



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2021 – 04:05 AM EDT

PDB ID : 3DGV
Title : Crystal structure of thrombin activatable fibrinolysis inhibitor (TAFI)
Authors : Anand, K.; Pallares, I.; Valnickova, Z.; Christensen, T.; Schreuder, H.; Enghild, J.
Deposited on : 2008-06-16
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

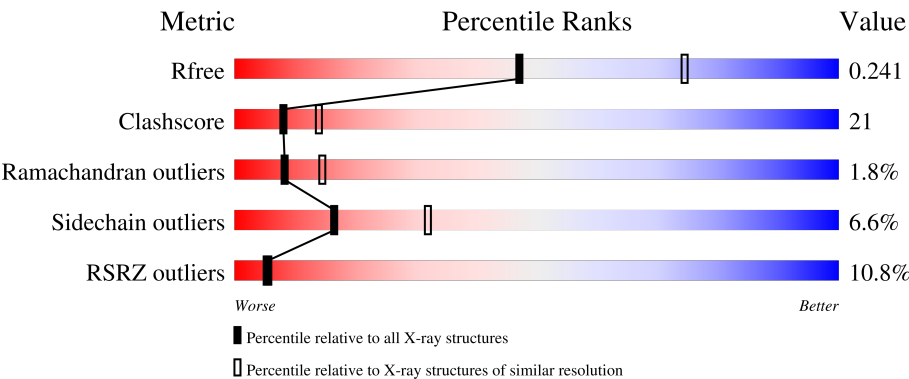
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



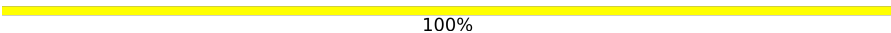


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	401	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>71%25%.</div></div>
1	B	401	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>69%29%.</div></div>
1	C	401	<div><div>28%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>37%51%7%5%</div></div>
2	D	2	<div><div></div><div><div></div></div><div>100%</div></div>
2	I	2	<div><div></div><div><div></div><div></div></div><div>50%50%</div></div>

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Mol	Chain	Length	Quality of chain
3	E	2	 50% 50%
4	F	2	 100%
4	J	2	 50% 50%
5	G	3	 67% 33%
6	H	3	 33% 67%

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
10	NAG	B	316	-	-	-	X
10	NAG	C	309	X	-	-	X
2	NDG	I	2	-	-	-	X
3	NAG	E	1	-	-	-	X
3	FUL	E	2	-	-	-	X
4	NAG	F	2	-	-	-	X
4	NAG	J	2	-	-	-	X
5	NAG	G	1	X	-	-	-
5	NAG	G	2	-	-	-	X
5	FUL	G	3	-	-	-	X
6	NAG	H	2	-	-	-	X
6	BMA	H	3	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 11015 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 Carboxypeptidase B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3278	2097	565	600	16			
1	B	401	Total	C	N	O	S	0	0	0
			3275	2094	564	601	16			
1	C	379	Total	C	N	O	S	0	0	0
			3068	1958	525	569	16			

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



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

- Molecule 3 is an oligosaccharide called beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			24	14	1	9			

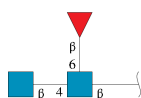
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



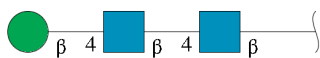
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is an oligosaccharide called 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	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		
7	B	1	Total	Zn	0	0
			1	1		
7	C	1	Total	Zn	0	0
			1	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



