CA-C	5.12	118.99	112.34
1	A	354	SER	N-CA-C	5.01	116.67	108.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	473	ASN	Peptide
1	D	473	ASN	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	3370	0	3313	149	0
1	D	3370	0	3313	149	0
2	B	1132	0	1094	55	0
2	E	1132	0	1094	69	0
3	C	61	0	52	1	0
4	F	83	0	70	1	0
5	G	28	0	25	2	0
5	J	28	0	25	1	0
6	H	61	0	52	3	0
7	I	83	0	70	5	0
8	A	14	0	13	0	0
8	D	14	0	13	0	0
9	A	45	0	0	4	0
9	B	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	50	0	0	0	0
9	E	5	0	0	1	0
10	A	46	0	0	2	0
10	B	9	0	0	0	0
10	D	44	0	0	2	0
10	E	13	0	0	1	0
All	All	9598	0	9134	416	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (416) 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:A:376:LYS:HD3	1:A:376:LYS:H	1.26	0.97
1:D:403:PRO:HG3	1:D:502:ILE:HD11	1.44	0.97
1:A:376:LYS:HD3	1:A:376:LYS:N	1.81	0.94
1:D:531:THR:HG21	1:D:533:GLU:OE2	1.71	0.90
2:B:86:GLY:HA2	2:B:136:TYR:HD1	1.37	0.90
2:B:66:ARG:HB3	2:B:67:PRO:HD3	1.54	0.89
1:A:602:THR:HG23	1:A:603:ALA:H	1.40	0.87
2:E:118:GLN:HE22	2:E:120:TYR:HB2	1.40	0.86
2:B:118:GLN:NE2	2:B:120:TYR:HB2	1.89	0.86
1:D:294:LEU:HB2	1:D:316:MET:HE2	1.60	0.84
1:D:376:LYS:H	1:D:376:LYS:HD3	1.42	0.84
2:E:66:ARG:HB3	2:E:67:PRO:HD3	1.57	0.84
2:B:66:ARG:HB3	2:B:67:PRO:CD	2.07	0.83
1:D:376:LYS:HD3	1:D:376:LYS:N	1.93	0.83
2:B:86:GLY:HA2	2:B:136:TYR:CD1	2.14	0.82
2:E:113:PHE:CE2	2:E:115:ILE:HG12	2.14	0.82
1:A:210:VAL:HG12	1:A:211:GLY:H	1.43	0.82
2:B:118:GLN:HG2	2:B:119:GLU:N	1.96	0.81
1:D:471:THR:HG23	1:D:474:PRO:O	1.81	0.81
1:D:422:GLU:CD	1:D:422:GLU:H	1.88	0.81
1:D:376:LYS:H	1:D:376:LYS:CD	1.95	0.79
2:E:113:PHE:HE2	2:E:115:ILE:HG12	1.45	0.78
1:A:363:TYR:CE2	1:A:415:LYS:HG3	2.18	0.77
2:E:141:SER:O	2:E:155:VAL:HG23	1.85	0.77
1:A:557:ASN:HB3	2:B:118:GLN:NE2	1.99	0.76
2:E:118:GLN:NE2	2:E:120:TYR:HB2	1.99	0.76
1:D:402:ARG:HH12	1:D:404:ASN:HB2	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:ARG:HG2	2:B:130:ARG:HH11	1.51	0.75
6:H:3:BMA:H2	6:H:4:BGC:H2	1.69	0.74
2:B:39:ASN:OD1	2:B:41:ARG:HB2	1.86	0.74
2:E:118:GLN:HG2	2:E:119:GLU:H	1.50	0.74
1:A:535:PRO:HG3	1:A:558:ALA:HB2	1.68	0.74
1:D:585:ASP:HB3	10:D:1515:HOH:O	1.88	0.73
1:D:557:ASN:HB3	2:E:118:GLN:NE2	2.03	0.72
1:D:531:THR:CG2	1:D:533:GLU:HG2	2.20	0.72
2:E:66:ARG:O	2:E:68:PRO:HD3	1.89	0.72
1:D:384:ILE:HD11	1:D:392:PRO:HA	1.72	0.71
1:A:535:PRO:HG3	1:A:558:ALA:CB	2.21	0.71
2:B:66:ARG:O	2:B:68:PRO:HD3	1.91	0.70
2:B:64:ARG:HD2	2:B:67:PRO:HD2	1.73	0.70
2:E:39:ASN:O	2:E:40:LYS:HB3	1.91	0.70
2:E:118:GLN:HG2	2:E:119:GLU:N	2.03	0.70
1:D:403:PRO:CG	1:D:502:ILE:HD11	2.21	0.70
2:E:79:TYR:HE2	2:E:155:VAL:HG21	1.56	0.70
1:A:224:MET:HE3	1:A:255:VAL:HG21	1.72	0.69
2:E:66:ARG:HB3	2:E:67:PRO:CD	2.22	0.69
2:E:64:ARG:CD	2:E:67:PRO:HD2	2.23	0.69
2:B:73:SER:HB2	2:B:74:PRO:HD2	1.73	0.69
1:D:242:ARG:HD3	2:E:126:GLY:O	1.92	0.68
6:H:3:BMA:C2	6:H:4:BGC:H2	2.20	0.68
1:A:223:ALA:HB3	1:A:230:ALA:HB3	1.75	0.68
1:D:471:THR:HG22	1:D:476:VAL:CG1	2.23	0.68
1:A:471:THR:HG22	1:A:476:VAL:HG13	1.77	0.67
2:E:88:GLN:NE2	2:E:95:PRO:HG3	2.10	0.67
1:D:370:LEU:HB3	1:D:408:ILE:HD11	1.76	0.67
1:D:531:THR:HG22	1:D:533:GLU:HG2	1.77	0.67
1:A:256:LEU:HD12	1:A:266:PHE:CD2	2.30	0.67
1:D:536:VAL:HG12	1:D:538:THR:HG22	1.77	0.66
1:D:240:CYS:SG	2:E:119:GLU:HG2	2.36	0.66
2:E:155:VAL:HG12	2:E:159:ARG:HB2	1.77	0.66
2:E:49:VAL:HG13	2:E:164:LEU:HD23	1.78	0.66
2:E:89:GLY:HA3	2:E:136:TYR:CD1	2.31	0.66
1:A:471:THR:HG23	1:A:474:PRO:O	1.96	0.66
2:E:85:GLU:HB2	2:E:88:GLN:HG3	1.78	0.66
1:A:215:THR:HG22	1:A:587:VAL:HG23	1.78	0.65
1:A:557:ASN:HB3	2:B:118:GLN:HE21	1.61	0.65
1:D:558:ALA:HA	1:D:579:GLU:O	1.96	0.65
1:A:206:THR:HG21	1:A:264:SER:OG	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:84:VAL:HG13	2:E:88:GLN:HB2	1.78	0.65
1:A:226:GLU:OE1	1:A:286:TYR:HE2	1.80	0.65
1:D:471:THR:HG22	1:D:476:VAL:HG12	1.78	0.65
1:A:508:TYR:HB3	1:A:560:LYS:HD3	1.77	0.64
1:D:372:ARG:NH2	1:D:397:LEU:HA	2.12	0.64
1:D:281:HIS:CD2	1:D:349:MET:HE1	2.33	0.64
2:B:66:ARG:HB2	2:B:107:PRO:O	1.98	0.64
2:B:105:ASP:HB2	2:B:106:ARG:HE	1.63	0.64
1:D:508:TYR:HB3	1:D:560:LYS:HD3	1.80	0.64
1:D:557:ASN:HB3	2:E:118:GLN:HE21	1.63	0.64
1:A:388:GLN:O	1:A:389:TYR:HB2	1.99	0.63
1:A:212:GLN:H	1:A:212:GLN:CD	2.07	0.63
2:E:88:GLN:HE22	2:E:95:PRO:HG3	1.64	0.63
2:E:105:ASP:HB2	2:E:106:ARG:HE	1.64	0.63
1:D:398:SER:OG	1:D:502:ILE:HA	1.99	0.63
1:D:535:PRO:HG3	1:D:558:ALA:HB2	1.81	0.62
1:D:437:SER:HB2	1:D:465:LYS:NZ	2.14	0.62
2:B:64:ARG:HD3	2:B:108:ASP:O	2.00	0.62
2:E:65:ALA:HB2	2:E:72:SER:HB2	1.79	0.62
2:B:118:GLN:HE22	2:B:120:TYR:HB2	1.64	0.62
2:E:80:LYS:HE2	2:E:103:THR:HG23	1.81	0.62
1:A:344:ARG:NH2	1:A:376:LYS:HD2	2.15	0.61
2:B:104:CYS:HA	2:B:111:LEU:HD12	1.81	0.61
2:E:79:TYR:CE2	2:E:155:VAL:HG21	2.35	0.61
1:D:388:GLN:O	1:D:389:TYR:HB2	1.98	0.61
1:D:512:PHE:CD2	1:D:565:CYS:HB2	2.36	0.61
1:D:210:VAL:HG12	1:D:211:GLY:H	1.65	0.61
1:D:310:TRP:CZ3	1:D:312:GLY:HA2	2.36	0.61
1:A:240:CYS:SG	2:B:119:GLU:HG2	2.41	0.60
1:A:224:MET:HE1	1:A:566:PHE:CE2	2.36	0.60
7:I:1:LXB:O4	7:I:1:LXB:O6	2.19	0.59
1:A:351:TYR:CE2	1:A:441:PRO:HD3	2.37	0.59
1:A:402:ARG:HD2	9:A:1368:SO4:O2	2.03	0.59
1:D:471:THR:CG2	1:D:476:VAL:HG12	2.32	0.59
1:A:405:SER:HA	9:A:1368:SO4:O2	2.02	0.59
2:E:86:GLY:HA2	2:E:136:TYR:HD1	1.67	0.59
1:A:372:ARG:HH21	1:A:397:LEU:HA	1.67	0.59
1:A:495:ARG:O	1:A:496:PHE:HB2	2.03	0.59
1:A:489:GLY:O	1:A:530:GLN:HA	2.02	0.58
2:B:39:ASN:O	2:B:40:LYS:HB3	2.03	0.58
1:A:242:ARG:HE	2:B:128:GLU:HG2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:PHE:HB2	1:A:551:LEU:HD21	1.86	0.58
1:A:210:VAL:HG12	1:A:211:GLY:N	2.17	0.58
1:A:577:LEU:C	1:A:577:LEU:HD23	2.29	0.58
1:A:231:TYR:OH	1:A:233:HIS:HD2	1.87	0.58
1:D:492:GLN:HE21	1:D:492:GLN:CA	2.17	0.58
1:A:205:TYR:CE1	1:A:206:THR:HG23	2.39	0.57
1:D:490:GLN:OE1	2:E:123:ASN:HB2	2.04	0.57
1:D:577:LEU:HD12	1:D:592:LEU:HD11	1.86	0.57
2:E:50:LEU:C	2:E:52:PRO:HD3	2.30	0.57
1:A:352:GLY:HA3	1:A:442:SER:O	2.03	0.57
1:A:348:VAL:HG21	1:A:428:PHE:HB2	1.86	0.56
1:A:184:LEU:HD12	1:D:472:VAL:HG23	1.86	0.56
1:A:281:HIS:CD2	1:A:349:MET:HE1	2.41	0.56
1:A:528:SER:OG	1:A:531:THR:HG22	2.05	0.56
1:D:484:VAL:HG23	1:D:485:ILE:HG12	1.87	0.56
1:A:408:ILE:HD12	1:A:408:ILE:C	2.30	0.56
1:D:348:VAL:HG11	1:D:414:LEU:HD21	1.87	0.56
7:I:3:GL0:H4	7:I:4:BGC:O5	2.05	0.56
1:A:372:ARG:NH2	1:A:397:LEU:HA	2.20	0.56
1:A:553:SER:OG	10:A:48:HOH:O	2.18	0.56
1:D:295:CYS:HB2	1:D:315:MET:HE2	1.87	0.56
1:A:232:SER:HA	1:A:249:ILE:O	2.07	0.55
10:D:1511:HOH:O	7:I:1:LXB:H8	2.07	0.55
2:B:30:LEU:HD11	2:B:52:PRO:HB3	1.87	0.55
1:A:600:GLN:HB3	1:A:602:THR:HG22	1.89	0.55
1:A:233:HIS:ND1	1:A:233:HIS:C	2.65	0.54
5:J:2:NAG:H82	5:J:2:NAG:O3	2.07	0.54
1:A:257:ASP:C	1:A:259:GLY:H	2.16	0.54
2:E:34:TYR:CE2	2:E:61:LEU:HD12	2.42	0.54
1:D:271:TRP:CZ3	1:D:273:PRO:HG3	2.42	0.54
1:A:251:GLY:HA3	1:A:267:MET:HE1	1.89	0.54
1:D:370:LEU:HB3	1:D:408:ILE:CD1	2.37	0.54
1:A:221:LEU:C	1:A:221:LEU:HD23	2.33	0.54
1:A:417:ASN:O	1:A:424:PRO:HB3	2.08	0.54
1:A:536:VAL:O	1:A:538:THR:HG22	2.08	0.54
1:D:417:ASN:HB3	1:D:420:ASP:HB2	1.90	0.54
2:E:134:ASP:HB3	2:E:164:LEU:HD11	1.90	0.54
2:E:80:LYS:HG2	2:E:103:THR:HG23	1.90	0.54
1:A:294:LEU:HD13	1:A:316:MET:HE3	1.90	0.53
1:A:338:ARG:HH11	1:A:423:ASN:HB3	1.72	0.53
1:D:344:ARG:NH2	1:D:376:LYS:HD2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:SER:OG	1:A:365:PRO:HD2	2.08	0.53
1:D:231:TYR:OH	1:D:233:HIS:HD2	1.92	0.53
1:A:372:ARG:NH1	1:A:405:SER:OG	2.42	0.53
1:D:397:LEU:HB3	1:D:502:ILE:HD12	1.91	0.53
1:D:269:ASN:HD22	1:D:323:PRO:HG3	1.73	0.53
1:D:470:LEU:CD1	1:D:478:ASN:HB2	2.39	0.53
1:D:437:SER:HB2	1:D:465:LYS:HZ3	1.72	0.52
2:B:141:SER:O	2:B:155:VAL:HG23	2.08	0.52
1:D:264:SER:HB3	1:D:266:PHE:CE2	2.44	0.52
1:D:309:TYR:CD2	6:H:1:NAG:H5	2.44	0.52
2:E:64:ARG:HD3	2:E:67:PRO:HD2	1.89	0.52
1:A:450:GLN:HG3	1:A:451:PRO:HD2	1.90	0.52
1:A:340:ILE:HA	1:A:426:VAL:HG23	1.90	0.52
1:D:230:ALA:HA	1:D:252:VAL:HG12	1.92	0.52
1:A:258:ARG:HG2	1:A:262:VAL:O	2.10	0.52
2:B:84:VAL:HG13	2:B:88:GLN:HB2	1.90	0.52
2:B:130:ARG:HH11	2:B:130:ARG:CG	2.22	0.52
1:D:408:ILE:HD12	1:D:408:ILE:O	2.10	0.52
1:A:401:ILE:HG22	1:A:504:TRP:CE2	2.45	0.52
2:E:50:LEU:O	2:E:52:PRO:HD3	2.09	0.52
1:D:491:SER:HB3	2:E:113:PHE:HB2	1.91	0.52
1:D:561:THR:HG22	1:D:578:VAL:HG13	1.92	0.52
1:A:449:GLY:HA3	1:D:449:GLY:HA3	1.92	0.51
1:D:351:TYR:HB2	1:D:367:VAL:HG12	1.92	0.51
1:A:328:GLY:HA2	10:A:15:HOH:O	2.11	0.51
1:D:237:ILE:HD11	1:D:246:LYS:HB2	1.91	0.51
1:D:480:ARG:HD3	1:D:519:TRP:CH2	2.46	0.51
2:E:106:ARG:HG2	2:E:111:LEU:HD11	1.92	0.51
1:D:397:LEU:CB	1:D:502:ILE:HD12	2.40	0.51
1:A:188:ILE:HG21	1:A:572:ILE:HD12	1.93	0.51
1:D:348:VAL:CG1	1:D:414:LEU:HD21	2.41	0.51
2:E:123:ASN:ND2	2:E:125:TRP:H	2.08	0.51
1:D:531:THR:HG21	1:D:533:GLU:HG2	1.92	0.51
2:E:66:ARG:HB2	2:E:107:PRO:O	2.11	0.51
2:B:118:GLN:HG2	2:B:120:TYR:H	1.75	0.51
1:D:335:LEU:N	1:D:335:LEU:HD12	2.23	0.51
2:B:85:GLU:HB2	2:B:88:GLN:CD	2.36	0.51
2:B:118:GLN:HG2	2:B:119:GLU:H	1.72	0.51
2:B:155:VAL:HA	2:B:158:THR:HB	1.93	0.51
1:A:422:GLU:CD	1:A:422:GLU:H	2.20	0.50
1:D:422:GLU:O	1:D:424:PRO:HD3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:ARG:HH21	1:D:397:LEU:HA	1.76	0.50
1:D:431:ILE:HA	1:D:475:LEU:HD23	1.94	0.50
1:D:401:ILE:HG13	1:D:402:ARG:HG3	1.91	0.50
9:A:1371:SO4:O2	5:G:2:NAG:H5	2.11	0.50
1:D:408:ILE:HD12	1:D:408:ILE:C	2.37	0.50
1:A:264:SER:HB3	1:A:266:PHE:CE2	2.46	0.50
2:E:80:LYS:HE2	2:E:103:THR:CG2	2.41	0.50
4:F:2:NGA:H62	4:F:7:GLC:H2	1.94	0.50
1:A:388:GLN:O	1:A:389:TYR:CB	2.59	0.50
1:A:429:ILE:HD13	1:A:473:ASN:HA	1.93	0.50
1:D:221:LEU:C	1:D:221:LEU:HD23	2.37	0.50
