



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:24 PM BST

PDB ID : 5JG8  
Title : Crystal structure of human acid sphingomyelinase  
Authors : Xiong, Z.J.; Prive, G.G.  
Deposited on : 2016-04-19  
Resolution : 2.80 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](mailto: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.

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

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

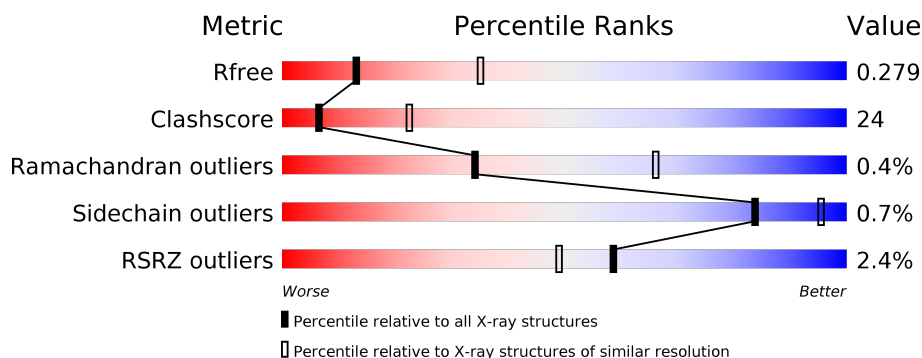
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.




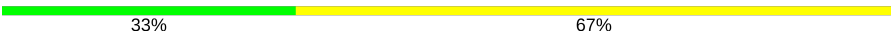
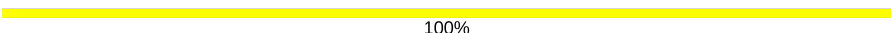
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	586	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>34%</div> <div>10%</div> </div> </div>
1	B	586	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>39%</div> <div>10%</div> </div> </div>
2	C	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	D	2	<div> <div></div> <div>100%</div> </div>
2	H	2	<div> <div></div> <div>100%</div> </div>
2	I	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	E	2	 50% 50%
4	F	3	 33% 67%
4	G	3	 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
6	ACT	A	703	-	-	X	-
6	ACT	B	703	-	-	X	-
7	NAG	A	704	-	-	-	X
7	NAG	A	705	-	-	-	X
7	NAG	B	705	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8676 atoms, of which 35 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 Sphingomyelin phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4165	2686	718	738	23			
1	B	530	Total	C	N	O	S	0	0	0
			4176	2695	719	739	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLY	-	expression tag	UNP P17405
A	45	ALA	-	expression tag	UNP P17405
A	46	PRO	-	expression tag	UNP P17405
A	629	SER	CYS	engineered mutation	UNP P17405
B	44	GLY	-	expression tag	UNP P17405
B	45	ALA	-	expression tag	UNP P17405
B	46	PRO	-	expression tag	UNP P17405
B	629	SER	CYS	engineered mutation	UNP P17405

- Molecule 2 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
2	C	2	Total	C	N	O		0	0	0
			28	16	2	10				
2	D	2	Total	C	H	N	O	0	0	0
			32	16	4	2	10			
2	H	2	Total	C	H	N	O	0	0	0
			32	16	4	2	10			

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

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



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

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

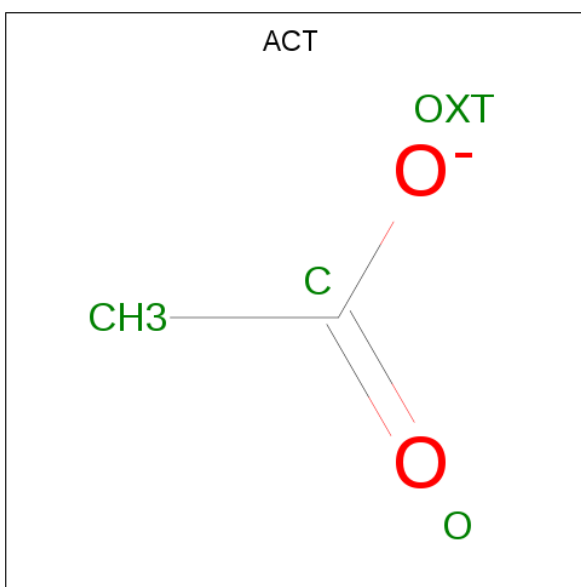


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	G	3	Total	C	H	N	O	0	0
			50	22	11	2	15		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

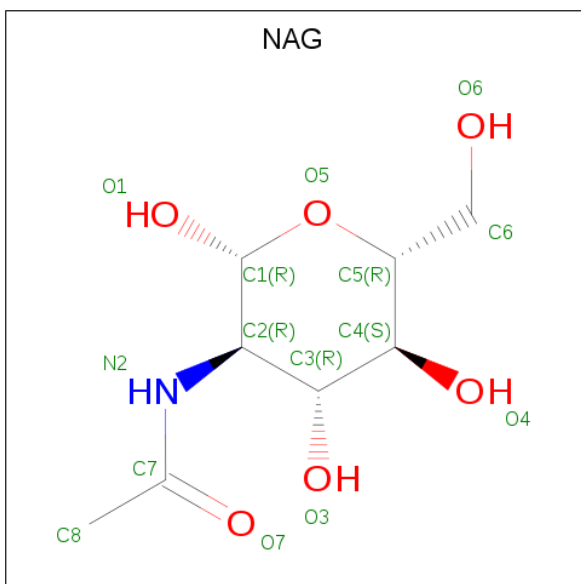
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Zn	0	0
			2	2		
5	A	2	Total	Zn	0	0
			2	2		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	0	0
			18	8	4	1	5		

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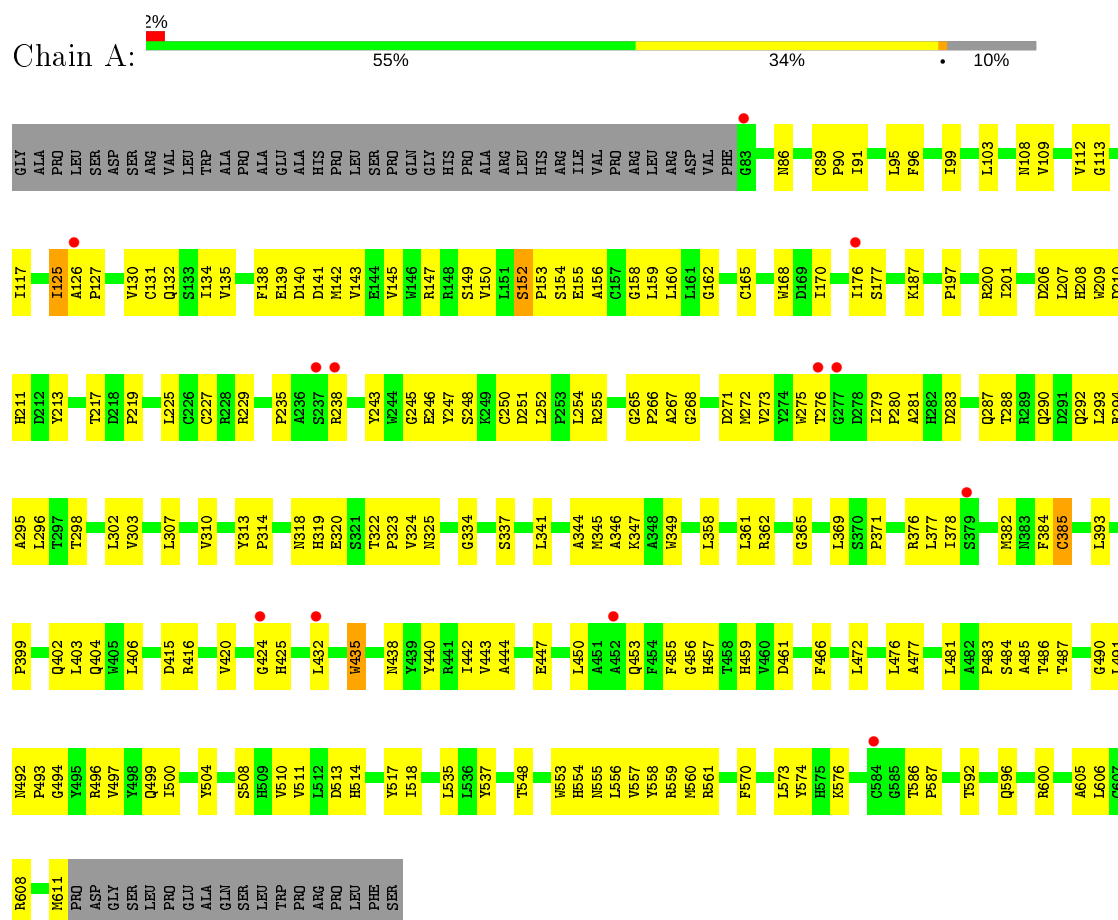
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	0	0
			18	8	4	1	5		
7	A	1	Total	C	N	O		0	0
			14	8	1	5			
7	B	1	Total	C	H	N	O	0	0
			18	8	4	1	5		
7	B	1	Total	C	H	N	O	0	0
			18	8	4	1	5		

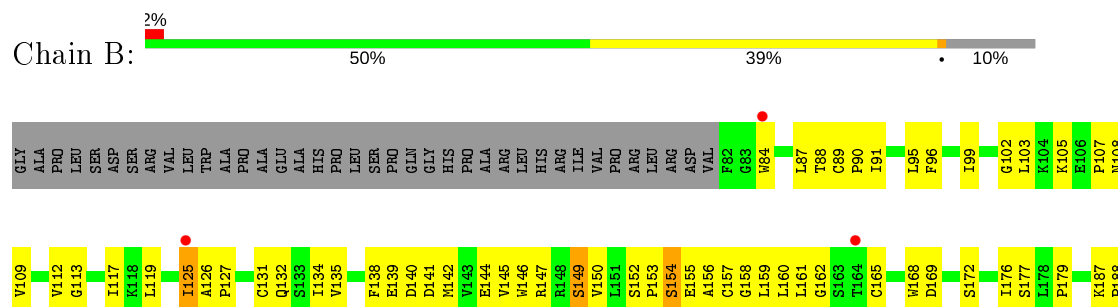
### 3 Residue-property plots

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

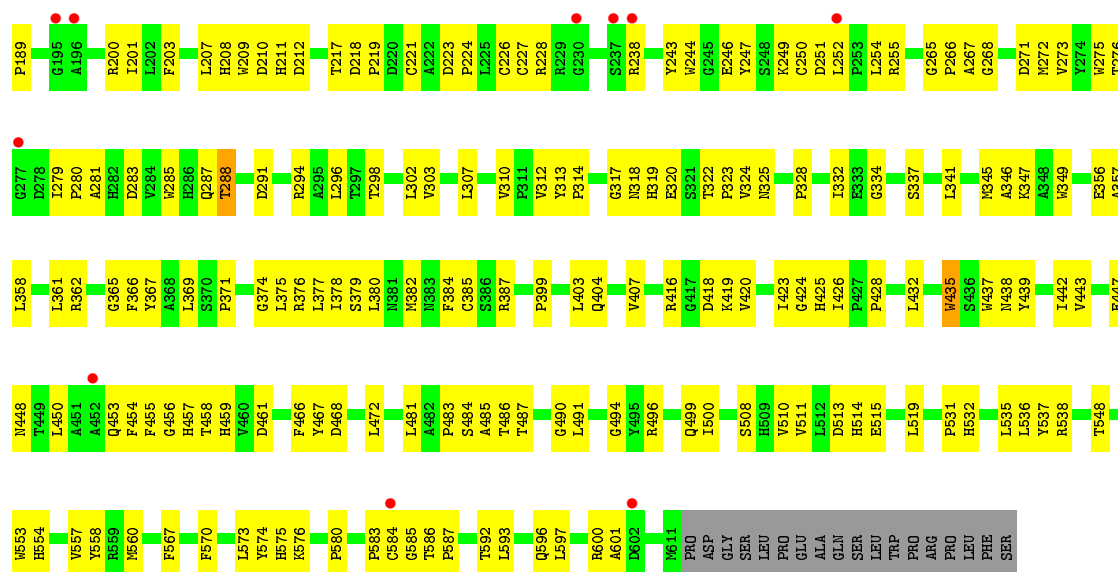
#### • Molecule 1: Spingomyelin phosphodiesterase