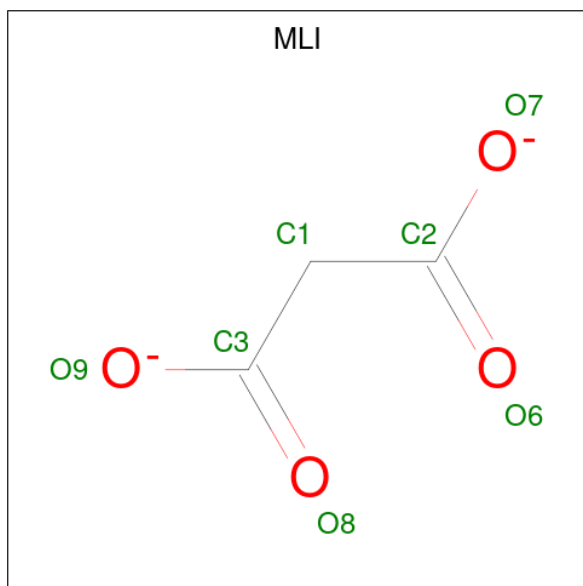
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is MALONATE ION (three-letter code: MLI) (formula: $\text{C}_3\text{H}_2\text{O}_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	3	4		
9	B	1	Total	C	O	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			7	3	4		