1:D:496:PHE:HD2	7:I:1:LXB:H5	1.76	0.49
1:A:185:PRO:HB3	1:A:567:LEU:HD21	1.93	0.49
1:D:434:GLN:O	1:D:435:ARG:C	2.55	0.49
1:D:460:TRP:CB	1:D:501:GLU:H	2.26	0.49
1:D:559:GLN:HB3	1:D:579:GLU:OE1	2.12	0.49
2:E:138:ILE:HG22	2:E:162:LYS:HB3	1.93	0.49
2:B:65:ALA:HB2	2:B:72:SER:HB2	1.93	0.49
1:A:389:TYR:CG	2:B:106:ARG:HD2	2.48	0.49
1:A:423:ASN:N	1:A:424:PRO:HD3	2.28	0.49
2:B:155:VAL:HG11	2:B:161:MET:SD	2.52	0.49
1:D:340:ILE:HG12	1:D:426:VAL:CG2	2.43	0.49
2:E:138:ILE:HG22	2:E:162:LYS:CB	2.43	0.49
1:D:447:SER:HB3	1:D:513:LEU:HD23	1.95	0.49
1:A:422:GLU:C	1:A:424:PRO:HD3	2.38	0.49
1:A:376:LYS:H	1:A:376:LYS:CD	2.13	0.49
1:A:192:LYS:HD2	1:A:545:ILE:O	2.13	0.48
1:D:324:LYS:O	1:D:326:ASN:N	2.43	0.48
1:D:486:SER:HB3	1:D:495:ARG:HG3	1.94	0.48
1:D:531:THR:HG21	1:D:533:GLU:CD	2.38	0.48
1:A:602:THR:HG23	1:A:603:ALA:N	2.19	0.48
1:D:349:MET:HB2	1:D:350:PRO:HD2	1.95	0.48
2:B:32:PRO:HB3	2:B:61:LEU:HD11	1.95	0.48
1:D:285:VAL:HG13	1:D:364:PHE:CZ	2.48	0.48
3:C:3:BMA:H2	3:C:4:BMA:O2	2.13	0.48
1:A:218:THR:HG21	1:A:240:CYS:HB3	1.95	0.48
2:B:76:TYR:CD1	2:B:107:PRO:HA	2.49	0.48
2:B:104:CYS:HA	2:B:111:LEU:CD1	2.43	0.48
1:D:257:ASP:OD2	1:D:261:GLU:HA	2.13	0.48
1:D:257:ASP:OD2	1:D:568:LEU:HD21	2.14	0.48
2:E:86:GLY:HA2	2:E:136:TYR:CD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:VAL:HG21	1:A:428:PHE:CB	2.43	0.48
1:D:417:ASN:O	1:D:424:PRO:HB3	2.14	0.48
2:E:85:GLU:HA	2:E:85:GLU:OE1	2.14	0.48
1:A:212:GLN:O	1:A:215:THR:HB	2.13	0.48
1:A:600:GLN:HA	1:A:600:GLN:NE2	2.29	0.48
1:D:460:TRP:HB3	1:D:501:GLU:H	1.78	0.48
1:D:486:SER:HB3	1:D:495:ARG:CG	2.44	0.48
1:A:470:LEU:HD13	1:A:478:ASN:HB2	1.94	0.48
1:D:234:LEU:HD11	1:D:245:SER:HB3	1.96	0.47
1:A:340:ILE:HG12	1:A:426:VAL:HG21	1.96	0.47
1:A:510:ASP:C	1:A:510:ASP:OD1	2.56	0.47
1:D:224:MET:HE3	1:D:255:VAL:HG21	1.95	0.47
1:D:254:GLU:HG3	1:D:256:LEU:HD11	1.96	0.47
1:D:495:ARG:O	1:D:496:PHE:HB2	2.14	0.47
1:A:294:LEU:HB2	1:A:316:MET:HE2	1.97	0.47
1:D:492:GLN:NE2	1:D:492:GLN:HA	2.28	0.47
1:D:535:PRO:HG3	1:D:558:ALA:CB	2.44	0.47
1:A:460:TRP:CD2	1:A:500:PRO:HA	2.49	0.47
1:A:573:TRP:CZ2	1:A:596:LYS:HB2	2.49	0.47
1:A:597:ILE:HA	1:A:598:PRO:HD3	1.70	0.47
1:D:345:TYR:CD1	1:D:370:LEU:HB2	2.50	0.47
2:E:158:THR:HG22	2:E:159:ARG:HG3	1.97	0.47
1:A:376:LYS:N	1:A:376:LYS:CD	2.63	0.47
1:D:283:SER:OG	1:D:365:PRO:HD2	2.15	0.47
2:E:159:ARG:HB2	2:E:161:MET:HG3	1.96	0.47
1:D:491:SER:HA	1:D:530:GLN:NE2	2.30	0.47
1:D:547:TYR:N	1:D:547:TYR:CD2	2.83	0.47
1:D:480:ARG:HD3	1:D:519:TRP:CZ3	2.49	0.46
2:E:85:GLU:HB2	2:E:88:GLN:CG	2.45	0.46
2:E:84:VAL:HG13	2:E:85:GLU:N	2.30	0.46
1:A:471:THR:CG2	1:A:476:VAL:HG13	2.45	0.46
1:D:488:PRO:HA	1:D:529:ASN:O	2.15	0.46
2:E:92:CYS:O	2:E:153:GLY:N	2.47	0.46
1:A:203:ILE:HG12	1:A:592:LEU:HB3	1.97	0.46
1:A:348:VAL:HG21	1:A:428:PHE:CG	2.51	0.46
2:B:64:ARG:CD	2:B:67:PRO:HD2	2.43	0.46
1:D:532:ALA:HB1	1:D:558:ALA:O	2.15	0.46
1:D:334:GLN:HE21	1:D:334:GLN:HB3	1.52	0.46
1:A:229:PHE:CD2	1:A:265:LEU:HD13	2.51	0.46
1:D:388:GLN:O	1:D:389:TYR:CB	2.64	0.46
1:D:585:ASP:OD1	1:D:585:ASP:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:90:ARG:C	2:E:92:CYS:H	2.23	0.46
1:A:268:THR:O	1:A:323:PRO:HG2	2.17	0.45
1:A:274:PRO:HG2	1:A:275:ASN:H	1.81	0.45
1:A:454:TYR:CE1	1:A:510:ASP:HA	2.51	0.45
1:D:492:GLN:CA	1:D:492:GLN:NE2	2.79	0.45
1:D:248:ARG:O	1:D:272:THR:HG22	2.16	0.45
1:D:470:LEU:HD11	1:D:478:ASN:HB2	1.99	0.45
1:A:275:ASN:ND2	1:A:278:THR:HG23	2.31	0.45
1:A:532:ALA:HB1	1:A:558:ALA:O	2.16	0.45
2:B:56:ASP:O	2:B:117:PHE:HD1	2.00	0.45
1:A:294:LEU:HB2	1:A:316:MET:CE	2.47	0.45
1:D:192:LYS:HA	1:D:546:LEU:HA	1.98	0.45
1:D:460:TRP:CG	1:D:500:PRO:HA	2.52	0.45
1:A:351:TYR:CZ	1:A:441:PRO:HD3	2.52	0.45
1:A:494:PRO:HD2	1:A:497:ASN:HB2	1.98	0.45
1:A:513:LEU:HD12	1:A:520:ILE:O	2.17	0.45
2:B:140:THR:HA	2:B:154:GLY:H	1.82	0.45
1:D:222:LEU:HD12	1:D:230:ALA:O	2.17	0.45
1:A:213:SER:OG	1:A:586:ASN:HB3	2.17	0.44
1:A:527:ASP:HB3	1:A:534:ASN:ND2	2.32	0.44
2:B:130:ARG:CG	2:B:130:ARG:NH1	2.80	0.44
1:D:355:GLY:HA2	1:D:444:ILE:HG23	1.99	0.44
1:D:496:PHE:CD2	7:I:1:LXB:H5	2.50	0.44
1:A:231:TYR:OH	1:A:233:HIS:CD2	2.68	0.44
2:B:82:TYR:CD2	2:B:98:PRO:HB2	2.52	0.44
1:D:370:LEU:HD23	1:D:408:ILE:HD11	1.99	0.44
1:D:460:TRP:CD2	1:D:500:PRO:HA	2.53	0.44
2:B:90:ARG:HD2	9:B:203:SO4:O4	2.18	0.44
1:D:487:ARG:NH2	1:D:493:CYS:O	2.44	0.44
1:A:592:LEU:HD12	1:A:592:LEU:HA	1.89	0.44
1:D:600:GLN:HA	1:D:600:GLN:NE2	2.32	0.44
1:A:412:GLY:HA3	1:A:429:ILE:O	2.17	0.44
1:A:569:LYS:O	1:A:571:LYS:HG3	2.18	0.44
1:A:271:TRP:CZ3	1:A:273:PRO:HG3	2.53	0.44
1:D:499:CYS:HA	1:D:500:PRO:HD3	1.91	0.44
2:E:159:ARG:HD2	2:E:161:MET:HE3	2.00	0.44
1:D:294:LEU:HD13	1:D:316:MET:CE	2.48	0.44
1:A:335:LEU:HG	1:A:337:LEU:H	1.82	0.44
2:B:63:PRO:O	2:B:64:ARG:C	2.60	0.44
2:B:83:LEU:HB2	2:B:101:LEU:HD11	2.00	0.44
2:E:66:ARG:CB	2:E:67:PRO:HD3	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:PHE:O	1:A:504:TRP:HA	2.18	0.44
2:E:158:THR:HG21	9:E:190:SO4:O3	2.18	0.44
1:D:409:LEU:HD12	1:D:438:ILE:HD11	1.99	0.43
1:D:528:SER:OG	1:D:531:THR:HB	2.17	0.43
1:A:375:PHE:CE2	1:A:377:TYR:HB2	2.53	0.43
1:A:401:ILE:HG13	1:A:402:ARG:HG3	2.00	0.43
1:A:191:GLN:HB2	1:A:601:CYS:SG	2.57	0.43
2:E:94:ALA:HA	2:E:95:PRO:HD3	1.85	0.43
1:A:229:PHE:CG	1:A:265:LEU:HD13	2.53	0.43
2:B:49:VAL:HG22	2:B:164:LEU:HB3	2.00	0.43
1:D:310:TRP:CE3	1:D:312:GLY:HA2	2.53	0.43
2:E:169:GLN:HG2	10:E:200:HOH:O	2.18	0.43
1:A:338:ARG:NH1	1:A:423:ASN:HB3	2.33	0.43
1:D:376:LYS:H	1:D:376:LYS:CE	2.31	0.43
2:E:105:ASP:HB2	2:E:106:ARG:NE	2.32	0.43
1:A:336:ALA:O	1:A:337:LEU:HB2	2.18	0.43
1:D:233:HIS:ND1	1:D:233:HIS:C	2.77	0.43
1:D:315:MET:HG2	1:D:316:MET:N	2.31	0.43
1:D:573:TRP:CZ2	1:D:596:LYS:HB2	2.54	0.43
1:A:205:TYR:N	1:A:205:TYR:CD1	2.86	0.43
1:A:319:LEU:HD22	1:A:332:GLN:HG2	2.01	0.43
1:D:470:LEU:HD13	1:D:478:ASN:HB2	2.01	0.43
1:D:255:VAL:HG22	1:D:265:LEU:HD22	2.01	0.43
1:D:271:TRP:CZ2	1:D:334:GLN:OE1	2.72	0.42
1:D:602:THR:OG1	1:D:603:ALA:N	2.51	0.42
1:A:358:GLN:HG3	1:D:570:ASN:ND2	2.34	0.42
2:B:66:ARG:CB	2:B:67:PRO:CD	2.91	0.42
1:D:420:ASP:HB3	1:D:424:PRO:HB3	2.01	0.42
1:A:326:ASN:HD22	1:A:326:ASN:HA	1.65	0.42
2:B:58:LEU:O	2:B:114:THR:HA	2.19	0.42
1:A:294:LEU:HD13	1:A:316:MET:CE	2.48	0.42
1:A:382:CYS:HA	1:A:383:PRO:HD3	1.78	0.42
1:A:466:PHE:CZ	1:A:519:TRP:HZ3	2.38	0.42
1:D:336:ALA:HB3	1:D:338:ARG:CZ	2.49	0.42
1:A:471:THR:HG22	1:A:476:VAL:CG1	2.47	0.42
1:A:370:LEU:HB3	1:A:408:ILE:HD11	2.01	0.42
1:A:434:GLN:HE21	1:A:434:GLN:HB3	1.65	0.42
2:B:76:TYR:CE1	2:B:107:PRO:HA	2.54	0.42
2:B:159:ARG:HD2	2:B:161:MET:HE3	2.01	0.42
1:D:185:PRO:HB3	1:D:567:LEU:HD21	2.01	0.42
1:D:384:ILE:O	1:D:384:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ALA:O	1:A:229:PHE:HA	2.20	0.42
2:E:60:LEU:O	2:E:112:ARG:HA	2.19	0.42
1:A:402:ARG:NH1	9:A:1368:SO4:O1	2.53	0.42
1:A:512:PHE:CD2	1:A:565:CYS:HB2	2.54	0.42
2:B:42:PHE:C	2:B:44:ALA:H	2.27	0.42
2:B:142:ASP:OD1	2:B:144:THR:HG23	2.20	0.42
2:E:146:GLU:H	2:E:146:GLU:CD	2.27	0.42
1:A:555:ASP:HB3	2:B:57:ARG:HH22	1.85	0.42
1:A:435:ARG:HG2	1:A:465:LYS:HE3	2.02	0.41
1:A:508:TYR:CZ	1:A:510:ASP:HB3	2.55	0.41
1:D:452:VAL:HG12	1:D:453:PHE:N	2.35	0.41
2:E:64:ARG:HD2	2:E:67:PRO:HD2	1.99	0.41
1:D:268:THR:O	1:D:323:PRO:HG2	2.20	0.41
1:A:384:ILE:HG13	1:A:390:SER:HB3	2.02	0.41
1:A:600:GLN:HA	1:A:600:GLN:HE21	1.85	0.41
1:D:248:ARG:HB3	1:D:273:PRO:HD2	2.01	0.41
1:A:198:LEU:HD22	1:A:595:VAL:HG11	2.01	0.41
1:A:465:LYS:HB3	1:A:465:LYS:HE2	1.85	0.41
1:A:470:LEU:CD1	1:A:478:ASN:HB2	2.51	0.41
1:A:335:LEU:HD23	1:A:337:LEU:HD22	2.03	0.41
1:D:508:TYR:CD2	1:D:508:TYR:C	2.99	0.41
2:E:97:ALA:N	2:E:98:PRO:HD3	2.36	0.41
2:E:152:GLN:O	2:E:153:GLY:C	2.63	0.41
1:A:265:LEU:N	1:A:265:LEU:HD23	2.34	0.41
1:A:284:ALA:HB2	1:A:293:VAL:HG22	2.01	0.41
1:D:288:ASN:O	1:D:289:GLU:HB2	2.20	0.41
1:D:422:GLU:C	1:D:424:PRO:HD3	2.45	0.41
1:A:286:TYR:O	1:A:357:LYS:HG2	2.21	0.41
1:A:300:VAL:O	1:A:300:VAL:HG23	2.21	0.41
1:A:355:GLY:HA3	1:A:363:TYR:O	2.21	0.41
1:D:224:MET:CE	1:D:255:VAL:HG21	2.51	0.41
2:E:50:LEU:HD12	2:E:163:VAL:HG11	2.03	0.41
1:A:221:LEU:HD23	1:A:222:LEU:N	2.36	0.41
1:A:263:PRO:HD3	1:A:568:LEU:HD23	2.03	0.41
1:A:316:MET:HG3	1:A:317:THR:N	2.35	0.41
1:A:434:GLN:O	1:A:435:ARG:C	2.64	0.41
1:A:487:ARG:HH11	1:A:506:GLY:HA3	1.85	0.41
1:D:218:THR:HG21	1:D:240:CYS:HB3	2.03	0.41
1:D:512:PHE:CE2	1:D:565:CYS:HB2	2.55	0.41
1:D:526:LEU:HA	1:D:534:ASN:O	2.21	0.41
2:E:43:GLN:OE1	2:E:159:ARG:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:73:SER:HB2	2:E:74:PRO:HD2	2.02	0.41
2:E:155:VAL:HG11	2:E:161:MET:SD	2.60	0.41
1:D:221:LEU:HB3	1:D:232:SER:HB3	2.03	0.41
2:E:59:ASP:HA	2:E:113:PHE:O	2.21	0.41
2:E:121:SER:HA	2:E:122:PRO:HD3	1.94	0.41
1:A:438:ILE:HD13	1:A:504:TRP:CD1	2.56	0.40
1:D:371:VAL:HG12	1:D:373:THR:HG23	2.02	0.40
1:A:454:TYR:CZ	1:A:510:ASP:HA	2.56	0.40
1:D:339:SER:C	1:D:340:ILE:HG13	2.45	0.40
2:B:130:ARG:HG2	2:B:130:ARG:NH1	2.26	0.40
1:D:203:ILE:HA	1:D:205:TYR:CE1	2.56	0.40
1:D:382:CYS:HA	1:D:383:PRO:HD3	1.70	0.40
1:D:508:TYR:O	1:D:508:TYR:HD2	2.04	0.40
2:B:84:VAL:CG1	2:B:88:GLN:HB2	2.50	0.40
1:A:221:LEU:HB3	1:A:232:SER:HB3	2.03	0.40
1:A:480:ARG:HA	5:G:1:NAG:H82	2.04	0.40
2:B:134:ASP:HB3	2:B:164:LEU:HD11	2.03	0.40
2:B:155:VAL:HG12	2:B:161:MET:HB2	2.02	0.40
1:D:269:ASN:ND2	1:D:323:PRO:HG3	2.36	0.40
2:E:134:ASP:OD1	2:E:166:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	426/428 (100%)	382 (90%)	40 (9%)	4 (1%)	14	48
1	D	426/428 (100%)	372 (87%)	50 (12%)	4 (1%)	14	48
2	B	139/141 (99%)	120 (86%)	13 (9%)	6 (4%)	2	12
2	E	139/141 (99%)	118 (85%)	17 (12%)	4 (3%)	3	20
All	All	1130/1138 (99%)	992 (88%)	120 (11%)	18 (2%)	7	34