#### • Molecule 1: Spingomyelin phosphodiesterase







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

Chain C: 50% 50%



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

Chain D: 100%



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

Chain H: 100%



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

Chain I: 50% 50%




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

Chain E:  50% 50%

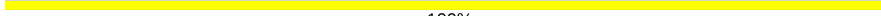
MAG1  
MAG2

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

Chain F:  33% 67%

MAG1  
MAG2  
MAG3

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

Chain G:  100%

MAG1  
MAG2  
MAG3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.53Å 143.66Å 193.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.76 – 2.80 28.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (26.76-2.80) 93.8 (28.84-2.80)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, $R_{free}$	0.230 , 0.279 0.230 , 0.279	Depositor DCC
$R_{free}$ test set	1977 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.9	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 36.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8676	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.29	0/4311	0.49	1/5909 (0.0%)
1	B	0.30	0/4323	0.50	3/5925 (0.1%)
All	All	0.29	0/8634	0.50	4/11834 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	SER	O-C-N	6.43	132.99	122.70
1	A	152	SER	C-N-CD	6.34	141.72	128.40
1	B	154	SER	N-CA-C	-5.92	95.01	111.00
1	B	189	PRO	C-N-CA	-5.55	107.82	121.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4165	0	4030	198	0
1	B	4176	0	4039	217	0
2	C	28	0	25	1	0
2	D	28	4	25	0	0
2	H	28	4	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	28	0	25	0	0
3	E	28	0	25	1	0
4	F	39	0	34	0	0
4	G	39	11	34	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	4	0	3	8	0
6	B	4	0	3	4	0
7	A	42	8	39	1	0
7	B	28	8	26	1	0
All	All	8641	35	8333	404	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 24.