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

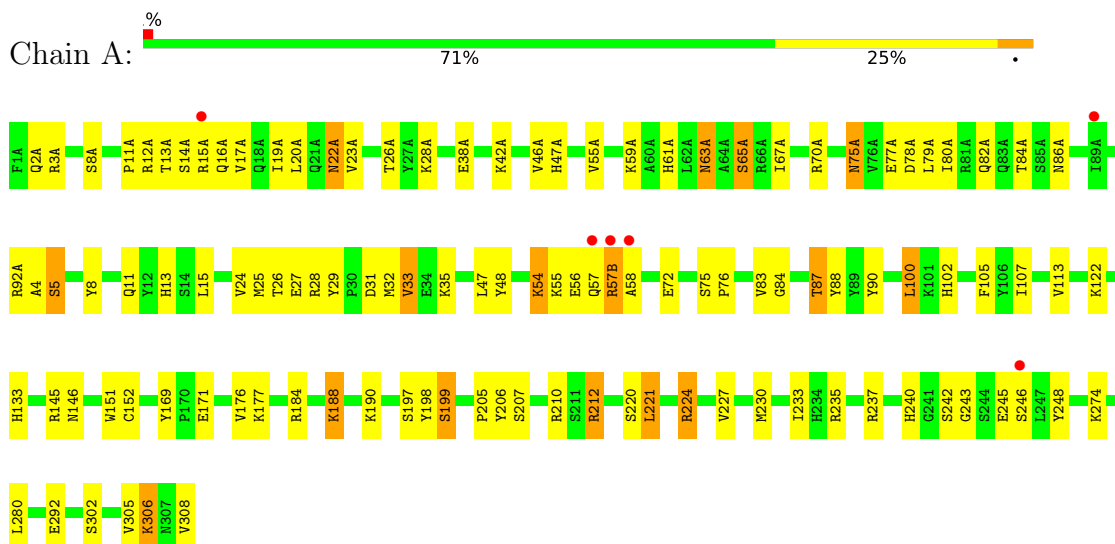
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	484	Total	O	0	0
			484	484		
11	B	417	Total	O	0	0
			417	417		
11	C	118	Total	O	0	0
			118	118		

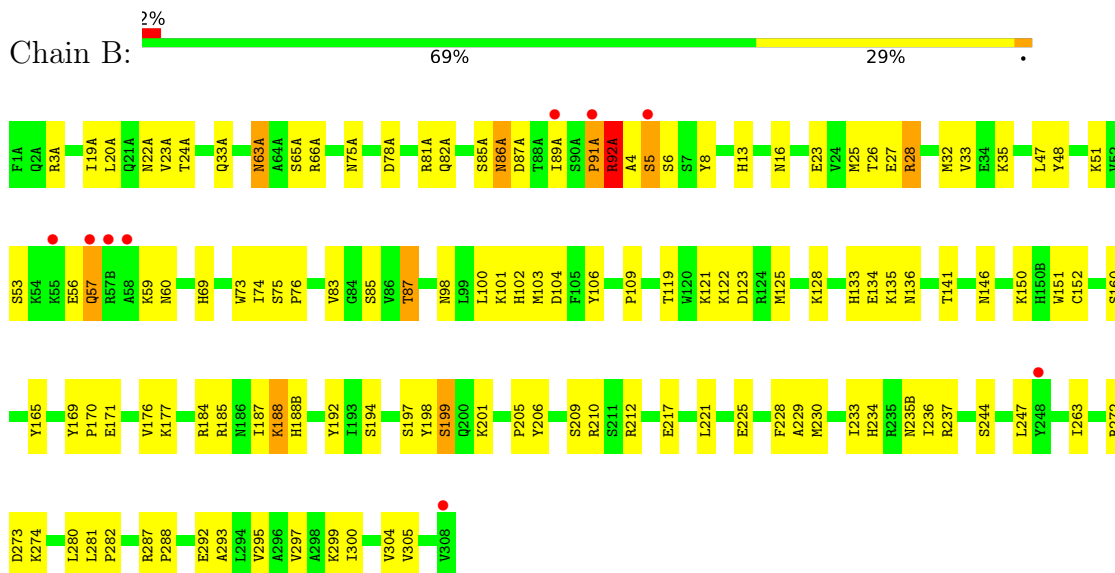
3 Residue-property plots [i](#)