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	64	ARG
2	E	64	ARG
1	A	338	ARG
2	B	45	GLU
2	B	153	GLY
2	B	158	THR
1	D	205	TYR
1	D	325	SER
2	E	153	GLY
1	A	258	ARG
2	B	66	ARG
1	A	474	PRO
1	D	385	THR
1	D	389	TYR
2	B	85	GLU
2	E	168	GLY
1	A	328	GLY
2	E	74	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/382 (100%)	341 (89%)	41 (11%)	6	26
1	D	382/382 (100%)	331 (87%)	51 (13%)	4	18
2	B	121/121 (100%)	113 (93%)	8 (7%)	15	46
2	E	121/121 (100%)	101 (84%)	20 (16%)	2	12
All	All	1006/1006 (100%)	886 (88%)	120 (12%)	5	22

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	VAL
1	A	194	SER

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Mol	Chain	Res	Type
1	A	201	LYS
1	A	203	ILE
1	A	204	SER
1	A	205	TYR
1	A	209	VAL
1	A	215	THR
1	A	233	HIS
1	A	241	SER
1	A	264	SER
1	A	265	LEU
1	A	272	THR
1	A	285	VAL
1	A	291	TYR
1	A	300	VAL
1	A	307	SER
1	A	316	MET
1	A	326	ASN
1	A	337	LEU
1	A	348	VAL
1	A	351	TYR
1	A	357	LYS
1	A	358	GLN
1	A	376	LYS
1	A	385	THR
1	A	393	GLU
1	A	411	SER
1	A	422	GLU
1	A	426	VAL
1	A	466	PHE
1	A	470	LEU
1	A	476	VAL
1	A	487	ARG
1	A	492	GLN
1	A	519	TRP
1	A	538	THR
1	A	541	LYS
1	A	582	ASP
1	A	592	LEU
1	A	600	GLN
2	B	41	ARG
2	B	58	LEU
2	B	109	LEU

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Mol	Chain	Res	Type
2	B	112	ARG
2	B	119	GLU
2	B	121	SER
2	B	130	ARG
2	B	167	VAL
1	D	201	LYS
1	D	205	TYR
1	D	209	VAL
1	D	210	VAL
1	D	215	THR
1	D	233	HIS
1	D	237	ILE
1	D	241	SER
1	D	264	SER
1	D	270	VAL
1	D	279	VAL
1	D	285	VAL
1	D	291	TYR
1	D	308	THR
1	D	311	SER
1	D	324	LYS
1	D	325	SER
1	D	332	GLN
1	D	334	GLN
1	D	335	LEU
1	D	337	LEU
1	D	348	VAL
1	D	356	ILE
1	D	373	THR
1	D	376	LYS
1	D	385	THR
1	D	393	GLU
1	D	411	SER
1	D	422	GLU
1	D	431	ILE
1	D	437	SER
1	D	440	SER
1	D	466	PHE
1	D	470	LEU
1	D	487	ARG
1	D	490	GLN
1	D	492	GLN

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Mol	Chain	Res	Type
1	D	502	ILE
1	D	507	VAL
1	D	531	THR
1	D	538	THR
1	D	543	ASN
1	D	547	TYR
1	D	553	SER
1	D	570	ASN
1	D	582	ASP
1	D	583	THR
1	D	585	ASP
1	D	587	VAL
1	D	592	LEU
1	D	602	THR
2	E	41	ARG
2	E	48	TYR
2	E	49	VAL
2	E	58	LEU
2	E	64	ARG
2	E	66	ARG
2	E	84	VAL
2	E	103	THR
2	E	105	ASP
2	E	109	LEU
2	E	112	ARG
2	E	115	ILE
2	E	119	GLU
2	E	121	SER
2	E	123	ASN
2	E	128	GLU
2	E	145	ARG
2	E	146	GLU
2	E	155	VAL
2	E	158	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
1	A	277	ASN
1	A	326	ASN
1	A	332	GLN

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Mol	Chain	Res	Type
1	A	334	GLN
1	A	358	GLN
1	A	394	ASN
1	A	434	GLN
1	A	473	ASN
1	A	497	ASN
1	A	518	ASN
1	A	534	ASN
1	A	570	ASN
2	B	118	GLN
2	B	127	HIS
2	B	169	GLN
1	D	233	HIS
1	D	269	ASN
1	D	326	ASN
1	D	332	GLN
1	D	334	GLN
1	D	358	GLN
1	D	423	ASN
1	D	434	GLN
1	D	473	ASN
1	D	492	GLN
1	D	518	ASN
1	D	570	ASN
1	D	600	GLN
2	E	118	GLN
2	E	123	ASN
2	E	132	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 ⓘ