All (404) 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:457:HIS:CE1	6:A:703:ACT:H2	1.71	1.25
1:B:457:HIS:CE1	6:B:703:ACT:H1	1.73	1.23
1:B:117:ILE:HG12	1:B:135:VAL:HG11	1.25	1.13
1:A:117:ILE:HG12	1:A:135:VAL:HG11	1.29	1.12
1:A:125:ILE:HG12	7:B:704:NAG:H62	1.36	1.07
1:A:457:HIS:HE1	6:A:703:ACT:H2	0.92	1.06
1:A:176:ILE:HD11	1:A:404:GLN:HB2	1.38	1.03
1:A:483:PRO:HB2	1:A:576:LYS:HD3	1.41	0.99
1:B:96:PHE:HB2	1:B:153:PRO:HB3	1.48	0.95
1:B:210:ASP:OD1	1:B:228:ARG:NH1	2.00	0.95
1:A:346:ALA:HB2	1:A:361:LEU:HD23	1.51	0.92
1:A:201:ILE:HD12	1:A:500:ILE:HD12	1.53	0.90
1:B:483:PRO:HB2	1:B:576:LYS:HD3	1.52	0.89
1:B:384:PHE:HB3	1:B:399:PRO:HB2	1.55	0.89
1:B:243:TYR:O	1:B:255:ARG:NH1	2.05	0.89
1:B:273:VAL:HG21	1:B:307:LEU:HD22	1.54	0.89
1:A:243:TYR:O	1:A:255:ARG:NH1	2.06	0.88
1:B:176:ILE:HD11	1:B:404:GLN:HB2	1.55	0.88
1:B:187:LYS:HD2	1:B:188:PRO:HD2	1.56	0.87
1:B:267:ALA:HB1	1:B:268:GLY:HA2	1.56	0.86
1:B:126:ALA:HB1	1:B:127:PRO:HD2	1.58	0.85
1:A:273:VAL:HG21	1:A:307:LEU:HD22	1.57	0.85
1:A:142:MET:HG2	1:B:91:ILE:HG21	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ALA:HB1	1:A:127:PRO:HD2	1.58	0.83
1:A:131:CYS:O	1:A:135:VAL:HG12	1.78	0.83
1:B:265:GLY:O	1:B:267:ALA:HA	1.78	0.83
1:B:361:LEU:HD12	1:B:365:GLY:HA2	1.60	0.82
1:A:457:HIS:HE1	6:A:703:ACT:CH3	1.87	0.81
1:B:126:ALA:HB1	1:B:127:PRO:CD	2.10	0.81
1:B:416:ARG:HD2	1:B:418:ASP:OD2	1.81	0.80
1:A:457:HIS:CE1	6:A:703:ACT:CH3	2.60	0.80
1:B:131:CYS:O	1:B:135:VAL:HG12	1.81	0.80
1:A:117:ILE:CG1	1:A:135:VAL:HG11	2.10	0.79
1:B:201:ILE:HD12	1:B:500:ILE:HD12	1.65	0.79
1:A:126:ALA:HB1	1:A:127:PRO:CD	2.12	0.78
1:B:117:ILE:CG1	1:B:135:VAL:HG11	2.12	0.78
1:A:384:PHE:HB3	1:A:399:PRO:HB2	1.64	0.78
1:B:457:HIS:HE1	6:B:703:ACT:H1	1.49	0.77
1:A:201:ILE:HD12	1:A:500:ILE:CD1	2.15	0.76
1:A:156:ALA:O	1:A:160:LEU:HD12	1.84	0.76
1:B:356:GLU:OE1	1:B:356:GLU:N	2.19	0.75
1:B:153:PRO:HA	1:B:154:SER:OG	1.86	0.75
2:H:1:NAG:H62	2:H:2:NAG:O5	1.87	0.74
1:B:575:HIS:CD2	1:B:580:PRO:HD3	2.22	0.74
1:B:250:CYS:O	1:B:487:THR:HG23	1.87	0.74
1:A:210:ASP:HA	1:A:281:ALA:HB2	1.70	0.73
1:B:320:GLU:HB3	1:B:341:LEU:HD21	1.70	0.73
1:A:266:PRO:HA	1:A:267:ALA:HB2	1.70	0.73
1:B:210:ASP:HA	1:B:281:ALA:HB2	1.69	0.73
1:A:296:LEU:HD11	1:A:345:MET:HG2	1.70	0.72
1:B:247:TYR:O	1:B:490:GLY:HA2	1.88	0.72
1:A:109:VAL:O	1:A:112:VAL:HG22	1.89	0.72
1:B:276:THR:CG2	1:B:425:HIS:HA	2.19	0.72
1:B:154:SER:CB	1:B:157:CYS:H	2.03	0.71
1:A:511:VAL:O	1:A:548:THR:OG1	2.08	0.71
1:B:457:HIS:CE1	6:B:703:ACT:CH3	2.66	0.70
1:A:318:ASN:HD21	6:A:703:ACT:H3	1.57	0.70
1:B:271:ASP:O	1:B:272:MET:HG3	1.92	0.70
1:A:361:LEU:HD12	1:A:365:GLY:HA2	1.72	0.70
1:A:267:ALA:HB1	1:A:268:GLY:O	1.92	0.70
1:B:154:SER:HB3	1:B:157:CYS:N	2.07	0.70
1:A:273:VAL:HG21	1:A:307:LEU:CD2	2.22	0.70
1:B:89:CYS:HB3	1:B:90:PRO:HD3	1.73	0.70
1:B:154:SER:HB3	1:B:157:CYS:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LEU:HD23	1:A:606:LEU:HD23	1.74	0.69
1:B:200:ARG:NH1	1:B:499:GLN:HE21	1.90	0.69
1:B:443:VAL:HG21	1:B:466:PHE:CD2	2.27	0.69
1:A:265:GLY:O	1:A:267:ALA:HA	1.92	0.69
1:A:247:TYR:OH	1:A:492:ASN:OD1	2.05	0.69
1:B:458:THR:O	1:B:459:HIS:HB2	1.92	0.68
1:B:438:ASN:O	1:B:442:ILE:HG13	1.94	0.68
1:B:152:SER:O	1:B:154:SER:HA	1.92	0.68
1:B:307:LEU:O	1:B:310:VAL:HG22	1.94	0.68
1:B:149:SER:OG	1:B:150:VAL:N	2.26	0.68
1:A:96:PHE:HB2	1:A:153:PRO:HB3	1.74	0.68
1:B:103:LEU:HD12	1:B:147:ARG:HD3	1.76	0.68
1:A:208:HIS:O	1:A:251:ASP:HB3	1.94	0.67
1:B:187:LYS:CD	1:B:188:PRO:HD2	2.25	0.67
1:A:152:SER:O	1:A:155:GLU:HB2	1.95	0.67
1:A:271:ASP:O	1:A:272:MET:HG3	1.95	0.67
1:B:283:ASP:O	1:B:287:GLN:HG3	1.94	0.67
1:B:307:LEU:HB3	1:B:310:VAL:CG2	2.25	0.67
1:A:113:GLY:O	1:A:117:ILE:HG13	1.94	0.66
1:A:283:ASP:O	1:A:287:GLN:HG3	1.95	0.66
1:A:154:SER:HA	1:A:155:GLU:HB2	1.77	0.66
1:A:307:LEU:O	1:A:310:VAL:HG22	1.95	0.66
1:A:438:ASN:O	1:A:442:ILE:HG13	1.95	0.66
1:A:288:THR:HG22	1:A:290:GLN:H	1.61	0.66
3:E:1:NAG:O4	3:E:2:NAG:O5	2.09	0.66
1:A:307:LEU:HB3	1:A:310:VAL:CG2	2.25	0.66
1:B:515:GLU:OE2	1:B:538:ARG:NH1	2.29	0.65
1:A:318:ASN:HD21	6:A:703:ACT:CH3	2.09	0.65
1:A:176:ILE:HD11	1:A:404:GLN:CB	2.23	0.65
1:A:89:CYS:HB3	1:A:90:PRO:HD3	1.78	0.65
1:B:103:LEU:HD11	1:B:147:ARG:HB2	1.79	0.64
1:B:419:LYS:HD2	1:B:508:SER:O	1.97	0.64
1:A:138:PHE:HE1	1:A:323:PRO:HB3	1.60	0.64
1:A:103:LEU:HD12	1:A:147:ARG:HD3	1.80	0.64
1:A:313:TYR:CD2	1:A:377:LEU:HD13	2.32	0.64
1:A:138:PHE:CE1	1:A:323:PRO:HB3	2.33	0.64
1:A:484:SER:HB2	1:A:486:THR:HG22	1.80	0.64
1:B:176:ILE:HD11	1:B:404:GLN:CB	2.28	0.64
1:B:152:SER:O	1:B:155:GLU:HB2	1.98	0.63
1:B:459:HIS:HA	1:B:484:SER:HB3	1.79	0.63
1:A:143:VAL:HG22	1:B:95:LEU:CD1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LEU:O	1:A:362:ARG:HG3	1.99	0.63
1:A:415:ASP:O	1:A:416:ARG:HB3	1.99	0.62
1:A:443:VAL:HG21	1:A:466:PHE:CD2	2.34	0.62
1:A:103:LEU:HD11	1:A:147:ARG:HB2	1.80	0.62
1:A:276:THR:CG2	1:A:425:HIS:HA	2.29	0.62
1:A:99:ILE:HG21	1:B:99:ILE:HD13	1.82	0.62
1:B:267:ALA:HB1	1:B:268:GLY:CA	2.27	0.61
1:B:96:PHE:CB	1:B:153:PRO:HB3	2.27	0.61
1:B:346:ALA:CB	1:B:358:LEU:HD22	2.31	0.61
1:A:201:ILE:CD1	1:A:500:ILE:HD12	2.30	0.61
1:A:440:TYR:CD2	1:A:600:ARG:HB2	2.35	0.61
1:B:450:LEU:HD21	1:B:453:GLN:HE21	1.65	0.61
1:B:155:GLU:O	1:B:158:GLY:N	2.34	0.61
1:B:294:ARG:O	1:B:298:THR:HG23	2.00	0.61
1:A:153:PRO:HA	1:A:154:SER:OG	2.00	0.61
1:B:346:ALA:HB1	1:B:358:LEU:HD22	1.82	0.60
1:B:201:ILE:HD12	1:B:500:ILE:CD1	2.30	0.60
1:A:444:ALA:O	1:A:447:GLU:HG3	2.01	0.60
1:B:158:GLY:O	1:B:162:GLY:HA2	2.01	0.60
1:A:138:PHE:CD2	1:B:87:LEU:HD12	2.37	0.60
1:A:508:SER:OG	1:A:510:VAL:HG22	2.01	0.60
1:B:508:SER:OG	1:B:510:VAL:HG22	2.01	0.60
1:A:556:LEU:HG	1:A:560:MET:HE2	1.84	0.60
1:B:103:LEU:CD1	1:B:147:ARG:HD3	2.31	0.60
1:B:273:VAL:HG21	1:B:307:LEU:CD2	2.31	0.60
1:A:130:VAL:O	1:A:134:ILE:HG22	2.02	0.59
1:A:294:ARG:O	1:A:298:THR:HG23	2.02	0.59
1:A:219:PRO:HB3	1:A:246:GLU:HG2	1.83	0.59
1:A:450:LEU:HD21	1:A:453:GLN:HE21	1.67	0.59
1:A:235:PRO:HD2	1:A:238:ARG:NH2	2.17	0.59
1:A:250:CYS:O	1:A:487:THR:HG23	2.02	0.59
1:B:154:SER:HB3	1:B:155:GLU:C	2.23	0.59
1:A:314:PRO:HG2	1:A:349:TRP:CD2	2.38	0.59
1:B:519:LEU:HD12	1:B:532:HIS:O	2.03	0.59
1:A:456:GLY:O	1:A:457:HIS:HB3	2.03	0.59
1:B:266:PRO:HA	1:B:267:ALA:HB2	1.85	0.59
1:A:103:LEU:CD1	1:A:147:ARG:HD3	2.33	0.59
1:B:288:THR:HG22	1:B:291:ASP:OD2	2.02	0.59
1:A:346:ALA:HB2	1:A:361:LEU:CD2	2.31	0.58
1:A:276:THR:HG22	1:A:425:HIS:HD1	1.69	0.58
1:B:484:SER:HB2	1:B:486:THR:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:TYR:CG	1:B:573:LEU:HD13	2.38	0.58
1:B:109:VAL:O	1:B:112:VAL:HG22	2.04	0.58
1:B:113:GLY:O	1:B:117:ILE:HG13	2.04	0.58
1:B:254:LEU:HD11	1:B:302:LEU:HD22	1.85	0.58
1:B:207:LEU:HD13	1:B:275:TRP:HE1	1.69	0.57
1:A:142:MET:CG	1:B:91:ILE:HG21	2.33	0.57
1:B:158:GLY:HA2	1:B:165:CYS:O	2.05	0.57
1:A:275:TRP:O	1:A:314:PRO:HA	2.04	0.57
1:B:553:TRP:O	1:B:557:VAL:HG23	2.05	0.57
2:C:1:NAG:H61	2:C:2:NAG:N2	2.20	0.56
1:B:210:ASP:HA	1:B:281:ALA:CB	2.36	0.56
1:B:273:VAL:HB	1:B:312:VAL:HG22	1.86	0.56
1:A:472:LEU:HD23	1:A:606:LEU:CD2	2.34	0.56
1:B:142:MET:O	1:B:145:VAL:HG22	2.06	0.56
1:A:187:LYS:O	1:A:187:LYS:HG3	2.05	0.56
1:A:313:TYR:HD2	1:A:377:LEU:HD13	1.70	0.56
1:B:384:PHE:HB3	1:B:399:PRO:CB	2.32	0.56
1:B:428:PRO:HG3	1:B:439:TYR:CE2	2.40	0.56
1:A:134:ILE:HD11	1:A:138:PHE:CZ	2.41	0.56
1:A:459:HIS:HA	1:A:484:SER:HB3	1.86	0.56
1:B:209:TRP:CZ2	1:B:211:HIS:HB2	2.40	0.56
1:B:275:TRP:O	1:B:314:PRO:HA	2.06	0.56
1:B:403:LEU:HD21	1:B:435:TRP:CH2	2.40	0.56
1:B:461:ASP:CG	1:B:496:ARG:HH22	2.08	0.56
1:B:511:VAL:O	1:B:548:THR:OG1	2.24	0.56
1:A:553:TRP:O	1:A:557:VAL:HG23	2.06	0.56
1:B:102:GLY:O	1:B:108:ASN:ND2	2.37	0.55
1:B:456:GLY:O	1:B:457:HIS:HB3	2.06	0.55
1:A:318:ASN:ND2	1:A:319:HIS:CD2	2.74	0.55
1:A:267:ALA:HB1	1:A:268:GLY:C	2.27	0.55
1:B:458:THR:HG21	1:B:481:LEU:HD23	1.88	0.55
1:A:456:GLY:O	1:A:457:HIS:CB	2.55	0.55
1:A:200:ARG:NH1	1:A:499:GLN:HE21	2.05	0.55
1:A:209:TRP:NE1	1:A:254:LEU:HB2	2.22	0.55
1:B:154:SER:HA	1:B:155:GLU:HB2	1.89	0.55
1:A:210:ASP:O	1:A:211:HIS:HB3	2.06	0.55
1:A:424:GLY:O	1:A:455:PHE:HA	2.07	0.55
1:B:125:ILE:O	1:B:125:ILE:HG23	2.06	0.55
1:A:248:SER:O	1:A:250:CYS:SG	2.64	0.55
1:A:152:SER:O	1:A:154:SER:HA	2.06	0.54
1:B:461:ASP:OD2	1:B:496:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:GLU:HG3	1:B:448:ASN:H	1.72	0.54
1:B:210:ASP:O	1:B:211:HIS:HB3	2.08	0.54
1:A:125:ILE:O	1:A:125:ILE:HG23	2.06	0.54
1:A:90:PRO:HB3	1:B:119:LEU:HB2	1.90	0.53
1:A:95:LEU:O	1:A:99:ILE:HG13	2.08	0.53
1:B:380:LEU:HB3	1:B:382:MET:HE1	1.90	0.53
1:B:324:VAL:O	1:B:325:ASN:HB2	2.09	0.53
1:B:84:TRP:CZ3	1:B:88:THR:HG22	2.43	0.53
1:A:208:HIS:HB2	1:A:486:THR:HB	1.90	0.53
1:A:491:LEU:HB3	1:A:576:LYS:HE3	1.90	0.53
1:A:86:ASN:OD1	7:A:704:NAG:N2	2.41	0.53
1:A:307:LEU:HD23	1:A:310:VAL:HG21	1.91	0.53
1:A:296:LEU:HD11	1:A:345:MET:CG	2.37	0.53
1:A:376:ARG:O	1:A:420:VAL:HA	2.09	0.53
1:A:555:ASN:O	1:A:559:ARG:HB2	2.10	0.52
1:B:447:GLU:HG3	1:B:448:ASN:N	2.24	0.52
1:B:322:THR:HA	1:B:323:PRO:C	2.30	0.52