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

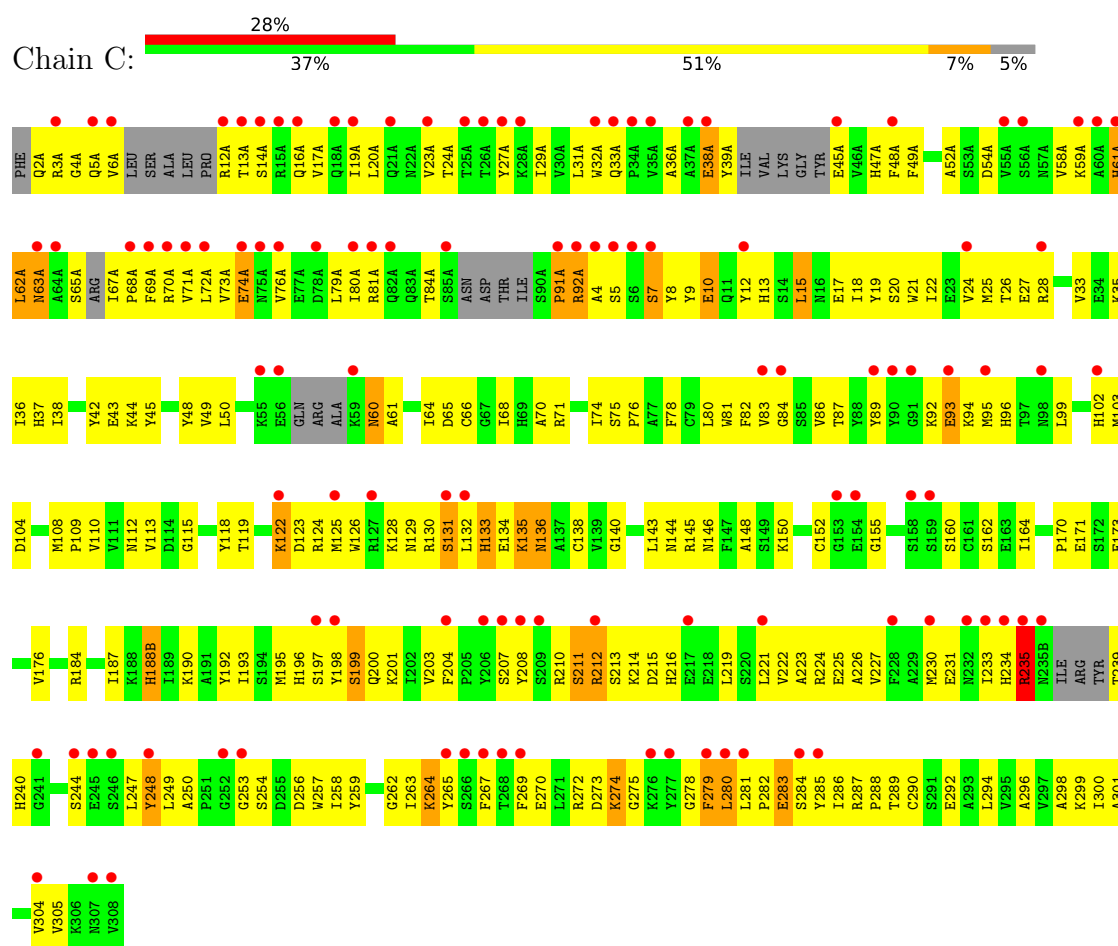
- Molecule 1: Carboxypeptidase B2



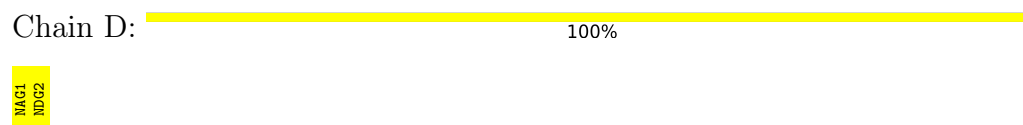
- Molecule 1: Carboxypeptidase B2



- Molecule 1: Carboxypeptidase B2



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



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



- Molecule 3: beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain F:  100%

MAG1
MAG2

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

Chain J:  50% 50%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  67% 33%

MAG1
MAG2
FOLL3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33% 67%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	146.47Å 146.47Å 231.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 2.50 19.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.86-2.50) 99.7 (19.86-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.243 0.203 , 0.241	Depositor DCC
R_{free} test set	4345 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 83.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11015	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FUL, SO4, NDG, NAG, MLI, BMA, ZN

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	0.37	0/3367	0.51	0/4560
1	B	0.34	0/3364	0.49	0/4557
1	C	0.24	0/3147	0.43	0/4261
All	All	0.32	0/9878	0.48	0/13378

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	92(A)	ARG	Peptide

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	3278	0	3194	99	0
1	B	3275	0	3183	96	0
1	C	3068	0	2926	218	0
2	D	28	0	24	0	0
2	I	28	0	24	1	0
3	E	24	0	22	1	0
4	F	28	0	25	2	0
4	J	28	0	25	2	0
5	G	38	0	34	0	0
6	H	39	0	34	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	45	0	0	2	0
8	B	55	0	0	0	0
8	C	10	0	0	1	0
9	A	7	0	2	0	0
9	B	7	0	2	1	0
9	C	7	0	2	0	0
10	B	14	0	13	2	0
10	C	14	0	13	0	0
11	A	484	0	0	19	0
11	B	417	0	0	19	0
11	C	118	0	0	17	0
All	All	11015	0	9523	415	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 21.