28 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	C	1	1,3	14,14,15	1.95	4 (28%)	17,19,21	2.03	5 (29%)
3	NAG	C	2	3	14,14,15	2.64	6 (42%)	17,19,21	1.44	4 (23%)
3	BMA	C	3	3	11,11,12	2.00	4 (36%)	15,15,17	1.54	2 (13%)
3	BMA	C	4	3	11,11,12	1.59	3 (27%)	15,15,17	1.72	4 (26%)
3	MAN	C	5	3	11,11,12	1.61	3 (27%)	15,15,17	1.47	2 (13%)
4	LXZ	F	1	1,4	14,14,15	2.40	4 (28%)	17,19,21	1.85	5 (29%)
4	NGA	F	2	4	14,14,15	2.39	6 (42%)	17,19,21	2.40	6 (35%)
4	GL0	F	3	4	11,11,12	2.37	4 (36%)	15,15,17	1.98	5 (33%)
4	BGC	F	4	4	11,11,12	1.63	3 (27%)	15,15,17	1.29	2 (13%)
4	GLC	F	5	4	11,11,12	1.61	4 (36%)	15,15,17	1.17	1 (6%)
4	BGC	F	6	4	11,11,12	1.29	2 (18%)	15,15,17	1.98	4 (26%)
4	GLC	F	7	4	11,11,12	1.52	3 (27%)	15,15,17	1.56	3 (20%)
5	NAG	G	1	1,5	14,14,15	2.01	5 (35%)	17,19,21	2.10	4 (23%)
5	NAG	G	2	5	14,14,15	2.31	4 (28%)	17,19,21	1.69	5 (29%)
6	NAG	H	1	6,1	14,14,15	2.06	6 (42%)	17,19,21	1.39	2 (11%)
6	NAG	H	2	6	14,14,15	2.55	8 (57%)	17,19,21	1.70	5 (29%)
6	BMA	H	3	6	11,11,12	2.15	5 (45%)	15,15,17	1.42	4 (26%)
6	BGC	H	4	6	11,11,12	1.82	4 (36%)	15,15,17	2.30	6 (40%)
6	MAN	H	5	6	11,11,12	1.76	4 (36%)	15,15,17	1.05	1 (6%)
7	LXB	I	1	1,7	14,14,15	2.40	4 (28%)	17,19,21	1.60	4 (23%)
7	NGZ	I	2	7	14,14,15	2.51	7 (50%)	17,19,21	1.87	5 (29%)
7	GL0	I	3	7	11,11,12	2.36	4 (36%)	15,15,17	2.32	5 (33%)
7	BGC	I	4	7	11,11,12	1.55	3 (27%)	15,15,17	1.15	2 (13%)
7	GLC	I	5	7	11,11,12	1.55	2 (18%)	15,15,17	1.32	1 (6%)
7	BGC	I	6	7	11,11,12	1.26	1 (9%)	15,15,17	1.96	4 (26%)
7	GXL	I	7	7	11,11,12	1.51	4 (36%)	15,15,17	1.12	0
5	NAG	J	1	1,5	14,14,15	2.04	4 (28%)	17,19,21	1.85	5 (29%)
5	NAG	J	2	5	14,14,15	2.40	4 (28%)	17,19,21	1.66	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	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	BMA	C	4	3	-	2/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
4	LXZ	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NGA	F	2	4	5/5/5/7	2/6/23/26	0/1/1/1
4	GL0	F	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	BGC	F	4	4	-	2/2/19/22	0/1/1/1
4	GLC	F	5	4	5/5/4/5	2/2/19/22	0/1/1/1
4	BGC	F	6	4	1/1/4/5	0/2/19/22	0/1/1/1
4	GLC	F	7	4	5/5/4/5	2/2/19/22	0/1/1/1
5	NAG	G	1	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	G	2	5	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	H	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	1/6/23/26	0/1/1/1
6	BMA	H	3	6	-	2/2/19/22	0/1/1/1
6	BGC	H	4	6	-	1/2/19/22	0/1/1/1
6	MAN	H	5	6	-	1/2/19/22	1/1/1/1
7	LXB	I	1	1,7	-	3/6/23/26	0/1/1/1
7	NGZ	I	2	7	1/1/5/7	0/6/23/26	0/1/1/1
7	GL0	I	3	7	1/1/4/5	0/2/19/22	0/1/1/1
7	BGC	I	4	7	-	0/2/19/22	0/1/1/1
7	GLC	I	5	7	5/5/4/5	2/2/19/22	0/1/1/1
7	BGC	I	6	7	1/1/4/5	2/2/19/22	0/1/1/1
7	GXL	I	7	7	1/1/4/5	2/2/19/22	0/1/1/1
5	NAG	J	1	1,5	2/2/5/7	5/6/23/26	0/1/1/1
5	NAG	J	2	5	1/1/5/7	2/6/23/26	0/1/1/1

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C1-C2	5.73	1.60	1.52
7	I	2	NGZ	C1-C2	5.66	1.60	1.52
5	J	2	NAG	C1-C2	5.37	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	2	NAG	C1-C2	5.11	1.59	1.52
6	H	2	NAG	C1-C2	5.01	1.59	1.52
7	I	1	LXB	C7-N2	4.85	1.50	1.34
3	C	2	NAG	C7-N2	4.83	1.49	1.34
4	F	1	LXZ	C7-N2	4.82	1.49	1.34
4	F	2	NGA	C1-C2	4.78	1.58	1.52
7	I	1	LXB	C4-C5	4.69	1.63	1.53
6	H	2	NAG	C7-N2	4.66	1.49	1.34
5	G	1	NAG	C7-N2	4.64	1.49	1.34
4	F	1	LXZ	C4-C5	4.62	1.62	1.53
5	J	1	NAG	C7-N2	4.51	1.48	1.34
7	I	3	GL0	O5-C1	4.41	1.51	1.43
5	J	2	NAG	C7-N2	4.39	1.48	1.34
4	F	3	GL0	O5-C1	4.35	1.51	1.43
4	F	2	NGA	C7-N2	4.27	1.48	1.34
5	G	2	NAG	C7-N2	4.14	1.47	1.34
6	H	1	NAG	C7-N2	4.09	1.47	1.34
7	I	2	NGZ	C7-N2	4.07	1.47	1.34
3	C	1	NAG	C7-N2	3.93	1.47	1.34
4	F	1	LXZ	C4-C3	3.88	1.62	1.52
7	I	1	LXB	C4-C3	3.76	1.62	1.52
7	I	3	GL0	C1-C2	3.75	1.61	1.52
6	H	3	BMA	O5-C5	3.75	1.50	1.43
4	F	3	GL0	C1-C2	3.54	1.60	1.52
6	H	1	NAG	C3-C2	3.46	1.59	1.52
5	J	1	NAG	C1-C2	3.43	1.57	1.52
6	H	5	MAN	O5-C1	3.43	1.49	1.43
3	C	3	BMA	O5-C5	3.39	1.50	1.43
5	J	2	NAG	O5-C1	3.39	1.49	1.43
4	F	3	GL0	C2-C3	3.37	1.57	1.52
4	F	3	GL0	O5-C5	3.31	1.49	1.43
5	G	2	NAG	O5-C1	3.28	1.49	1.43
6	H	4	BGC	C2-C3	3.27	1.57	1.52
7	I	3	GL0	C2-C3	3.27	1.57	1.52
3	C	1	NAG	C3-C2	3.21	1.59	1.52
4	F	2	NGA	O5-C1	3.15	1.49	1.43
3	C	4	BMA	C2-C3	3.12	1.57	1.52
7	I	3	GL0	O5-C5	3.09	1.49	1.43
7	I	2	NGZ	O5-C1	3.04	1.48	1.43
4	F	4	BGC	O5-C1	3.02	1.48	1.43
6	H	2	NAG	O5-C1	3.01	1.48	1.43
4	F	7	GLC	O5-C1	2.96	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	4	BGC	O5-C1	2.94	1.48	1.43
6	H	3	BMA	C2-C3	2.93	1.57	1.52
3	C	5	MAN	O5-C1	2.91	1.48	1.43
6	H	4	BGC	O5-C1	2.89	1.48	1.43
6	H	3	BMA	C4-C5	2.88	1.59	1.53
7	I	7	GXL	O5-C1	2.85	1.48	1.43
6	H	1	NAG	C4-C3	2.85	1.59	1.52
4	F	5	GLC	C2-C3	2.78	1.56	1.52
3	C	1	NAG	C4-C3	2.75	1.59	1.52
3	C	2	NAG	C3-C2	2.74	1.58	1.52
7	I	5	GLC	C2-C3	2.73	1.56	1.52
3	C	3	BMA	C4-C5	2.69	1.58	1.53
3	C	2	NAG	C8-C7	2.69	1.56	1.50
3	C	2	NAG	C2-N2	2.67	1.50	1.46
6	H	2	NAG	C8-C7	2.64	1.56	1.50
7	I	2	NGZ	C3-C2	2.63	1.58	1.52
3	C	3	BMA	C2-C3	2.63	1.56	1.52
4	F	4	BGC	C1-C2	2.62	1.58	1.52
4	F	7	GLC	O5-C5	2.59	1.48	1.43
6	H	1	NAG	C4-C5	2.56	1.58	1.53
3	C	2	NAG	O5-C1	2.56	1.48	1.43
4	F	2	NGA	O5-C5	2.55	1.48	1.43
3	C	5	MAN	C2-C3	2.54	1.56	1.52
4	F	4	BGC	O5-C5	2.45	1.48	1.43
6	H	5	MAN	C1-C2	2.45	1.58	1.52
7	I	6	BGC	C2-C3	2.44	1.56	1.52
6	H	4	BGC	C1-C2	2.40	1.57	1.52
6	H	5	MAN	C2-C3	2.40	1.56	1.52
4	F	2	NGA	C3-C2	2.38	1.57	1.52
5	J	1	NAG	C3-C2	2.36	1.57	1.52
6	H	1	NAG	C1-C2	2.36	1.55	1.52
6	H	2	NAG	C2-N2	2.36	1.50	1.46
7	I	2	NGZ	O5-C5	2.35	1.48	1.43
5	G	1	NAG	C8-C7	2.32	1.55	1.50
7	I	7	GXL	C1-C2	2.31	1.57	1.52
3	C	1	NAG	C4-C5	2.29	1.57	1.53
3	C	5	MAN	C1-C2	2.29	1.57	1.52
6	H	3	BMA	O5-C1	2.29	1.47	1.43
5	G	1	NAG	C1-C2	2.29	1.55	1.52
7	I	4	BGC	C1-C2	2.27	1.57	1.52
6	H	4	BGC	O5-C5	2.26	1.47	1.43
7	I	7	GXL	O5-C5	2.26	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	5	GLC	O5-C5	2.25	1.47	1.43
7	I	4	BGC	O5-C5	2.25	1.47	1.43
4	F	1	LXZ	C8-C7	2.25	1.55	1.50
4	F	7	GLC	C1-C2	2.23	1.57	1.52
6	H	2	NAG	C3-C2	2.22	1.57	1.52
6	H	3	BMA	C4-C3	2.21	1.58	1.52
5	G	2	NAG	O5-C5	2.21	1.47	1.43
3	C	4	BMA	C1-C2	2.19	1.57	1.52
4	F	6	BGC	C2-C3	2.19	1.55	1.52
5	J	2	NAG	O5-C5	2.17	1.47	1.43
3	C	4	BMA	O5-C1	2.17	1.47	1.43
6	H	2	NAG	O5-C5	2.16	1.47	1.43
7	I	5	GLC	O5-C5	2.16	1.47	1.43
7	I	2	NGZ	C8-C7	2.16	1.55	1.50
3	C	3	BMA	C4-C3	2.13	1.57	1.52
5	G	1	NAG	C4-C3	2.12	1.57	1.52
6	H	2	NAG	C4-C5	2.09	1.57	1.53
4	F	2	NGA	C8-C7	2.09	1.54	1.50
5	J	1	NAG	C8-C7	2.09	1.54	1.50
4	F	5	GLC	O5-C1	2.08	1.47	1.43
6	H	5	MAN	O5-C5	2.08	1.47	1.43
7	I	2	NGZ	O4-C4	2.07	1.48	1.43
7	I	7	GXL	C2-C3	2.06	1.55	1.52
6	H	1	NAG	O4-C4	2.04	1.48	1.43
4	F	6	BGC	C1-C2	2.03	1.57	1.52
5	G	1	NAG	C3-C2	2.02	1.56	1.52
4	F	5	GLC	C1-C2	2.02	1.57	1.52
7	I	1	LXB	C6-C5	2.01	1.58	1.51