1:B:457:HIS:ND1	6:B:703:ACT:H1	2.16	0.52
1:A:138:PHE:HD2	1:B:87:LEU:HD12	1.73	0.52
1:A:149:SER:OG	1:A:150:VAL:N	2.41	0.52
1:B:382:MET:HE2	1:B:382:MET:HA	1.91	0.52
1:B:296:LEU:HD11	1:B:345:MET:HG2	1.92	0.52
1:A:142:MET:O	1:A:145:VAL:HG22	2.10	0.52
1:A:455:PHE:O	1:A:481:LEU:HA	2.10	0.52
1:A:461:ASP:CG	1:A:496:ARG:HH22	2.14	0.52
1:B:208:HIS:O	1:B:251:ASP:HB3	2.09	0.51
1:A:537:TYR:CG	1:A:573:LEU:HD13	2.45	0.51
1:B:491:LEU:HB3	1:B:576:LYS:HE3	1.92	0.51
1:A:322:THR:HA	1:A:323:PRO:C	2.30	0.51
1:B:537:TYR:CD1	1:B:573:LEU:HD13	2.46	0.51
1:B:208:HIS:CD2	1:B:486:THR:HG21	2.46	0.51
1:A:345:MET:O	1:A:346:ALA:HB3	2.11	0.51
1:A:159:LEU:HD13	1:A:168:TRP:CD2	2.46	0.51
1:A:213:TYR:CZ	1:A:245:GLY:HA2	2.46	0.50
1:B:208:HIS:HB2	1:B:486:THR:HB	1.94	0.50
1:A:450:LEU:HD23	1:A:450:LEU:O	2.11	0.50
1:B:575:HIS:NE2	1:B:580:PRO:HD3	2.26	0.50
1:A:143:VAL:HG22	1:B:95:LEU:HD11	1.92	0.50
1:A:197:PRO:HD2	1:A:504:TYR:CD1	2.46	0.50
1:B:369:LEU:HD12	1:B:371:PRO:HD3	1.94	0.50
1:A:369:LEU:HD12	1:A:371:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:LYS:HG2	1:B:249:LYS:O	2.12	0.50
1:A:378:ILE:HG21	1:A:406:LEU:HD13	1.93	0.50
1:A:155:GLU:O	1:A:158:GLY:N	2.45	0.49
1:A:554:HIS:CE1	1:A:558:TYR:HE2	2.30	0.49
1:B:345:MET:O	1:B:346:ALA:HB3	2.11	0.49
1:A:415:ASP:O	1:A:416:ARG:CB	2.58	0.49
1:A:377:LEU:HD23	1:A:378:ILE:N	2.27	0.49
1:B:485:ALA:HA	1:B:494:GLY:O	2.12	0.49
1:A:99:ILE:CG2	1:B:99:ILE:HD13	2.41	0.49
1:A:403:LEU:HD21	1:A:435:TRP:CH2	2.47	0.49
1:B:456:GLY:O	1:B:457:HIS:CB	2.60	0.49
1:B:554:HIS:CE1	1:B:558:TYR:HE2	2.28	0.49
1:B:224:PRO:HB2	1:B:285:TRP:HZ3	1.77	0.49
1:A:605:ALA:O	1:A:608:ARG:HG2	2.13	0.49
1:A:276:THR:CG2	1:A:425:HIS:HD1	2.26	0.49
1:A:586:THR:OG1	1:A:587:PRO:HD3	2.13	0.49
1:A:208:HIS:CD2	1:A:486:THR:HG21	2.48	0.49
1:A:217:THR:OG1	1:A:227:CYS:HA	2.13	0.49
1:A:320:GLU:HB3	1:A:341:LEU:HD21	1.95	0.49
1:A:252:LEU:HD11	1:A:485:ALA:O	2.13	0.49
1:A:158:GLY:HA2	1:A:165:CYS:O	2.12	0.48
1:A:303:VAL:HG13	1:A:307:LEU:HD13	1.95	0.48
1:B:212:ASP:O	1:B:228:ARG:HA	2.12	0.48
1:B:583:PRO:O	1:B:584:CYS:HB3	2.12	0.48
1:B:537:TYR:CD1	1:B:573:LEU:HD22	2.49	0.48
1:A:324:VAL:O	1:A:325:ASN:HB2	2.13	0.48
1:A:247:TYR:O	1:A:490:GLY:HA2	2.14	0.48
1:B:154:SER:CB	1:B:157:CYS:HB2	2.44	0.48
1:B:221:CYS:SG	1:B:223:ASP:HB2	2.54	0.47
1:A:197:PRO:HD2	1:A:504:TYR:CE1	2.49	0.47
1:B:209:TRP:CE2	1:B:211:HIS:HB2	2.50	0.47
1:B:328:PRO:HB2	1:B:332:ILE:HB	1.96	0.47
1:A:267:ALA:HB1	1:A:268:GLY:CA	2.44	0.47
1:B:437:TRP:CD2	1:B:600:ARG:HD2	2.49	0.47
1:A:210:ASP:HA	1:A:281:ALA:CB	2.42	0.47
1:B:131:CYS:O	1:B:134:ILE:HG22	2.15	0.47
1:B:244:TRP:CZ2	1:B:531:PRO:HG3	2.50	0.47
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.97	0.47
1:B:303:VAL:HG13	1:B:307:LEU:HD13	1.97	0.47
1:A:556:LEU:HG	1:A:560:MET:CE	2.45	0.47
1:B:126:ALA:CB	1:B:127:PRO:CD	2.85	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:GLY:HA2	1:B:425:HIS:CG	2.50	0.47
1:B:584:CYS:SG	1:B:585:GLY:N	2.88	0.47
1:B:380:LEU:HB3	1:B:382:MET:CE	2.45	0.46
1:B:95:LEU:O	1:B:99:ILE:HG13	2.15	0.46
1:B:380:LEU:CB	1:B:382:MET:HE1	2.45	0.46
1:B:513:ASP:OD1	1:B:514:HIS:N	2.43	0.46
1:B:176:ILE:O	1:B:177:SER:OG	2.30	0.46
1:B:560:MET:HE3	1:B:570:PHE:HB3	1.96	0.46
1:A:91:ILE:O	1:A:95:LEU:HB2	2.16	0.46
1:A:279:ILE:HB	1:A:280:PRO:HD3	1.97	0.46
1:B:217:THR:OG1	1:B:227:CYS:HA	2.15	0.46
1:A:143:VAL:HG22	1:B:95:LEU:HD13	1.97	0.46
1:A:461:ASP:OD2	1:A:496:ARG:NH2	2.49	0.45
1:A:561:ARG:HH21	1:A:611:MET:HE2	1.81	0.45
1:B:425:HIS:NE2	1:B:457:HIS:ND1	2.65	0.45
1:B:208:HIS:HD2	1:B:486:THR:HG21	1.81	0.45
1:A:254:LEU:HD11	1:A:302:LEU:HD22	1.99	0.45
1:A:99:ILE:HD13	1:B:99:ILE:HG21	1.99	0.45
1:B:318:ASN:ND2	1:B:319:HIS:CD2	2.84	0.45
1:B:334:GLY:HA2	1:B:337:SER:H	1.81	0.45
1:A:176:ILE:O	1:A:177:SER:OG	2.33	0.45
1:A:90:PRO:HA	1:B:119:LEU:HD13	1.98	0.45
1:B:226:CYS:SG	1:B:249:LYS:HE3	2.56	0.45
1:B:314:PRO:HG2	1:B:349:TRP:CD2	2.52	0.45
1:B:346:ALA:HB2	1:B:361:LEU:HD23	1.98	0.45
1:B:450:LEU:O	1:B:450:LEU:HD23	2.15	0.45
1:A:139:GLU:HG3	1:A:140:ASP:N	2.31	0.45
1:A:318:ASN:ND2	6:A:703:ACT:CH3	2.78	0.45
1:B:374:GLY:HA2	1:B:418:ASP:HB3	1.98	0.45
1:B:468:ASP:O	1:B:472:LEU:HD23	2.17	0.45
1:B:134:ILE:HG23	1:B:135:VAL:N	2.31	0.45
1:B:153:PRO:CA	1:B:154:SER:OG	2.61	0.45
1:B:207:LEU:HD12	1:B:207:LEU:N	2.32	0.45
1:A:229:ARG:CZ	1:A:229:ARG:HB3	2.45	0.45
1:B:139:GLU:HG3	1:B:140:ASP:N	2.32	0.45
1:B:200:ARG:HH21	1:B:268:GLY:H	1.65	0.45
1:B:382:MET:HA	1:B:382:MET:CE	2.46	0.45
1:A:318:ASN:ND2	1:A:319:HIS:HD2	2.14	0.45
1:B:592:THR:O	1:B:596:GLN:HG2	2.17	0.45
1:A:108:ASN:O	1:A:112:VAL:HG13	2.17	0.44
1:A:141:ASP:O	1:A:145:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LYS:NZ	1:B:188:PRO:HG2	2.31	0.44
1:B:288:THR:CG2	1:B:291:ASP:OD2	2.66	0.44
1:B:160:LEU:C	1:B:161:LEU:HD23	2.38	0.44
1:A:276:THR:HG23	1:A:425:HIS:HA	1.99	0.44
1:B:219:PRO:HB3	1:B:246:GLU:HG2	1.98	0.44
1:A:142:MET:HB2	1:A:142:MET:HE2	1.88	0.44
1:B:560:MET:HE2	1:B:593:LEU:HD21	1.99	0.44
1:B:318:ASN:ND2	1:B:319:HIS:HD2	2.15	0.44
1:A:346:ALA:HB1	1:A:358:LEU:HD22	2.00	0.43
1:B:179:PRO:HD3	1:B:407:VAL:HG11	2.00	0.43
1:B:536:LEU:HD12	1:B:536:LEU:HA	1.88	0.43
1:A:158:GLY:O	1:A:162:GLY:HA2	2.17	0.43
1:B:384:PHE:CB	1:B:399:PRO:HB2	2.36	0.43
1:B:155:GLU:O	1:B:156:ALA:C	2.54	0.43
1:B:345:MET:C	1:B:347:LYS:H	2.22	0.43
1:B:376:ARG:O	1:B:420:VAL:HA	2.18	0.43
1:B:154:SER:HB2	1:B:157:CYS:HB2	2.01	0.43
1:A:207:LEU:N	1:A:207:LEU:HD12	2.34	0.43
1:A:288:THR:O	1:A:292:GLN:HG2	2.19	0.43
1:A:382:MET:O	1:A:385:CYS:HB3	2.19	0.43
1:B:138:PHE:CE1	1:B:323:PRO:HB3	2.54	0.43
1:A:209:TRP:CZ3	1:A:295:ALA:HA	2.54	0.43
1:A:334:GLY:HA2	1:A:337:SER:H	1.84	0.43
1:B:317:GLY:HA2	1:B:425:HIS:CB	2.49	0.43
1:A:208:HIS:HD2	1:A:486:THR:HG21	1.83	0.43
1:A:513:ASP:OD1	1:A:514:HIS:N	2.44	0.43
1:B:366:PHE:HB2	1:B:379:SER:O	2.18	0.43
1:B:387:ARG:HH21	1:B:601:ALA:HB1	1.84	0.43
1:B:387:ARG:NH2	1:B:601:ALA:HB1	2.34	0.43
1:B:586:THR:HB	1:B:587:PRO:HD3	2.01	0.43
1:A:293:LEU:HD22	1:A:344:ALA:CB	2.48	0.42
1:A:535:LEU:O	1:A:535:LEU:HG	2.19	0.42
1:A:134:ILE:HG23	1:A:135:VAL:N	2.35	0.42
1:A:313:TYR:CE2	1:A:371:PRO:HG3	2.54	0.42
1:B:357:ALA:HA	1:B:367:TYR:HB2	2.01	0.42
1:B:201:ILE:CD1	1:B:500:ILE:HD12	2.43	0.42
1:B:560:MET:HE2	1:B:567:PHE:HD1	1.84	0.42
1:A:345:MET:C	1:A:347:LYS:H	2.23	0.42
1:B:105:LYS:HB3	1:B:107:PRO:HD2	2.01	0.42
1:A:496:ARG:HG3	1:A:497:VAL:N	2.35	0.42
1:A:206:ASP:O	1:A:486:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:TRP:HZ3	1:A:295:ALA:HA	1.85	0.42
1:A:314:PRO:HB2	1:A:349:TRP:CH2	2.54	0.42
1:A:592:THR:O	1:A:596:GLN:HG2	2.20	0.42
1:A:95:LEU:HD12	1:A:95:LEU:HA	1.91	0.42
1:B:176:ILE:HD11	1:B:404:GLN:CA	2.49	0.42
1:A:493:PRO:O	1:A:518:ILE:HA	2.19	0.42
1:B:358:LEU:O	1:B:362:ARG:HG3	2.20	0.42
1:A:213:TYR:OH	1:A:245:GLY:HA2	2.20	0.41
1:A:450:LEU:C	1:A:450:LEU:HD23	2.40	0.41
1:A:494:GLY:HA2	1:A:517:TYR:O	2.20	0.41
1:B:141:ASP:O	1:B:144:GLU:HB3	2.20	0.41
1:B:560:MET:CE	1:B:567:PHE:HD1	2.33	0.41
1:A:95:LEU:HD23	1:B:146:TRP:CE3	2.55	0.41
1:B:424:GLY:O	1:B:455:PHE:HA	2.20	0.41
1:B:535:LEU:O	1:B:535:LEU:HG	2.19	0.41
1:A:170:ILE:HD12	1:A:393:LEU:O	2.21	0.41
1:A:476:LEU:O	1:A:477:ALA:HB2	2.20	0.41
1:B:346:ALA:HA	1:B:358:LEU:HD22	2.02	0.41
1:A:117:ILE:HD13	1:A:132:GLN:HA	2.01	0.41
1:B:187:LYS:HZ3	1:B:188:PRO:HG2	1.85	0.41
1:B:467:TYR:OH	1:B:597:LEU:HD22	2.20	0.41
1:B:117:ILE:HD13	1:B:132:GLN:HG3	2.03	0.41
1:B:218:ASP:CG	1:B:238:ARG:HH21	2.24	0.41
1:A:288:THR:HG22	1:A:290:GLN:N	2.31	0.41
1:B:426:ILE:HG12	1:B:457:HIS:CD2	2.56	0.41
1:B:91:ILE:O	1:B:95:LEU:HB2	2.20	0.41
1:A:265:GLY:C	1:A:267:ALA:HA	2.40	0.41
1:B:455:PHE:O	1:B:481:LEU:HA	2.21	0.41
1:B:574:TYR:HD2	1:B:575:HIS:CE1	2.39	0.41
1:A:518:ILE:HD12	1:A:518:ILE:C	2.41	0.41
1:B:296:LEU:C	1:B:296:LEU:HD23	2.41	0.41
1:A:126:ALA:CB	1:A:127:PRO:CD	2.86	0.41
1:B:159:LEU:HD13	1:B:168:TRP:CD2	2.55	0.41
1:B:87:LEU:O	1:B:90:PRO:HD2	2.21	0.41
1:B:203:PHE:CE1	1:B:454:PHE:HB3	2.55	0.41
1:B:377:LEU:HD21	1:B:423:ILE:CD1	2.51	0.41
1:A:318:ASN:CG	1:A:319:HIS:HD2	2.24	0.40
1:A:369:LEU:HD12	1:A:369:LEU:C	2.41	0.40
1:A:377:LEU:HD23	1:A:377:LEU:C	2.41	0.40
1:B:154:SER:OG	1:B:157:CYS:SG	2.77	0.40
1:B:169:ASP:O	1:B:172:SER:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:HD12	1:A:250:CYS:H	1.85	0.40
1:A:491:LEU:HD13	1:A:576:LYS:HE2	2.03	0.40
1:A:318:ASN:ND2	6:A:703:ACT:H3	2.32	0.40
1:B:252:LEU:HD11	1:B:485:ALA:O	2.21	0.40
1:B:377:LEU:HD23	1:B:378:ILE:N	2.36	0.40
1:A:99:ILE:HG23	1:B:99:ILE:HG23	2.03	0.40
1:A:276:THR:HG21	1:A:425:HIS:HA	2.02	0.40
1:A:570:PHE:O	1:A:574:TYR:HB2	2.22	0.40
1:A:159:LEU:HD13	1:A:168:TRP:CE3	2.56	0.40
1:B:200:ARG:NH1	1:B:499:GLN:NE2	2.65	0.40
1:B:313:TYR:CD1	1:B:369:LEU:HD21	2.57	0.40
1:B:375:LEU:HD12	1:B:419:LYS:O	2.21	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	527/586 (90%)	485 (92%)	40 (8%)	2 (0%)	34	66
1	B	528/586 (90%)	490 (93%)	36 (7%)	2 (0%)	34	66
All	All	1055/1172 (90%)	975 (92%)	76 (7%)	4 (0%)	34	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	432	LEU
1	B	432	LEU
1	B	125	ILE
1	A	125	ILE

### 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	448/496 (90%)	445 (99%)	3 (1%)	84	95
1	B	449/496 (90%)	446 (99%)	3 (1%)	84	95
All	All	897/992 (90%)	891 (99%)	6 (1%)	84	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	385	CYS
1	A	402	GLN
1	A	435	TRP
1	B	288	THR
1	B	385	CYS
1	B	435	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	HIS
1	A	453	GLN
1	A	499	GLN
1	B	319	HIS
1	B	499	GLN
1	B	555	ASN

### 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 ⓘ

16 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$
2	NAG	C	1	1,2	14,14,15	0.31	0	17,19,21	0.92	1 (5%)
2	NAG	C	2	2	14,14,15	0.28	0	17,19,21	0.85	0
2	NAG	D	1	1,2	14,14,15	0.31	0	17,19,21	0.89	0
2	NAG	D	2	2	14,14,15	0.30	0	17,19,21	0.75	0
3	NAG	E	1	1,3	14,14,15	0.31	0	17,19,21	1.52	2 (11%)
3	NAG	E	2	3	14,14,15	0.34	0	17,19,21	0.88	0
4	NAG	F	1	1,4	14,14,15	0.31	0	17,19,21	0.91	1 (5%)
4	NAG	F	2	4	14,14,15	0.27	0	17,19,21	0.79	0
4	MAN	F	3	4	11,11,12	0.29	0	15,15,17	0.78	1 (6%)
4	NAG	G	1	1,4	14,14,15	0.29	0	17,19,21	0.92	1 (5%)
4	NAG	G	2	4	14,14,15	0.35	0	17,19,21	0.89	1 (5%)
4	MAN	G	3	4	11,11,12	0.33	0	15,15,17	0.92	1 (6%)
2	NAG	H	1	1,2	14,14,15	0.34	0	17,19,21	1.47	2 (11%)
2	NAG	H	2	2	14,14,15	0.46	0	17,19,21	0.91	1 (5%)
2	NAG	I	1	1,2	14,14,15	0.42	0	17,19,21	1.20	1 (5%)
2	NAG	I	2	2	14,14,15	0.30	0	17,19,21	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	MAN	F	3	4	-	1/2/19/22	1/1/1/1
4	NAG	G	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	MAN	G	3	4	-	0/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	NAG	C1-O5-C5	5.22	119.27	112.19
3	E	1	NAG	C1-O5-C5	5.01	118.97	112.19
2	I	1	NAG	C4-C3-C2	3.87	116.69	111.02
3	E	1	NAG	C4-C3-C2	-2.83	106.86	111.02
2	H	2	NAG	C1-O5-C5	2.77	115.95	112.19
4	G	3	MAN	C1-O5-C5	2.55	115.64	112.19
4	F	3	MAN	C1-O5-C5	2.44	115.49	112.19
4	G	2	NAG	O5-C1-C2	-2.17	107.85	111.29
2	H	1	NAG	O4-C4-C5	2.10	114.50	109.30
2	C	1	NAG	C1-O5-C5	2.05	114.97	112.19
4	F	1	NAG	C1-O5-C5	2.03	114.95	112.19
4	G	1	NAG	O5-C1-C2	-2.03	108.08	111.29

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C1-C2-N2-C7
2	C	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
4	F	3	MAN	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
4	F	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6

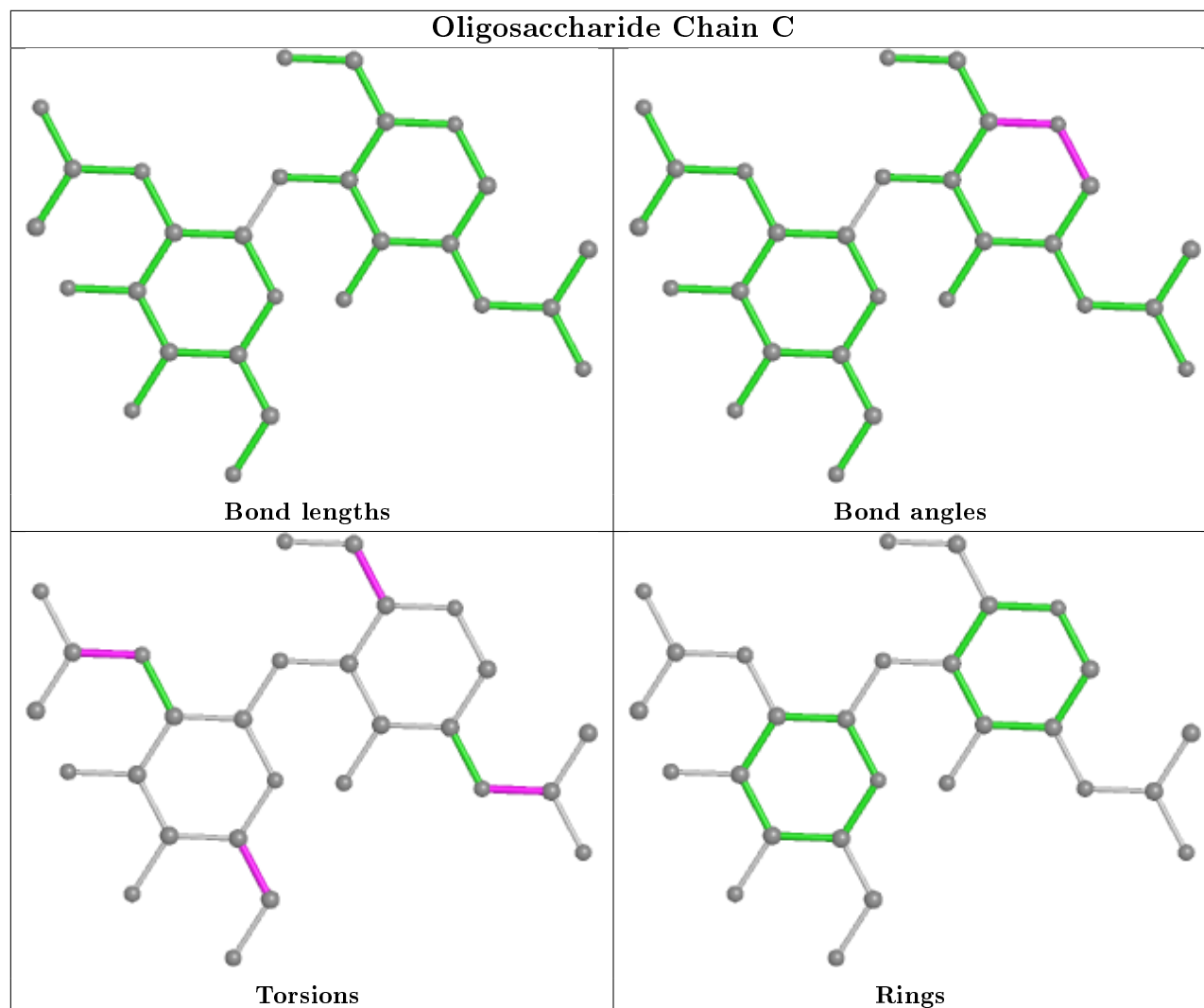
All (1) ring outliers are listed below:

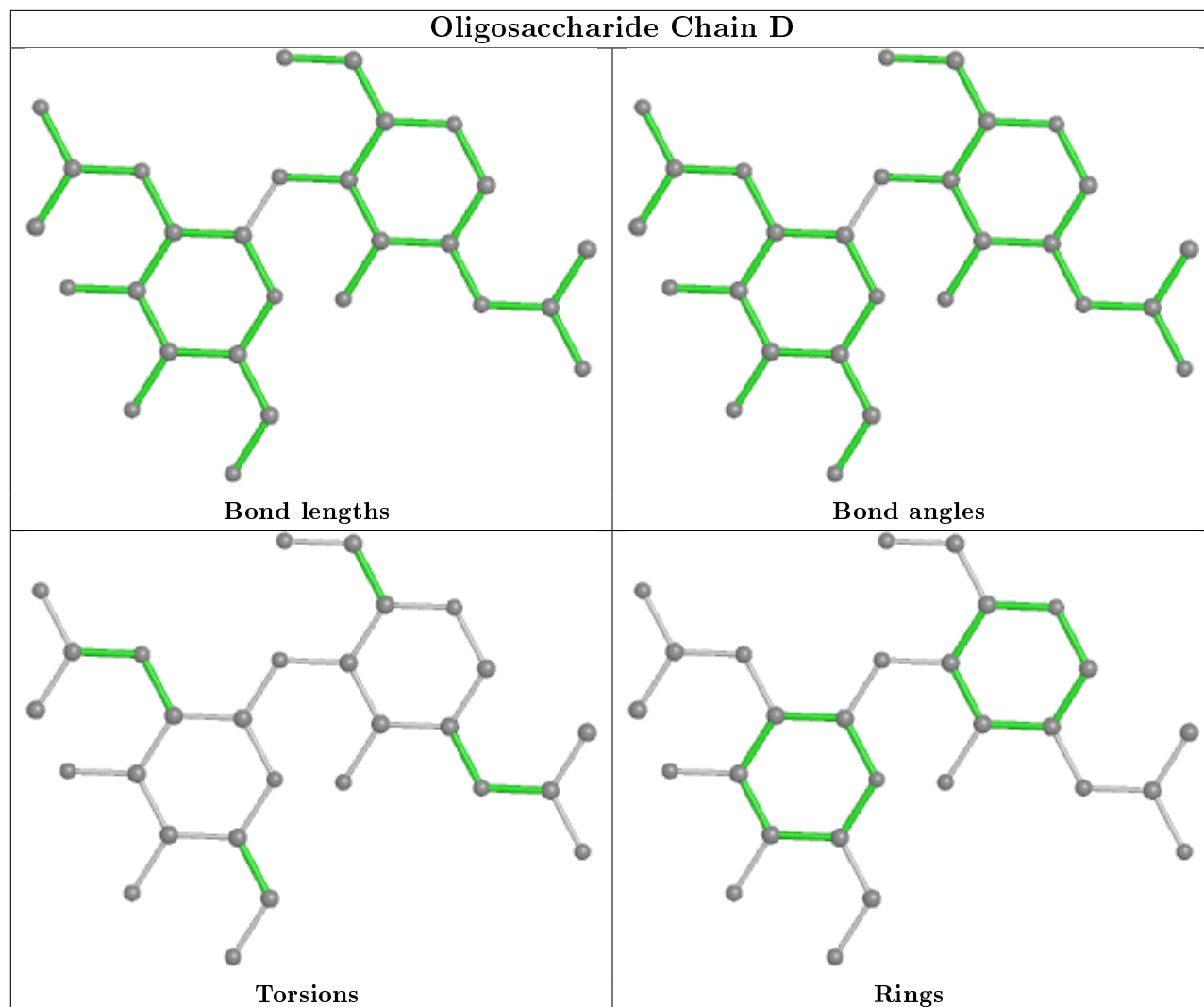
Mol	Chain	Res	Type	Atoms
4	F	3	MAN	C1-C2-C3-C4-C5-O5