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	1	NAG	C1-O5-C5	5.83	120.00	112.19
7	I	3	GL0	C1-C2-C3	5.56	117.74	109.64
4	F	2	NGA	O5-C1-C2	5.45	119.72	111.29
3	C	1	NAG	C1-O5-C5	5.05	118.95	112.19
6	H	4	BGC	C1-C2-C3	4.98	116.90	109.64
4	F	6	BGC	C1-C2-C3	4.84	116.69	109.64
7	I	6	BGC	C1-C2-C3	4.52	116.22	109.64
7	I	6	BGC	O5-C1-C2	4.49	121.50	110.79
3	C	4	BMA	C3-C4-C5	4.34	118.09	110.23
7	I	2	NGZ	C1-O5-C5	4.27	117.91	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3	GL0	C1-C2-C3	4.16	115.70	109.64
3	C	1	NAG	C2-N2-C7	-4.14	117.35	122.90
4	F	1	LXZ	C1-O5-C5	4.11	117.69	112.19
4	F	2	NGA	C4-C3-C2	4.01	116.89	111.02
7	I	3	GL0	C2-C3-C4	3.92	117.75	110.86
3	C	3	BMA	C1-O5-C5	3.90	117.41	112.19
3	C	5	MAN	C1-C2-C3	3.79	115.17	109.64
7	I	1	LXB	C4-C3-C2	3.72	116.47	111.02
4	F	2	NGA	C3-C4-C5	3.71	116.97	110.23
7	I	2	NGZ	O5-C1-C2	3.69	117.00	111.29
4	F	6	BGC	O5-C5-C6	3.68	114.83	107.66
6	H	4	BGC	C1-O5-C5	3.68	117.11	112.19
6	H	4	BGC	C3-C4-C5	3.68	116.90	110.23
4	F	2	NGA	C1-C2-N2	-3.63	104.72	110.43
5	J	1	NAG	C2-N2-C7	3.57	127.68	122.90
5	J	1	NAG	C1-O5-C5	3.55	116.95	112.19
4	F	3	GL0	C3-C4-C5	3.52	116.61	110.23
5	J	2	NAG	C8-C7-N2	3.52	121.95	116.12
7	I	5	GLC	C1-C2-C3	3.51	114.75	109.64
5	G	2	NAG	C4-C3-C2	3.48	116.11	111.02
3	C	1	NAG	C6-C5-C4	-3.38	104.72	113.02
5	J	2	NAG	C1-O5-C5	3.36	116.69	112.19
4	F	7	GLC	C1-O5-C5	3.32	116.64	112.19
4	F	2	NGA	C1-O5-C5	3.26	116.56	112.19
6	H	1	NAG	C1-O5-C5	3.22	116.50	112.19
3	C	2	NAG	C8-C7-N2	3.21	121.44	116.12
6	H	3	BMA	C1-O5-C5	3.15	116.40	112.19
4	F	3	GL0	O5-C5-C6	3.15	113.78	107.66
6	H	1	NAG	C2-N2-C7	-3.14	118.69	122.90
5	J	1	NAG	O5-C1-C2	3.12	116.12	111.29
5	G	1	NAG	C2-N2-C7	-3.11	118.73	122.90
7	I	3	GL0	C3-C4-C5	3.01	115.69	110.23
7	I	3	GL0	O5-C5-C6	2.99	113.48	107.66
4	F	1	LXZ	C3-C4-C5	2.97	115.63	110.23
5	J	1	NAG	C1-C2-N2	2.97	115.12	110.43
4	F	3	GL0	C2-C3-C4	2.96	116.06	110.86
3	C	5	MAN	C1-O5-C5	2.91	116.09	112.19
4	F	1	LXZ	O5-C5-C4	2.90	117.88	110.83
5	G	1	NAG	C8-C7-N2	2.89	120.92	116.12
7	I	1	LXB	C3-C4-C5	2.89	115.47	110.23
6	H	2	NAG	C2-N2-C7	-2.81	119.14	122.90
4	F	1	LXZ	C1-C2-N2	2.77	114.80	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	2	NAG	C1-O5-C5	2.77	115.89	112.19
4	F	4	BGC	C1-C2-C3	2.75	113.65	109.64
7	I	3	GL0	C1-O5-C5	2.75	115.87	112.19
4	F	5	GLC	C1-O5-C5	2.71	115.82	112.19
6	H	5	MAN	C1-O5-C5	2.64	115.72	112.19
6	H	4	BGC	C2-C3-C4	2.64	115.50	110.86
3	C	2	NAG	C2-N2-C7	-2.61	119.40	122.90
4	F	6	BGC	O5-C1-C2	2.61	117.02	110.79
6	H	2	NAG	C1-C2-N2	2.61	114.54	110.43
4	F	1	LXZ	C8-C7-N2	2.60	120.44	116.12
7	I	4	BGC	C1-O5-C5	2.57	115.63	112.19
6	H	4	BGC	O5-C5-C4	2.55	117.03	110.83
3	C	4	BMA	O5-C5-C4	2.52	116.95	110.83
5	G	2	NAG	C8-C7-N2	2.44	120.17	116.12
5	G	2	NAG	C1-O5-C5	2.44	115.45	112.19
4	F	7	GLC	C6-C5-C4	-2.42	107.09	113.02
6	H	2	NAG	C8-C7-N2	2.41	120.11	116.12
5	J	2	NAG	O5-C1-C2	2.37	114.96	111.29
6	H	3	BMA	O3-C3-C4	2.34	115.89	110.38
4	F	4	BGC	C1-O5-C5	2.33	115.31	112.19
4	F	6	BGC	O2-C2-C3	-2.33	105.33	110.15
3	C	4	BMA	C2-C3-C4	2.31	114.93	110.86
3	C	3	BMA	C3-C4-C5	2.31	114.42	110.23
6	H	2	NAG	O5-C5-C4	2.31	116.44	110.83
7	I	4	BGC	C1-C2-C3	2.30	112.99	109.64
6	H	3	BMA	O3-C3-C2	2.24	114.62	110.05
3	C	2	NAG	C1-C2-N2	2.22	113.94	110.43
3	C	1	NAG	C8-C7-N2	2.21	119.79	116.12
7	I	2	NGZ	O4-C4-C5	-2.21	103.88	109.32
7	I	6	BGC	O5-C5-C6	2.21	111.96	107.66
5	G	1	NAG	O5-C1-C2	2.20	114.70	111.29
4	F	7	GLC	O5-C5-C4	2.19	116.17	110.83
7	I	2	NGZ	C8-C7-N2	2.19	119.75	116.12
7	I	2	NGZ	O5-C5-C4	2.19	116.16	110.83
6	H	3	BMA	C1-C2-C3	-2.18	106.47	109.64
4	F	2	NGA	C8-C7-N2	2.13	119.66	116.12
7	I	6	BGC	C1-O5-C5	2.13	115.05	112.19
7	I	1	LXB	O7-C7-C8	-2.13	118.26	122.05
6	H	4	BGC	O5-C5-C6	2.13	111.80	107.66
4	F	3	GL0	O5-C1-C2	2.12	115.83	110.79
7	I	1	LXB	O5-C5-C6	2.09	111.72	107.66
5	G	2	NAG	O5-C1-C2	2.07	114.50	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	O7-C7-C8	-2.05	118.41	122.05
5	J	1	NAG	O7-C7-C8	-2.04	118.41	122.05
3	C	1	NAG	C3-C4-C5	2.03	113.92	110.23
5	J	2	NAG	C1-C2-N2	-2.02	107.24	110.43
3	C	4	BMA	C1-C2-C3	2.01	112.58	109.64
5	G	2	NAG	C2-N2-C7	-2.01	120.21	122.90

All (31) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	2	NGA	C4
4	F	2	NGA	C1
4	F	2	NGA	C2
4	F	2	NGA	C3
4	F	2	NGA	C5
4	F	3	GL0	C1
4	F	5	GLC	C4
4	F	5	GLC	C1
4	F	5	GLC	C2
4	F	5	GLC	C3
4	F	5	GLC	C5
4	F	6	BGC	C5
4	F	7	GLC	C4
4	F	7	GLC	C1
4	F	7	GLC	C2
4	F	7	GLC	C3
4	F	7	GLC	C5
5	G	1	NAG	C1
5	G	2	NAG	C1
5	J	1	NAG	C2
5	J	1	NAG	C1
5	J	2	NAG	C1
7	I	2	NGZ	C1
7	I	3	GL0	C1
7	I	5	GLC	C4
7	I	5	GLC	C1
7	I	5	GLC	C2
7	I	5	GLC	C3
7	I	5	GLC	C5
7	I	6	BGC	C5
7	I	7	GXL	C4

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	1	NAG	C1-C2-N2-C7
5	J	1	NAG	O7-C7-N2-C2
3	C	3	BMA	O5-C5-C6-O6
7	I	7	GXL	O5-C5-C6-O6
7	I	7	GXL	C4-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	5	MAN	O5-C5-C6-O6
3	C	4	BMA	O5-C5-C6-O6
6	H	3	BMA	O5-C5-C6-O6
4	F	3	GL0	C4-C5-C6-O6
3	C	4	BMA	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
7	I	1	LXB	O5-C5-C6-O6
4	F	7	GLC	C4-C5-C6-O6
4	F	7	GLC	O5-C5-C6-O6
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
4	F	1	LXZ	O5-C5-C6-O6
7	I	1	LXB	C4-C5-C6-O6
4	F	5	GLC	C4-C5-C6-O6
4	F	4	BGC	O5-C5-C6-O6
4	F	4	BGC	C4-C5-C6-O6
3	C	5	MAN	C4-C5-C6-O6
4	F	3	GL0	O5-C5-C6-O6
6	H	5	MAN	O5-C5-C6-O6
7	I	6	BGC	O5-C5-C6-O6
4	F	5	GLC	O5-C5-C6-O6
6	H	3	BMA	C4-C5-C6-O6
7	I	5	GLC	C4-C5-C6-O6
7	I	6	BGC	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
4	F	1	LXZ	C3-C2-N2-C7
4	F	2	NGA	C3-C2-N2-C7
7	I	5	GLC	O5-C5-C6-O6
4	F	2	NGA	C1-C2-N2-C7
6	H	2	NAG	O5-C5-C6-O6
7	I	1	LXB	O7-C7-N2-C2
6	H	4	BGC	O5-C5-C6-O6

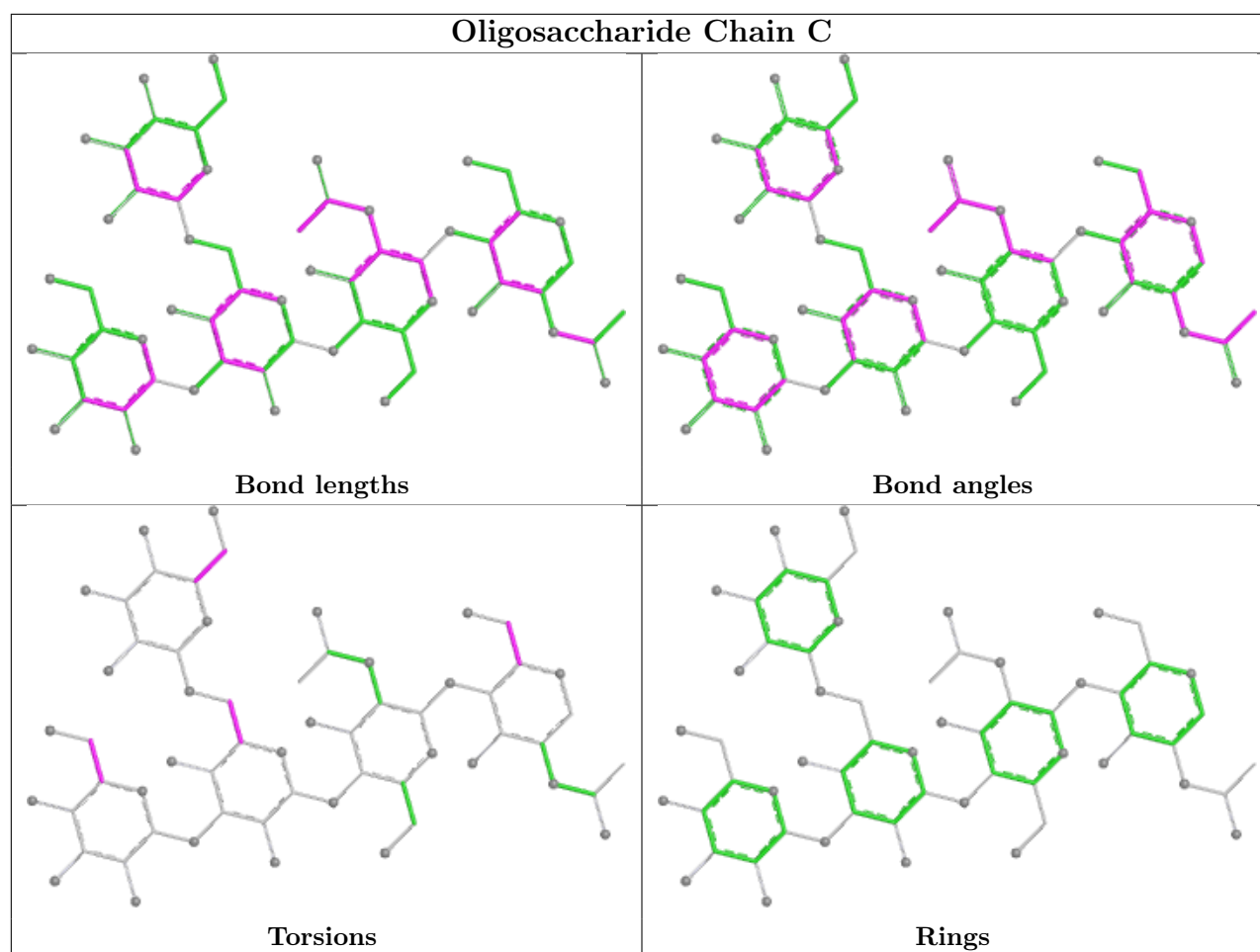
All (1) ring outliers are listed below:

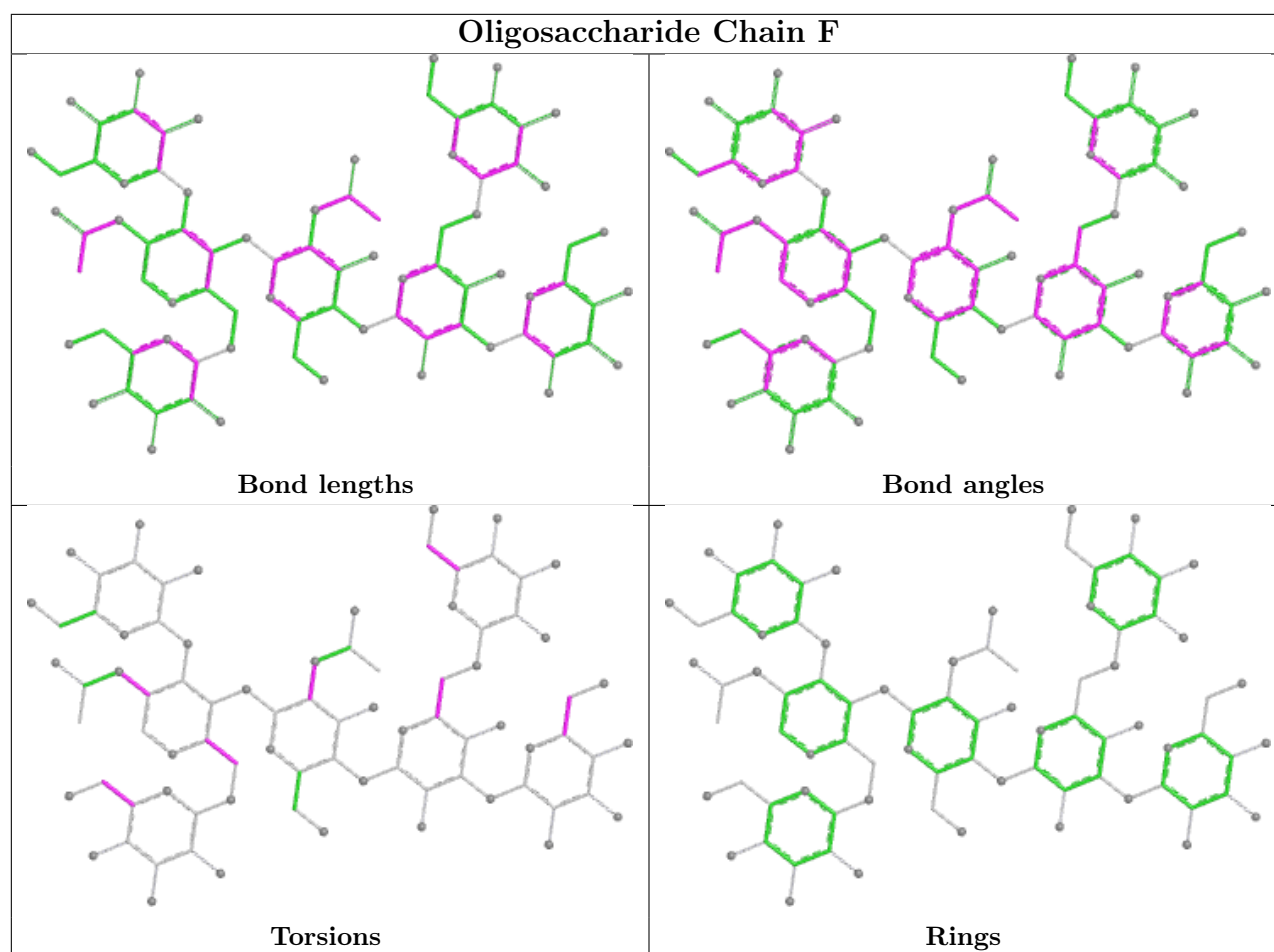
Mol	Chain	Res	Type	Atoms
6	H	5	MAN	C1-C2-C3-C4-C5-O5

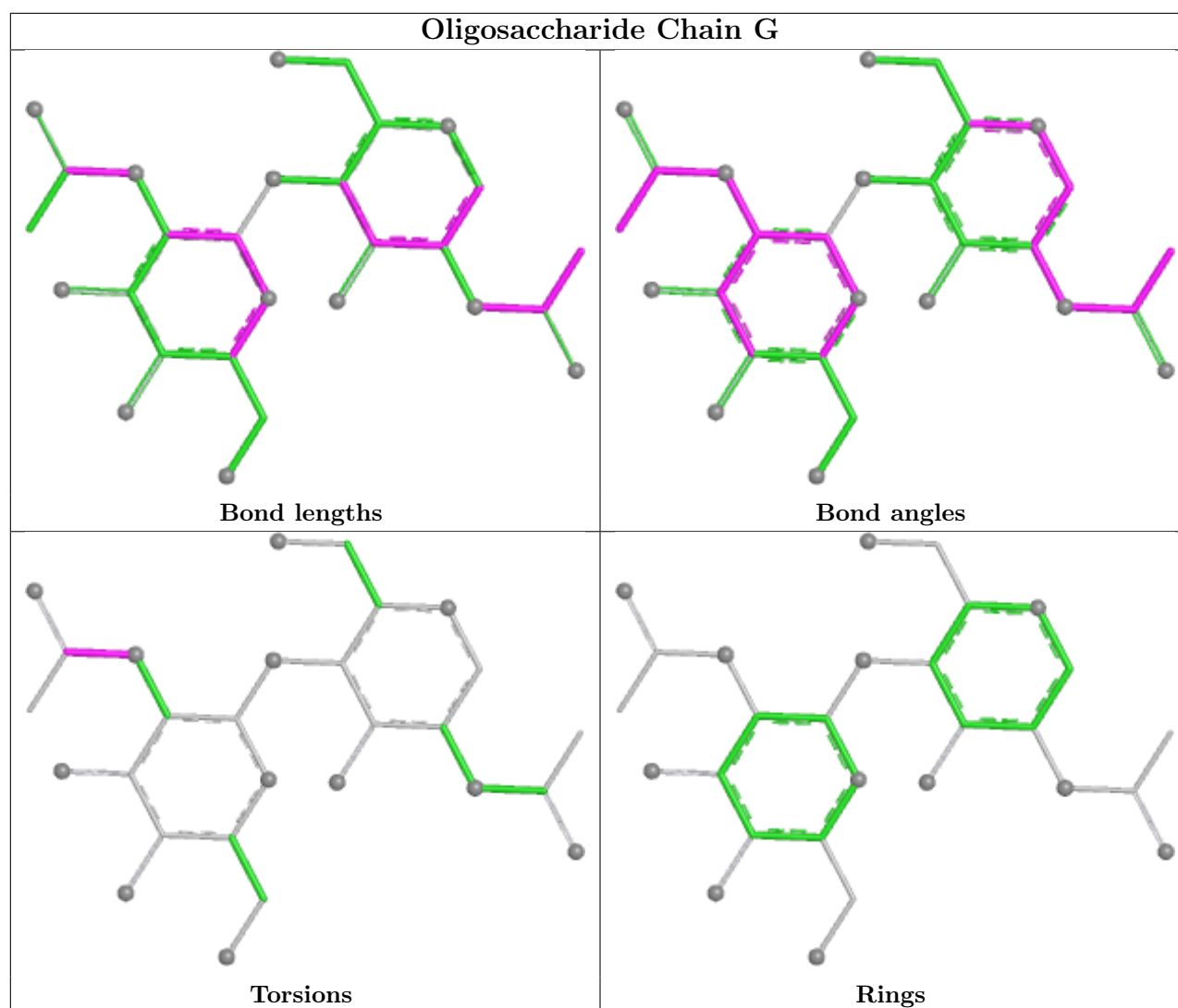
13 monomers are involved in 13 short contacts:

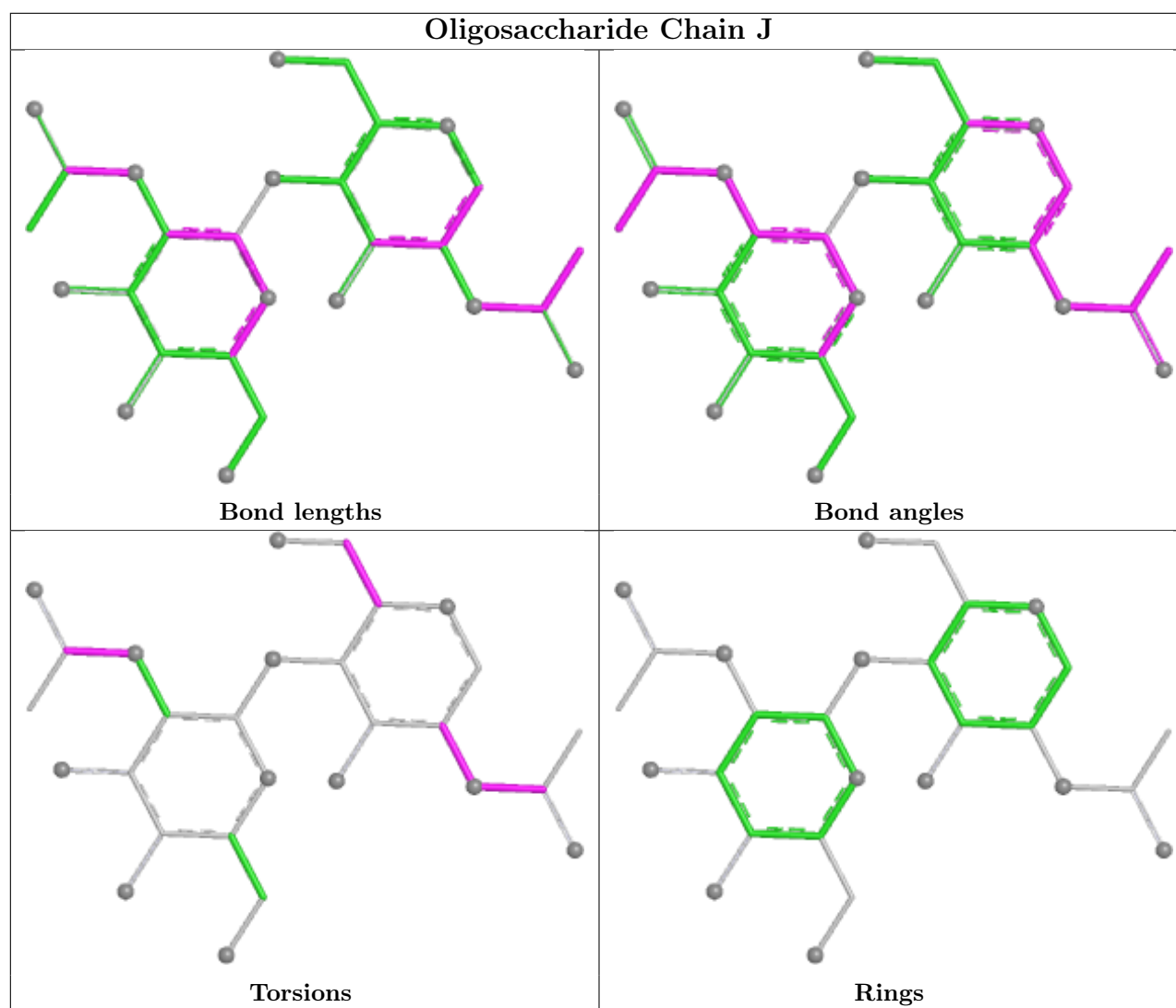
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2	NAG	1	0
4	F	2	NGA	1	0
7	I	3	GL0	1	0
3	C	3	BMA	1	0
5	J	2	NAG	1	0
6	H	1	NAG	1	0
7	I	1	LXB	4	0
5	G	1	NAG	1	0
4	F	7	GLC	1	0
3	C	4	BMA	1	0
6	H	3	BMA	2	0
7	I	4	BGC	1	0
6	H	4	BGC	2	0

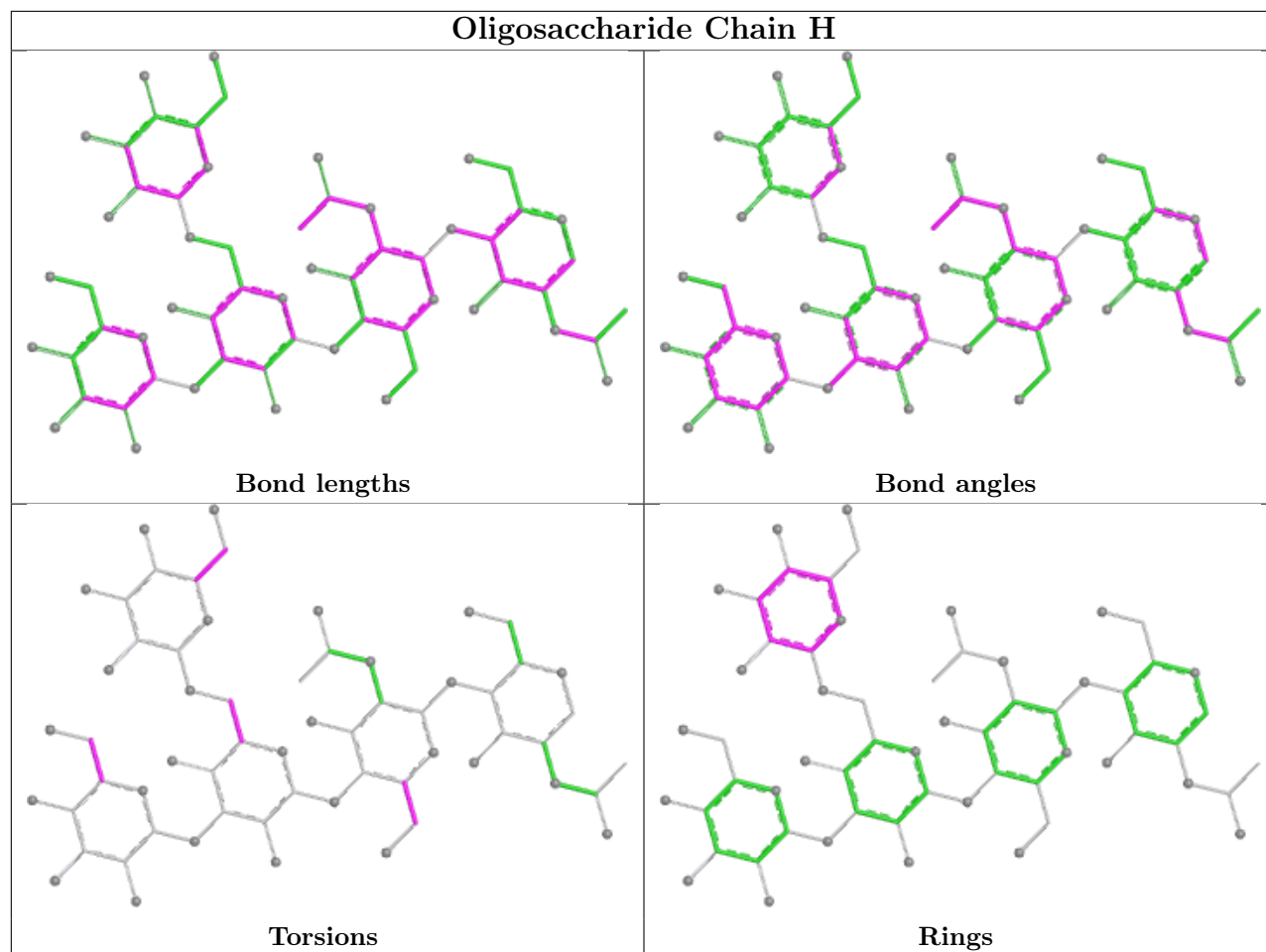
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