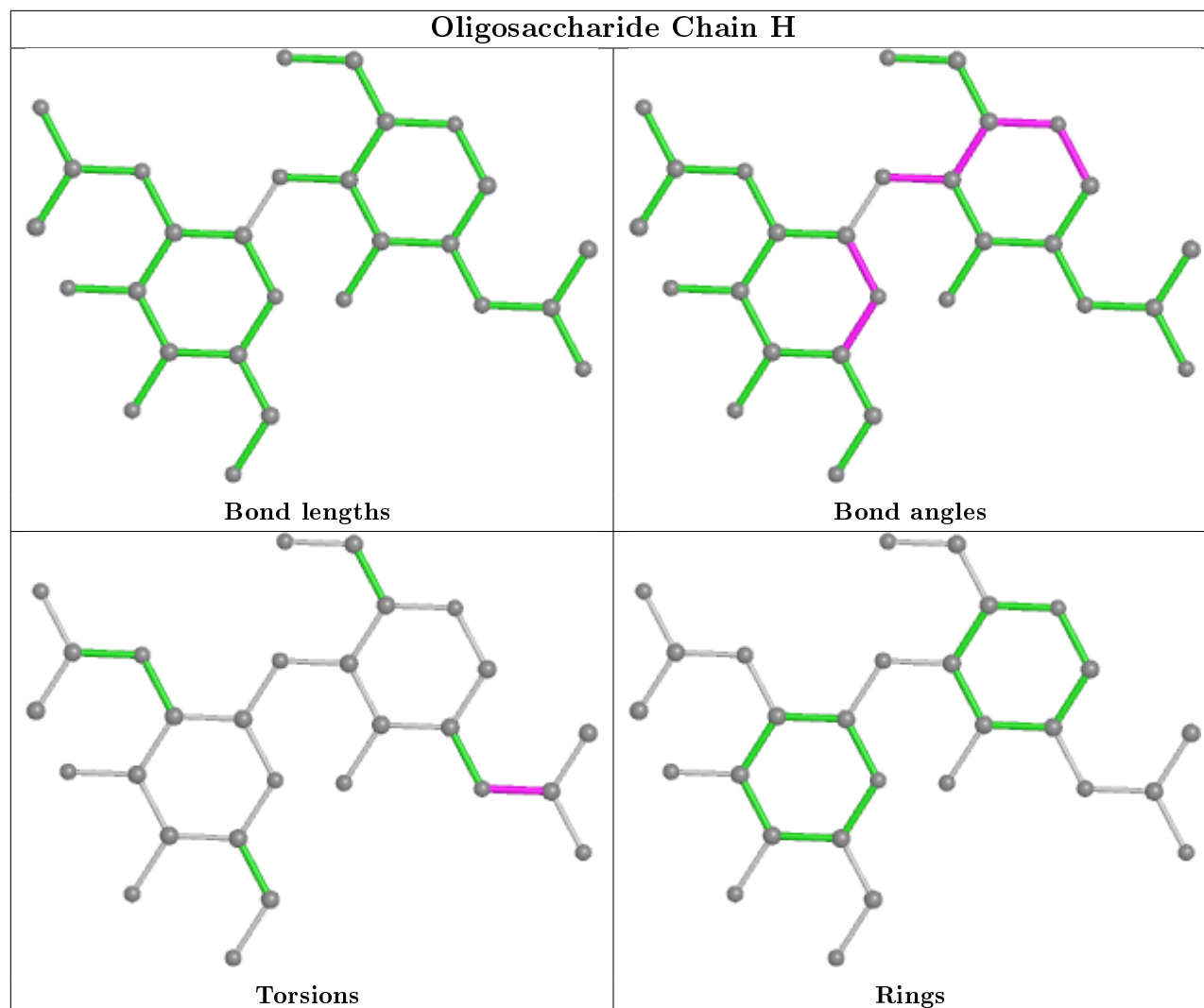
6 monomers are involved in 3 short contacts:

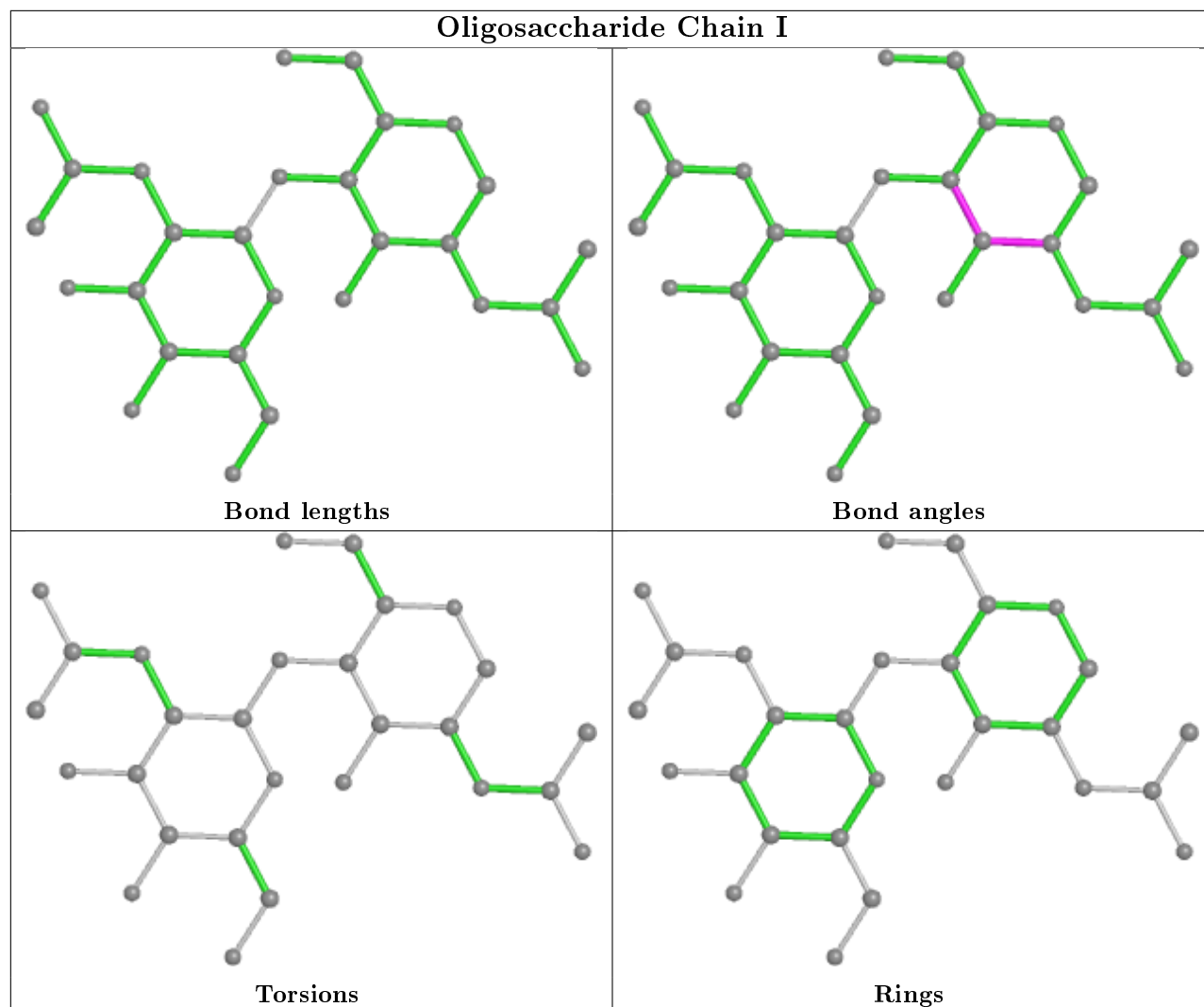
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0
2	H	2	NAG	1	0
3	E	1	NAG	1	0
2	C	2	NAG	1	0
2	C	1	NAG	1	0
3	E	2	NAG	1	0

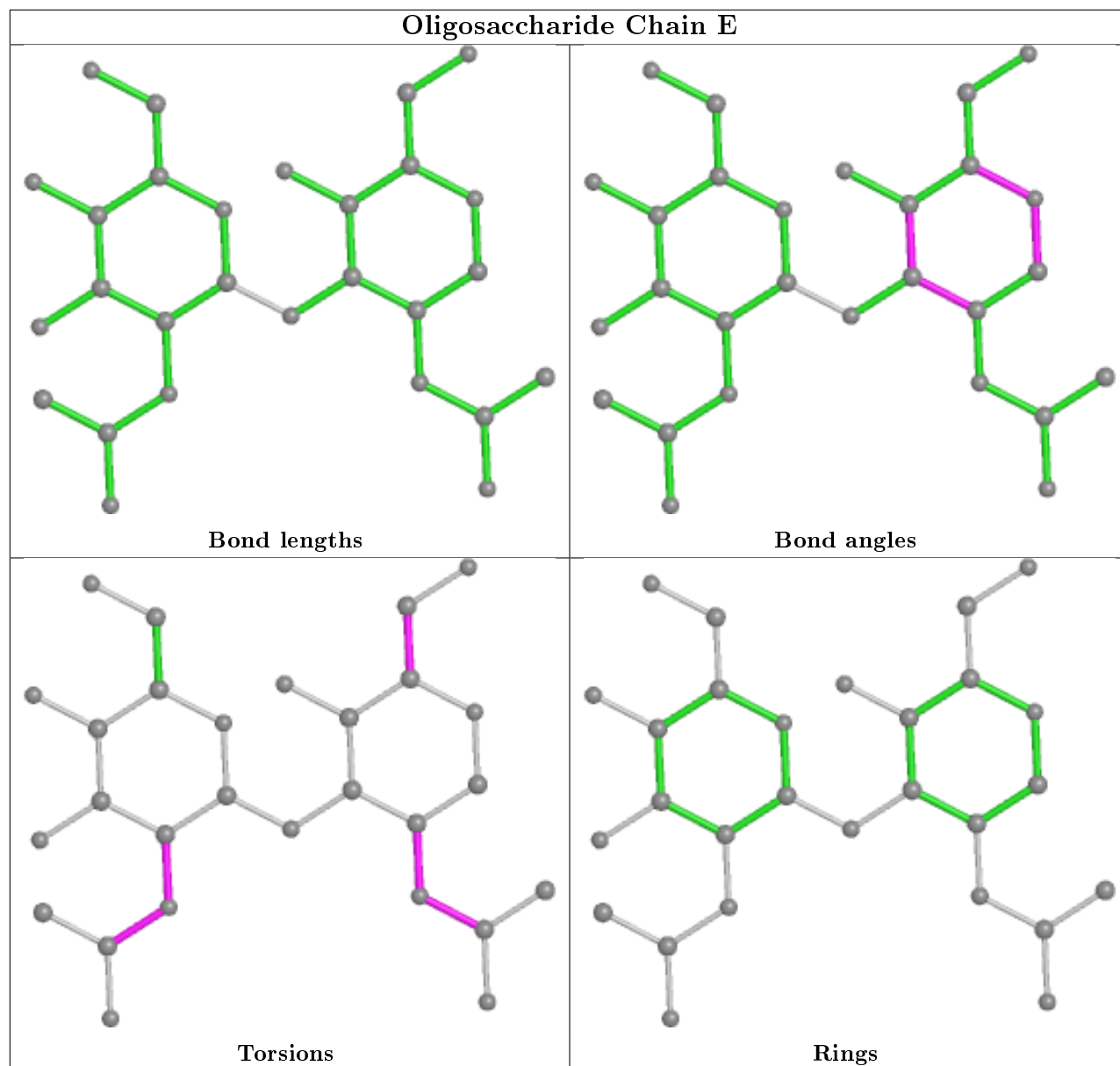
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



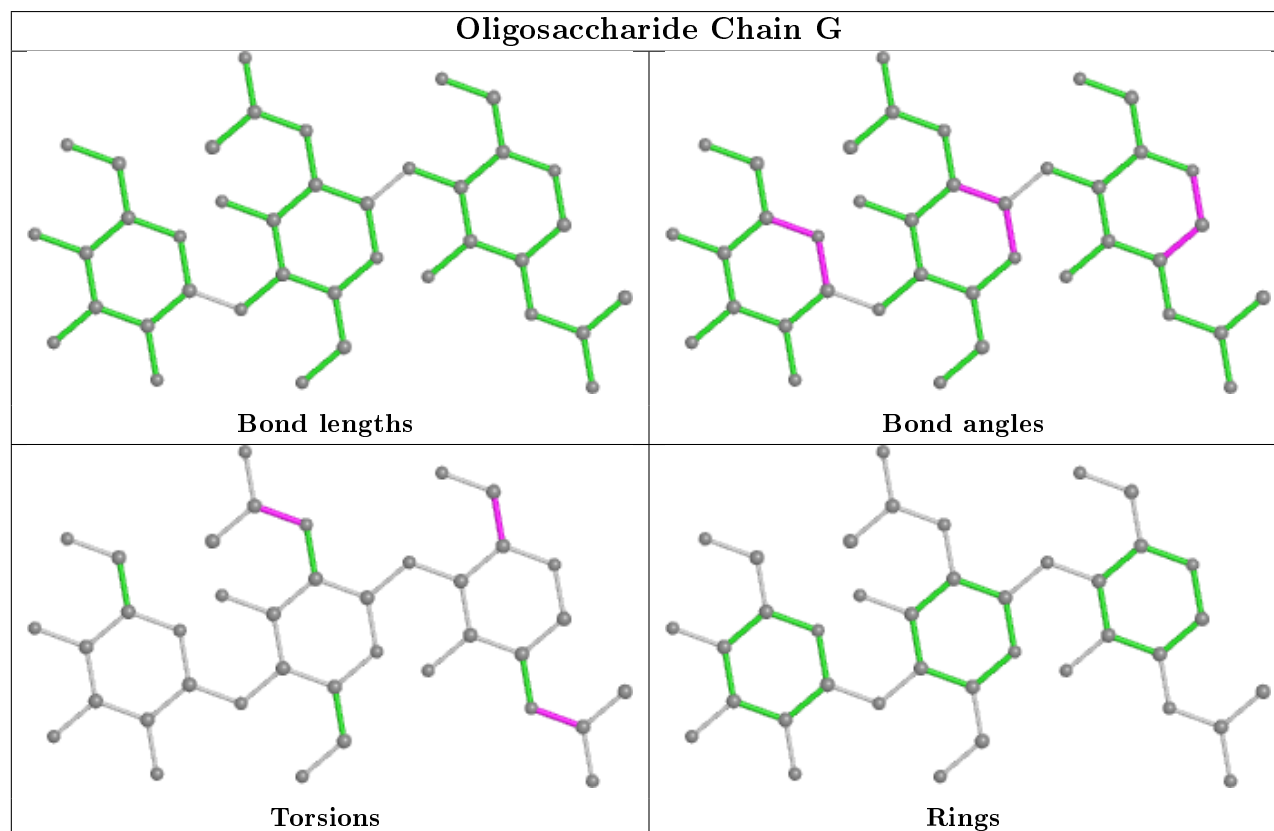
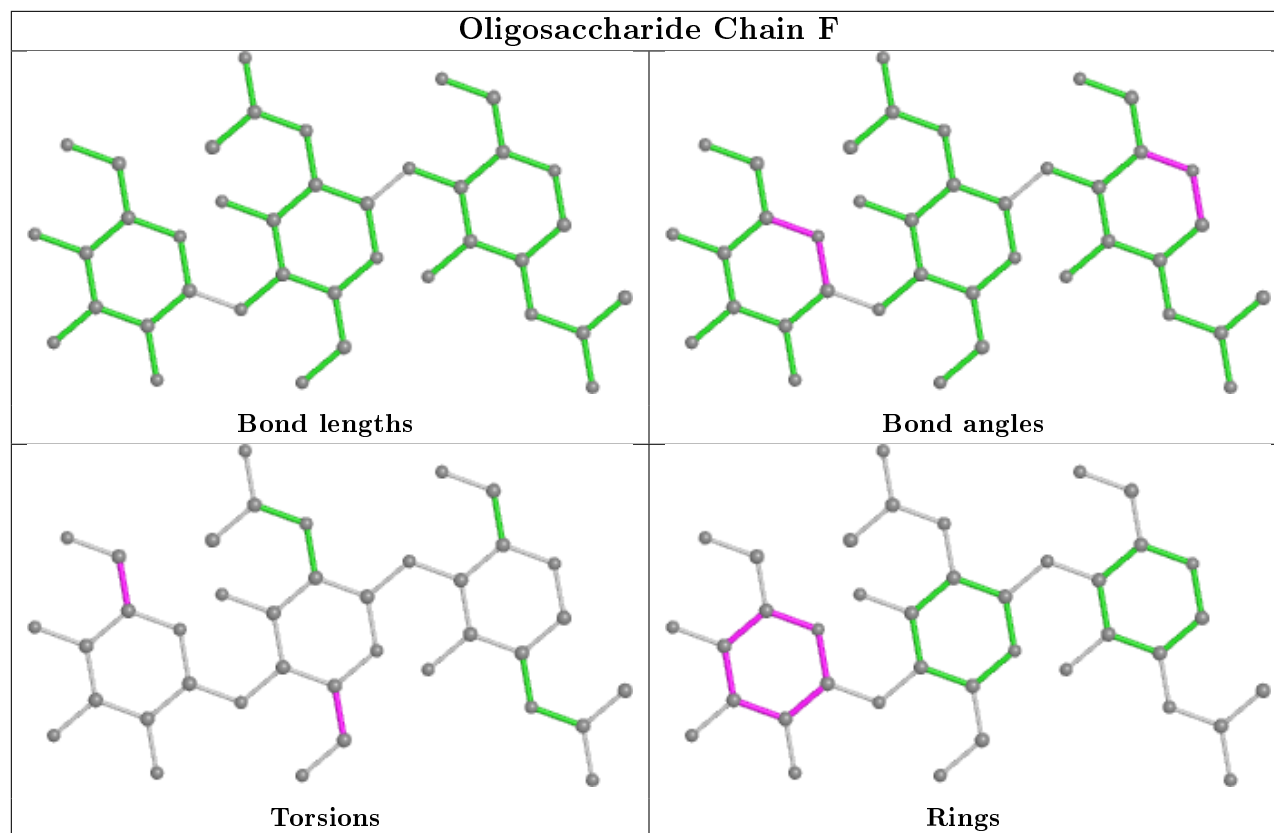












## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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
6	ACT	A	703	5	1,3,3	4.03	1 (100%)	0,3,3	0.00	-
6	ACT	B	703	5	1,3,3	1.85	0	0,3,3	0.00	-
7	NAG	B	704	1	14,14,15	0.37	0	17,19,21	1.31	1 (5%)
7	NAG	A	705	1	14,14,15	0.52	0	17,19,21	1.09	1 (5%)
7	NAG	A	712	1	14,14,15	0.28	0	17,19,21	0.73	0
7	NAG	A	704	1	14,14,15	0.38	0	17,19,21	1.26	2 (11%)
7	NAG	B	705	1	14,14,15	0.31	0	17,19,21	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	704	1	-	4/6/23/26	0/1/1/1
7	NAG	A	704	1	-	0/6/23/26	0/1/1/1
7	NAG	A	712	1	-	2/6/23/26	0/1/1/1
7	NAG	B	705	1	-	0/6/23/26	0/1/1/1
7	NAG	A	705	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703	ACT	CH3-C	4.03	1.53	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	704	NAG	C1-O5-C5	4.99	118.95	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	704	NAG	C1-O5-C5	4.39	118.14	112.19
7	A	705	NAG	C4-C3-C2	2.72	115.00	111.02
7	A	704	NAG	O5-C1-C2	2.23	114.81	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	712	NAG	C8-C7-N2-C2
7	A	712	NAG	O7-C7-N2-C2
7	B	704	NAG	C4-C5-C6-O6
7	B	704	NAG	C1-C2-N2-C7
7	B	704	NAG	O5-C5-C6-O6
7	B	704	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	703	ACT	8	0
6	B	703	ACT	4	0
7	B	704	NAG	1	0
7	A	704	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	529/586 (90%)	-0.10	12 (2%)	60 51	34, 57, 89, 125	0
1	B	530/586 (90%)	-0.08	13 (2%)	57 47	33, 58, 91, 133	0
All	All	1059/1172 (90%)	-0.09	25 (2%)	59 49	33, 57, 91, 133	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	452	ALA	3.4
1	A	237	SER	3.3
1	A	238	ARG	2.8
1	B	452	ALA	2.8
1	B	84	TRP	2.7
1	A	83	GLY	2.7
1	B	277	GLY	2.7
1	B	164	THR	2.6
1	B	125	ILE	2.6
1	B	230	GLY	2.5
1	B	238	ARG	2.4
1	A	424	GLY	2.4
1	B	252	LEU	2.3
1	B	195	GLY	2.3
1	A	432	LEU	2.3
1	B	584	CYS	2.2
1	B	237	SER	2.2
1	A	276	THR	2.2
1	A	126	ALA	2.2
1	A	176	ILE	2.2
1	A	379	SER	2.1
1	A	584	CYS	2.1
1	B	602	ASP	2.1
1	B	196	ALA	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	277	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

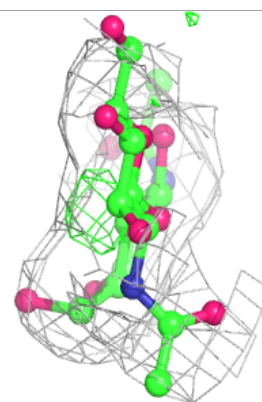
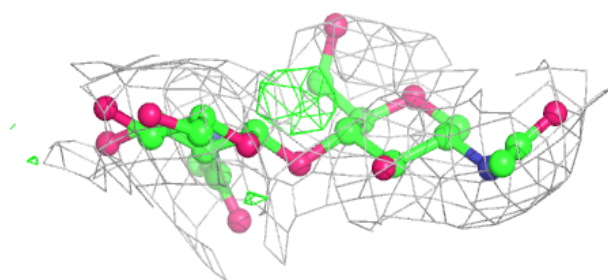
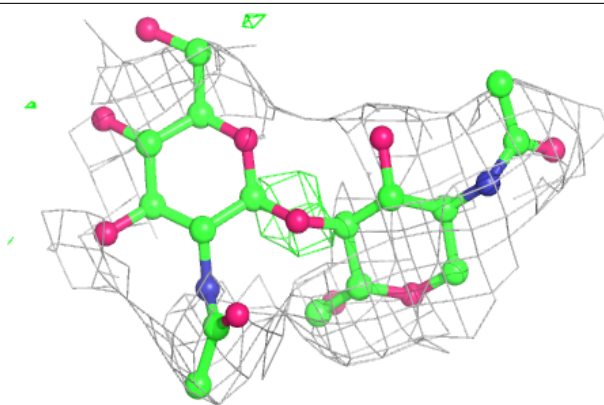
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MAN	F	3	11/12	0.70	0.24	76,92,110,117	0
3	NAG	E	2	14/15	0.78	0.22	60,88,109,116	0
4	MAN	G	3	11/12	0.81	0.34	107,135,161,163	0
2	NAG	I	2	14/15	0.82	0.36	111,132,142,147	0
2	NAG	D	2	14/15	0.83	0.43	105,126,149,153	0
2	NAG	H	2	14/15	0.85	0.29	94,114,134,154	0
2	NAG	D	1	14/15	0.86	0.29	65,84,106,114	0
2	NAG	I	1	14/15	0.86	0.22	31,90,119,126	0
2	NAG	H	1	14/15	0.87	0.19	80,98,108,119	0
2	NAG	C	2	14/15	0.88	0.18	74,98,111,116	0
4	NAG	G	1	14/15	0.88	0.23	75,87,100,100	0
4	NAG	G	2	14/15	0.89	0.21	69,99,121,125	0
3	NAG	E	1	14/15	0.92	0.12	52,78,88,97	0
4	NAG	F	2	14/15	0.94	0.10	47,71,88,91	0
4	NAG	F	1	14/15	0.94	0.10	35,42,47,54	0
2	NAG	C	1	14/15	0.95	0.12	40,62,69,71	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.