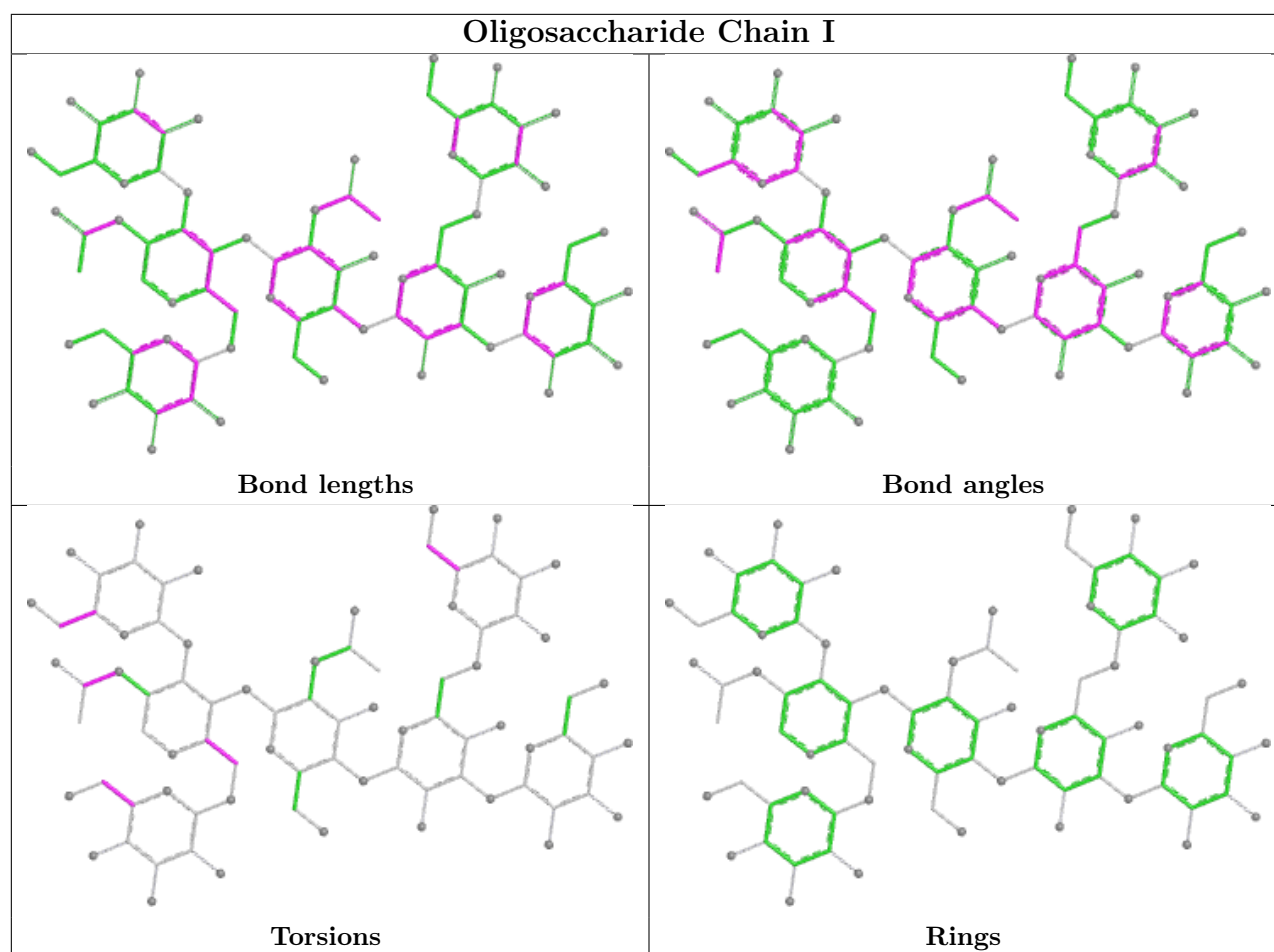












5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
9	SO4	A	1372	-	4,4,4	0.36	0	6,6,6	0.09	0
9	SO4	D	1472	-	4,4,4	0.28	0	6,6,6	0.19	0
8	NAG	A	1210	1	14,14,15	1.77	3 (21%)	17,19,21	1.61	4 (23%)
9	SO4	A	1368	-	4,4,4	0.35	0	6,6,6	0.27	0
9	SO4	A	1373	-	4,4,4	0.30	0	6,6,6	0.18	0
9	SO4	D	1475	-	4,4,4	0.33	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	D	1473	-	4,4,4	0.29	0	6,6,6	0.14	0
9	SO4	D	1474	-	4,4,4	0.39	0	6,6,6	0.30	0
9	SO4	D	1470	-	4,4,4	0.29	0	6,6,6	0.12	0
9	SO4	B	203	-	4,4,4	0.28	0	6,6,6	0.11	0
9	SO4	B	202	-	4,4,4	0.31	0	6,6,6	0.11	0
9	SO4	A	1376	-	4,4,4	0.31	0	6,6,6	0.12	0
9	SO4	A	1371	-	4,4,4	0.28	0	6,6,6	0.13	0
9	SO4	D	1471	-	4,4,4	0.34	0	6,6,6	0.16	0
9	SO4	A	1375	-	4,4,4	0.40	0	6,6,6	0.39	0
9	SO4	D	1469	-	4,4,4	0.27	0	6,6,6	0.10	0
9	SO4	A	1369	-	4,4,4	0.38	0	6,6,6	0.31	0
9	SO4	A	1370	-	4,4,4	0.30	0	6,6,6	0.12	0
9	SO4	D	1468	-	4,4,4	0.34	0	6,6,6	0.13	0
8	NAG	D	1310	1	14,14,15	1.80	3 (21%)	17,19,21	1.23	3 (17%)
9	SO4	A	1374	-	4,4,4	0.32	0	6,6,6	0.23	0
9	SO4	D	1476	-	4,4,4	0.28	0	6,6,6	0.18	0
9	SO4	E	190	-	4,4,4	0.26	0	6,6,6	0.20	0
9	SO4	D	1477	-	4,4,4	0.27	0	6,6,6	0.14	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
8	NAG	A	1210	1	-	6/6/23/26	0/1/1/1
8	NAG	D	1310	1	1/1/5/7	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1210	NAG	C7-N2	4.13	1.47	1.34
8	D	1310	NAG	C7-N2	3.97	1.47	1.34
8	D	1310	NAG	C1-C2	3.43	1.57	1.52
8	A	1210	NAG	C1-C2	3.29	1.56	1.52
8	D	1310	NAG	C3-C2	2.08	1.56	1.52
8	A	1210	NAG	C8-C7	2.07	1.54	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1210	NAG	C8-C7-N2	3.47	121.87	116.12
8	A	1210	NAG	C1-O5-C5	3.44	116.80	112.19
8	D	1310	NAG	O5-C1-C2	2.23	114.74	111.29
8	D	1310	NAG	C1-O5-C5	2.17	115.09	112.19
8	A	1210	NAG	C6-C5-C4	-2.14	107.76	113.02
8	A	1210	NAG	O7-C7-N2	-2.04	118.38	121.98
8	D	1310	NAG	C8-C7-N2	2.01	119.46	116.12

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	D	1310	NAG	C1

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1210	NAG	C8-C7-N2-C2
8	A	1210	NAG	O5-C5-C6-O6
8	A	1210	NAG	O7-C7-N2-C2
8	A	1210	NAG	C4-C5-C6-O6
8	D	1310	NAG	C4-C5-C6-O6
8	D	1310	NAG	O5-C5-C6-O6
8	A	1210	NAG	C3-C2-N2-C7
8	A	1210	NAG	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1368	SO4	3	0
9	B	203	SO4	1	0
9	A	1371	SO4	1	0
9	E	190	SO4	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	428/428 (100%)	-0.09	6 (1%)	73	51	43, 59, 85, 110	0
1	D	428/428 (100%)	0.01	7 (1%)	70	47	45, 61, 86, 104	0
2	B	141/141 (100%)	0.21	3 (2%)	63	40	45, 72, 94, 106	0
2	E	141/141 (100%)	0.10	1 (0%)	84	66	48, 70, 97, 99	0
All	All	1138/1138 (100%)	0.01	17 (1%)	72	49	43, 63, 90, 110	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	336	ALA	3.5
1	D	327	GLY	3.3
1	D	335	LEU	3.2
1	D	473	ASN	3.2
1	D	209	VAL	3.2
1	A	335	LEU	3.1
2	B	65	ALA	3.0
1	D	210	VAL	2.7
1	A	603	ALA	2.5
1	A	473	ASN	2.5
2	B	67	PRO	2.5
1	A	209	VAL	2.4
1	A	208	PRO	2.2
2	B	153	GLY	2.2
1	D	312	GLY	2.1
1	D	208	PRO	2.1
2	E	47	GLY	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 ⓘ

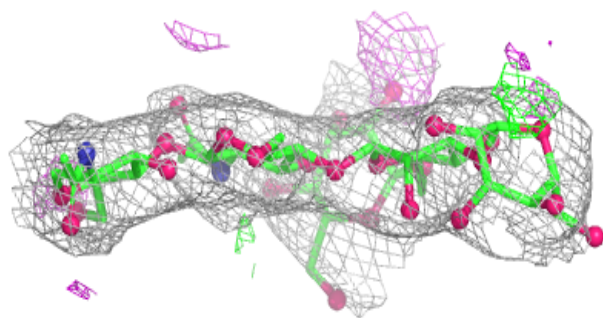
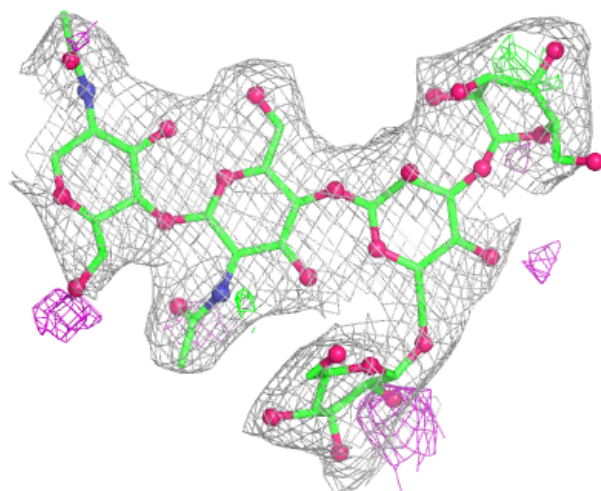
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	C	1	14/15	-	-	55,59,65,67	0
3	NAG	C	2	14/15	-	-	60,67,72,73	0
3	BMA	C	3	11/12	-	-	75,81,86,89	0
3	BMA	C	4	11/12	-	-	86,90,93,93	0
3	MAN	C	5	11/12	-	-	87,91,96,96	0
6	BMA	H	3	11/12	0.49	0.17	101,110,116,117	0
6	MAN	H	5	11/12	0.52	0.19	108,118,121,122	0
6	BGC	H	4	11/12	0.56	0.20	75,98,105,106	0
7	BGC	I	4	11/12	0.56	0.17	113,120,124,125	0
6	NAG	H	2	14/15	0.57	0.20	90,103,113,116	0
7	GLC	I	5	11/12	0.60	0.16	98,107,112,113	0
4	BGC	F	4	11/12	0.65	0.15	93,103,106,106	0
7	GL0	I	3	11/12	0.72	0.13	110,116,119,121	0
5	NAG	J	2	14/15	0.74	0.17	89,102,109,110	0
4	LXZ	F	1	14/15	0.75	0.16	65,70,80,81	0
4	GLC	F	5	11/12	0.77	0.16	87,97,101,101	0
4	GL0	F	3	11/12	0.78	0.12	93,97,99,101	0
4	BGC	F	6	11/12	0.79	0.14	75,81,87,90	0
5	NAG	G	2	14/15	0.80	0.15	85,95,100,100	0
6	NAG	H	1	14/15	0.82	0.15	85,90,100,104	0
7	NGZ	I	2	14/15	0.83	0.13	70,92,99,106	0
7	BGC	I	6	11/12	0.86	0.12	79,82,87,89	0
5	NAG	J	1	14/15	0.87	0.12	72,83,92,104	0
5	NAG	G	1	14/15	0.87	0.11	62,79,89,97	0
4	NGA	F	2	14/15	0.88	0.14	71,80,84,91	0
7	GXL	I	7	11/12	0.88	0.16	69,79,90,91	0
4	GLC	F	7	11/12	0.91	0.14	69,75,82,90	0
7	LXB	I	1	14/15	0.92	0.10	73,76,80,85	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.