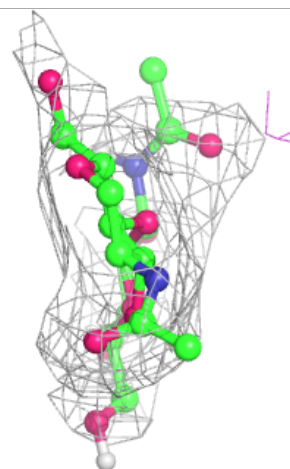
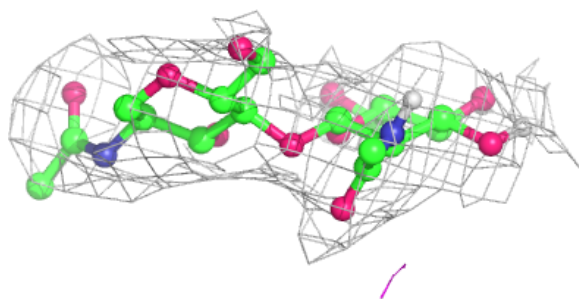
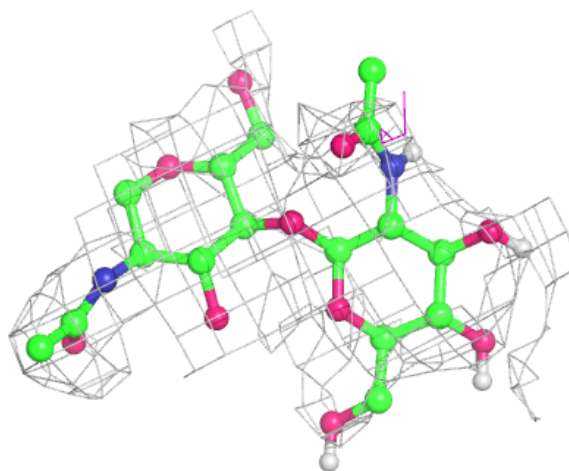
**Electron density around Chain C:**

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



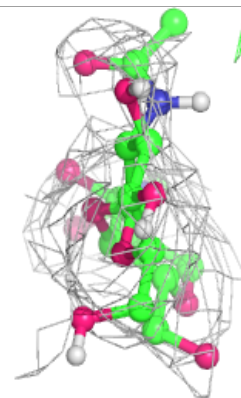
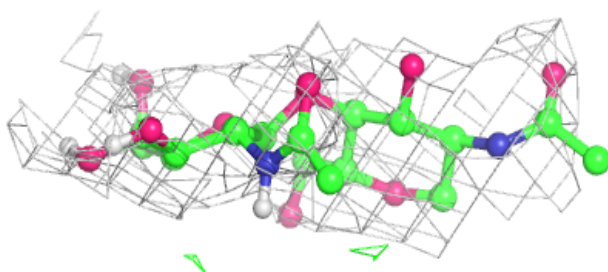
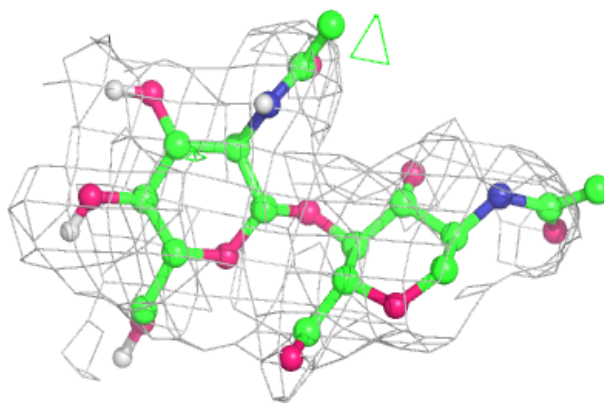
**Electron density around Chain D:**

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

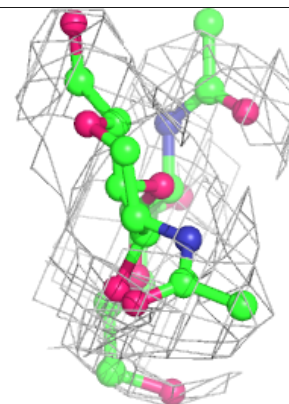
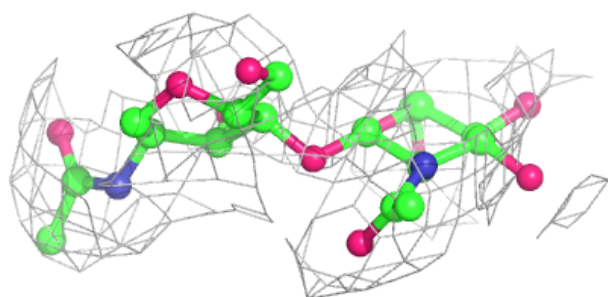
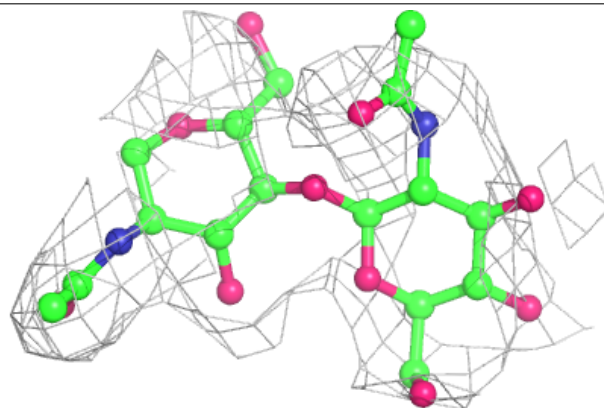


**Electron density around Chain H:**

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

**Electron density around Chain I:**

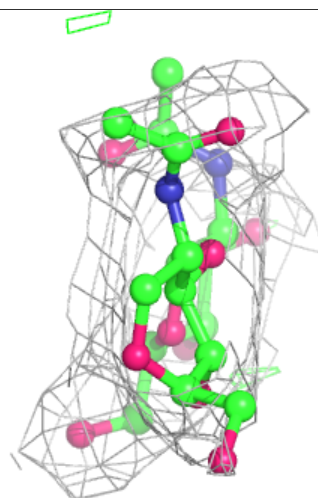
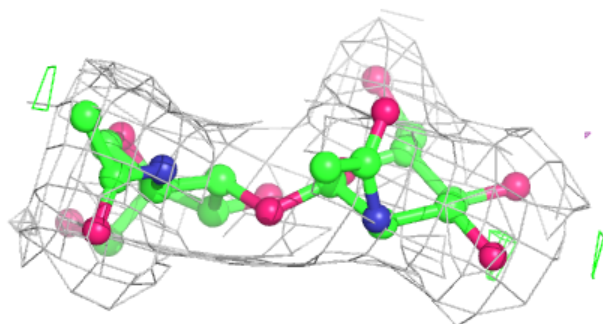
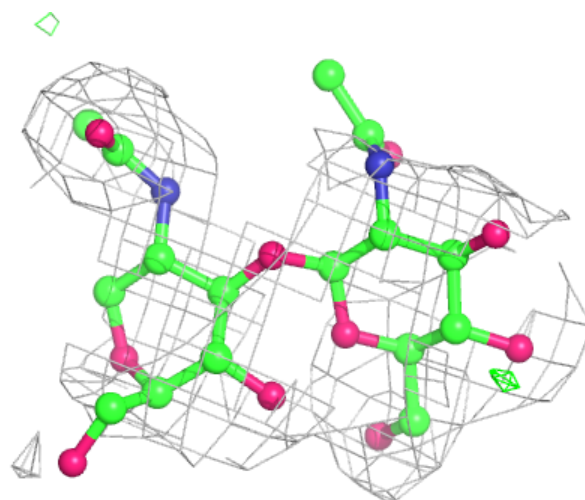
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





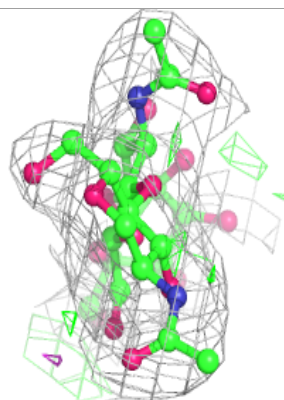
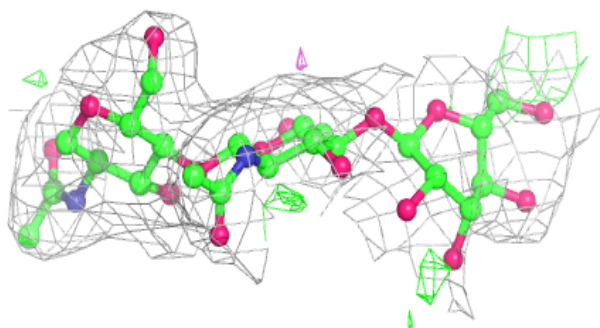
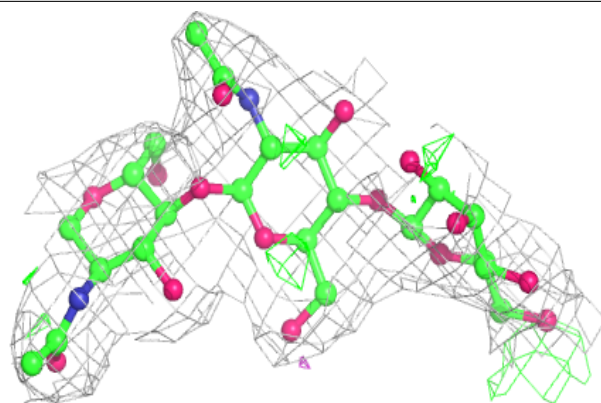
**Electron density around Chain E:**

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

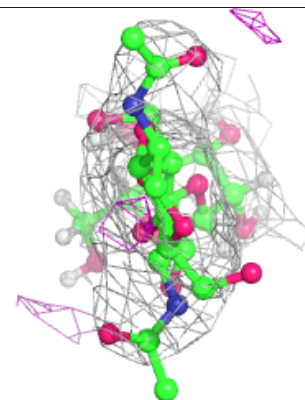
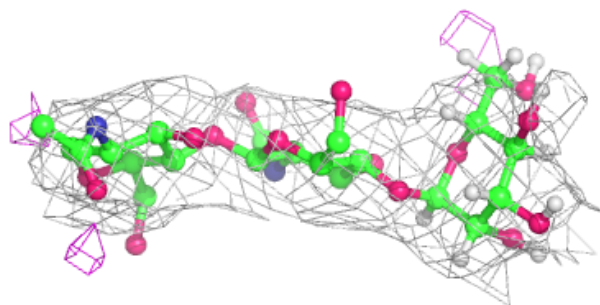
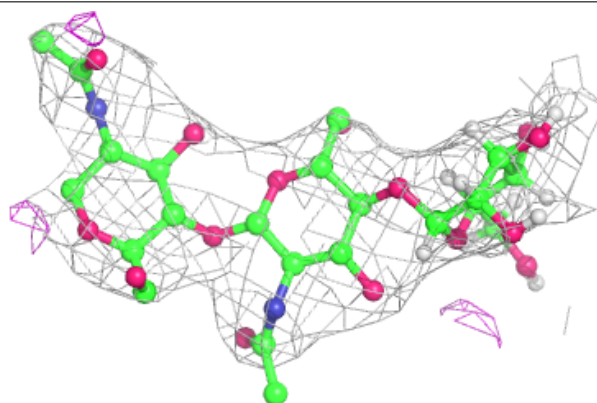


**Electron density around Chain F:**

$2mF_o - DF_c$  (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)



## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	NAG	A	704	14/15	0.56	0.44	98,150,180,194	0
7	NAG	B	705	14/15	0.64	0.55	114,143,172,173	0
7	NAG	A	705	14/15	0.72	0.53	80,110,131,156	0
7	NAG	B	704	14/15	0.78	0.34	115,136,170,171	0
7	NAG	A	712	14/15	0.87	0.13	77,94,107,108	0
6	ACT	A	703	4/4	0.89	0.27	53,62,80,81	0
5	ZN	B	701	1/1	0.92	0.09	45,45,45,45	0
5	ZN	A	702	1/1	0.95	0.06	90,90,90,90	0
5	ZN	B	702	1/1	0.97	0.06	98,98,98,98	0
5	ZN	A	701	1/1	0.97	0.16	55,55,55,55	0
6	ACT	B	703	4/4	0.98	0.21	46,68,72,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.