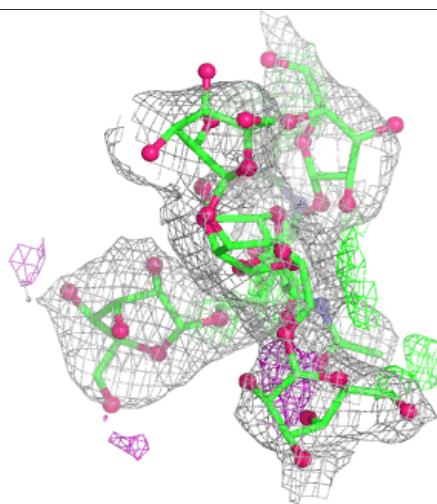
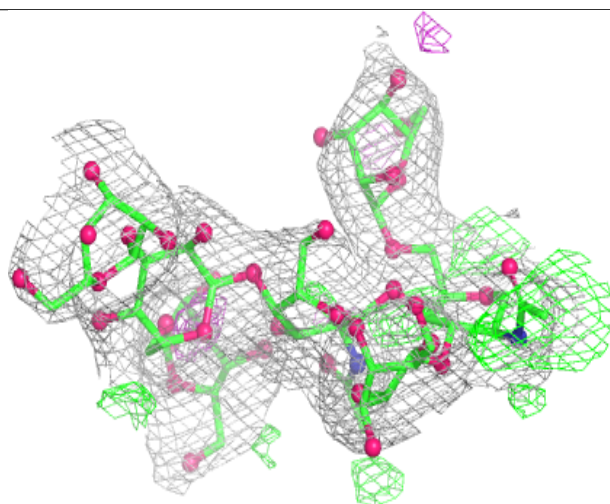
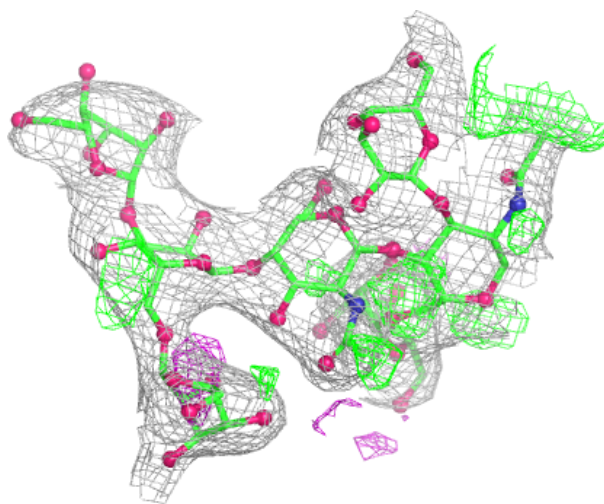
Electron density around Chain C:

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



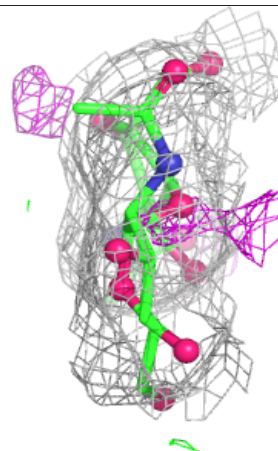
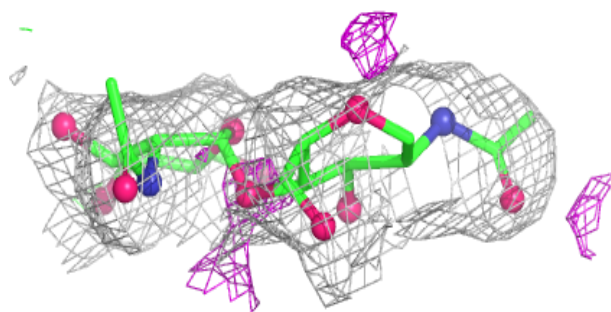
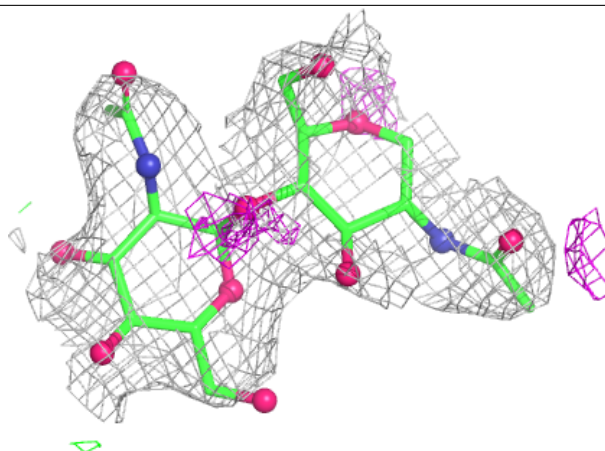
Electron density around Chain F:

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

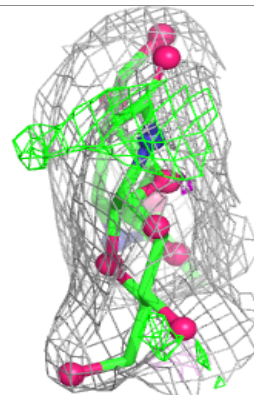
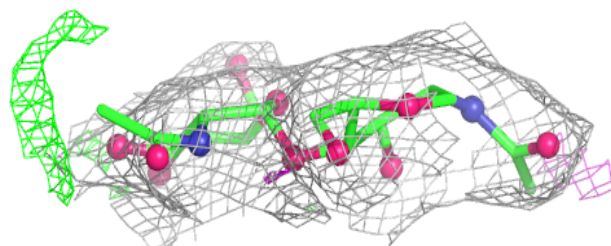
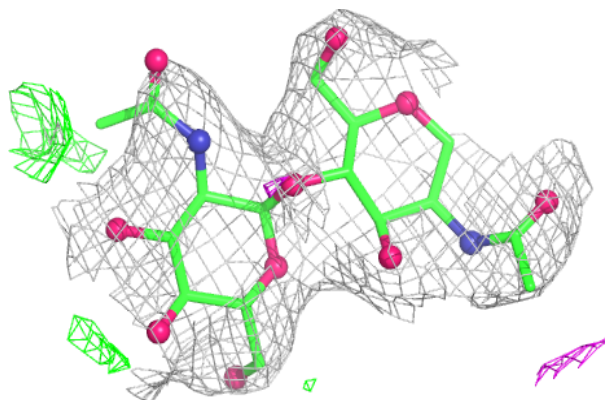


Electron density around Chain G:

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

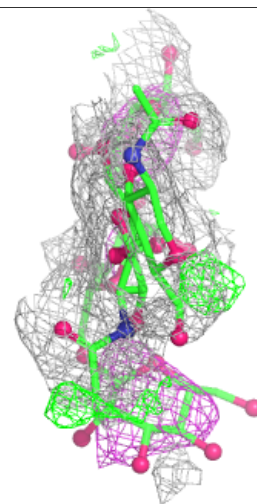
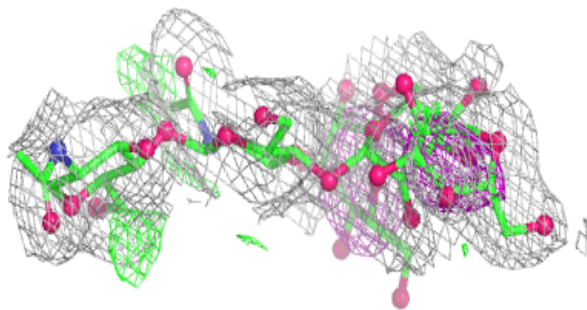
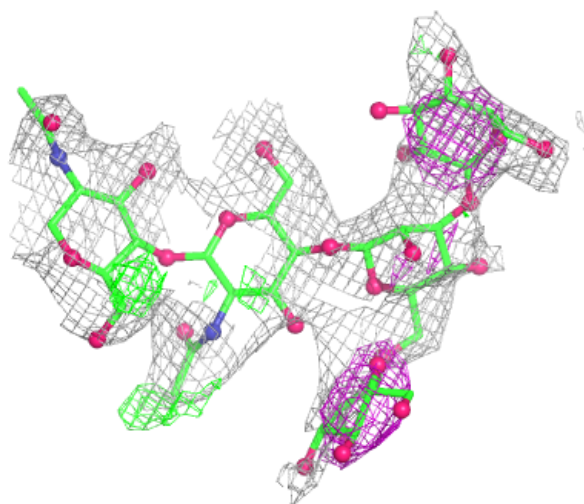
**Electron density around Chain J:**

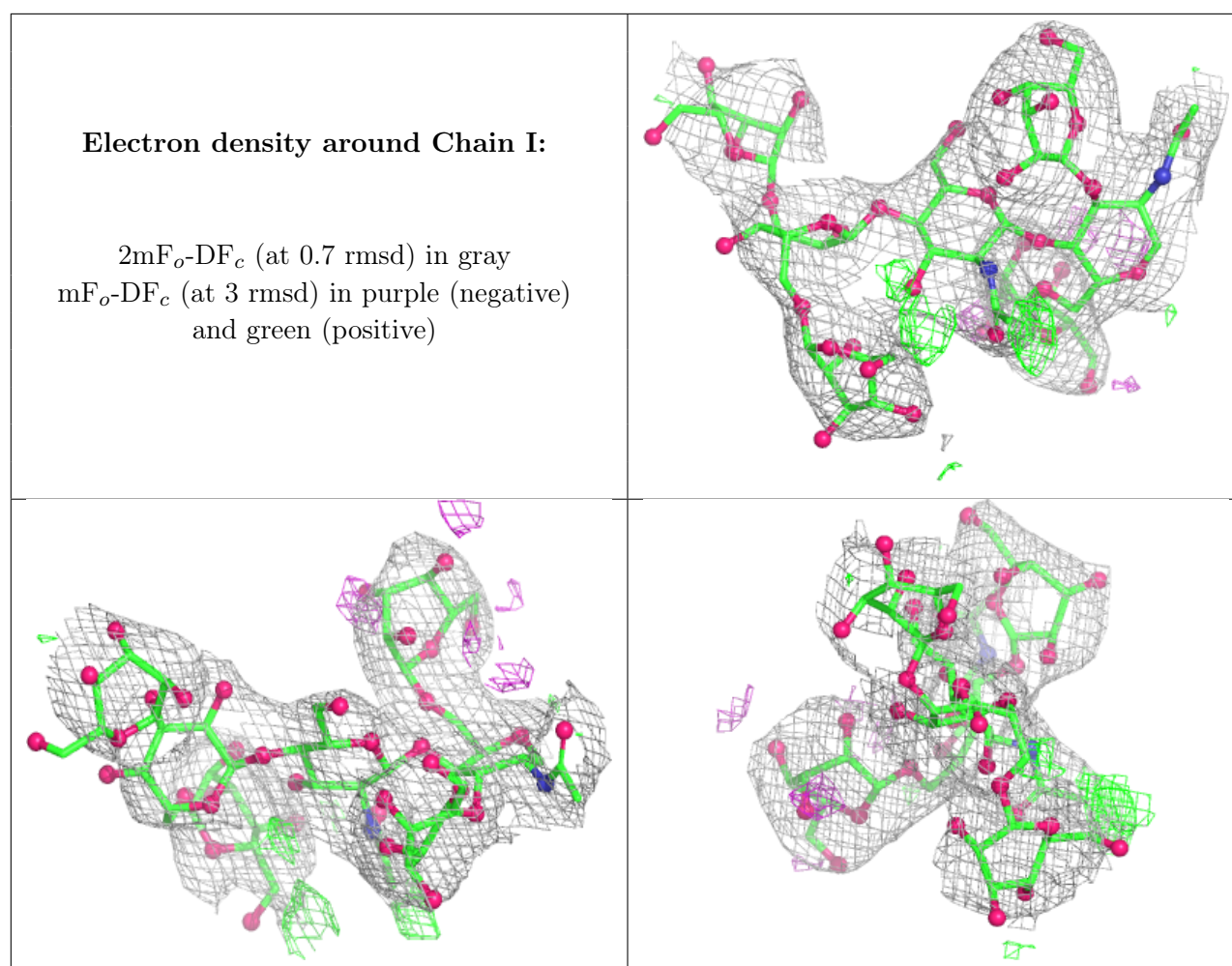
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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($\text{\AA}^2$)	Q<0.9
9	SO4	A	1370	5/5	0.57	0.15	116,121,126,139	0
9	SO4	D	1470	5/5	0.62	0.16	109,117,128,134	0
9	SO4	E	190	5/5	0.64	0.25	105,109,123,130	0
8	NAG	D	1310	14/15	0.65	0.19	95,105,108,108	0
9	SO4	D	1469	5/5	0.65	0.19	124,128,134,144	0
8	NAG	A	1210	14/15	0.68	0.16	88,92,97,97	0
9	SO4	A	1371	5/5	0.70	0.17	108,110,117,129	0
9	SO4	D	1474	5/5	0.73	0.32	90,95,109,114	0
9	SO4	D	1473	5/5	0.74	0.29	105,111,123,131	0
9	SO4	A	1374	5/5	0.75	0.22	92,99,110,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SO4	D	1472	5/5	0.76	0.32	98,103,119,121	0
9	SO4	B	202	5/5	0.78	0.20	102,106,112,126	0
9	SO4	D	1471	5/5	0.79	0.30	84,97,109,120	0
9	SO4	B	203	5/5	0.80	0.18	108,108,125,130	0
9	SO4	D	1477	5/5	0.80	0.20	105,107,117,130	0
9	SO4	A	1373	5/5	0.80	0.24	93,99,118,124	0
9	SO4	A	1375	5/5	0.82	0.30	82,83,103,104	0
9	SO4	A	1372	5/5	0.83	0.18	81,92,102,116	0
9	SO4	A	1376	5/5	0.83	0.16	86,88,100,108	0
9	SO4	D	1476	5/5	0.86	0.12	86,89,99,105	0
9	SO4	D	1475	5/5	0.88	0.15	88,88,100,108	0
9	SO4	D	1468	5/5	0.89	0.11	81,86,90,97	0
9	SO4	A	1368	5/5	0.95	0.08	58,60,64,67	0
9	SO4	A	1369	5/5	0.96	0.10	57,66,73,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.