All (415) 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:75(A):ASN:ND2	1:A:78(A):ASP:H	1.55	1.03
1:C:281:LEU:HD12	1:C:282:PRO:HD2	1.54	0.89
1:C:201:LYS:H	1:C:270:GLU:HB2	1.39	0.87
1:C:136:ASN:HB2	1:C:160:SER:OG	1.77	0.84
1:C:75:SER:HB3	1:C:76:PRO:HD3	1.60	0.83
1:A:75:SER:HB3	1:A:76:PRO:HD3	1.61	0.83
1:A:57:GLN:HA	11:A:604:HOH:O	1.79	0.82
1:B:134:GLU:HG2	1:B:135:LYS:HG2	1.60	0.82
1:C:79(A):LEU:HD23	1:C:280:LEU:HD13	1.62	0.81
1:C:207:SER:HB3	1:C:250:ALA:HB3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:VAL:O	1:B:87:THR:HB	1.82	0.80
1:C:89:TYR:HA	1:C:92:LYS:HD2	1.65	0.79
1:C:281:LEU:HD11	1:C:285:TYR:HB2	1.66	0.78
1:A:237:ARG:HG2	1:B:237:ARG:HH21	1.50	0.77
10:B:316:NAG:H5	11:B:541:HOH:O	1.84	0.76
1:A:75(A):ASN:HD21	1:A:78(A):ASP:H	1.33	0.76
1:C:212:ARG:HH11	1:C:216:HIS:HB3	1.52	0.74
1:A:83:VAL:O	1:A:87:THR:HB	1.87	0.74
1:C:115:GLY:HA2	11:C:407:HOH:O	1.88	0.73
1:C:119:THR:HA	1:C:124:ARG:H	1.54	0.73
1:C:280:LEU:HD12	1:C:280:LEU:H	1.54	0.73
1:C:223:ALA:O	1:C:227:VAL:HG23	1.89	0.72
1:B:201:LYS:HD3	11:B:637:HOH:O	1.88	0.72
1:C:146:ASN:OD1	1:C:176:VAL:HG11	1.90	0.72
1:B:4:ALA:O	1:B:6:SER:N	2.23	0.71
1:A:102:HIS:HB3	1:A:305:VAL:HG11	1.72	0.71
1:C:272:ARG:HB2	1:C:289:THR:HG22	1.72	0.71
1:B:300:ILE:O	1:B:304:VAL:HG23	1.91	0.71
1:B:287:ARG:HB3	1:B:288:PRO:HD3	1.72	0.71
1:C:197:SER:HB2	1:C:198:TYR:HB3	1.73	0.71
1:C:272:ARG:HB3	1:C:273:ASP:HA	1.75	0.69
1:C:68(A):PRO:HD3	11:C:347:HOH:O	1.93	0.69
1:A:92(A):ARG:HG2	1:A:24:VAL:HG21	1.75	0.69
1:A:274:LYS:HG3	11:B:403:HOH:O	1.92	0.68
1:C:36:ILE:HG12	1:C:49:VAL:O	1.93	0.68
1:A:75(A):ASN:C	1:A:75(A):ASN:HD22	1.98	0.67
1:C:124:ARG:HH21	1:C:280:LEU:HB3	1.60	0.67
1:C:230:MET:O	1:C:233:ILE:HG22	1.95	0.67
1:B:23:GLU:O	1:B:26:THR:HG22	1.97	0.65
1:C:22:ILE:HG23	1:C:50:LEU:HD21	1.78	0.65
1:A:22(A):ASN:O	1:A:26(A):THR:HG23	1.97	0.65
1:C:301:ALA:O	1:C:305:VAL:HG23	1.98	0.64
1:A:198:TYR:O	1:A:199:SER:HB3	1.97	0.64
1:C:64:ILE:HD11	1:C:78:PHE:HE2	1.63	0.64
1:A:198:TYR:O	1:A:199:SER:CB	2.45	0.63
1:C:32(A):TRP:CZ3	1:C:278:GLY:HA3	2.32	0.63
1:B:8:TYR:O	1:B:13:HIS:HE1	1.80	0.63
1:C:62(A):LEU:HD23	1:C:63(A):ASN:N	2.14	0.62
1:B:233:ILE:HD11	1:B:292:GLU:HA	1.82	0.62
1:C:64:ILE:HD11	1:C:195:MET:HE2	1.80	0.62
1:A:227:VAL:HA	1:A:230:MET:HE2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:HD11	1:A:292:GLU:HA	1.79	0.62
1:C:264:LYS:HD3	1:C:264:LYS:N	2.14	0.62
1:C:275:GLY:HA3	11:C:364:HOH:O	2.00	0.62
1:C:71(A):VAL:HG22	11:C:404:HOH:O	2.00	0.62
1:B:63(A):ASN:OD1	2:I:1:NAG:N2	2.32	0.61
1:C:144:ASN:O	1:C:253:GLY:HA2	2.01	0.61
1:C:264:LYS:HD3	1:C:264:LYS:H	1.66	0.61
1:B:5:SER:HB3	1:B:8:TYR:HB2	1.81	0.61
1:B:4:ALA:C	1:B:6:SER:H	2.04	0.61
1:C:281:LEU:HD21	1:C:285:TYR:O	2.01	0.60
1:B:81(A):ARG:HD3	11:B:445:HOH:O	2.01	0.60
1:B:91(A):PRO:HD2	1:B:5:SER:OG	2.02	0.60
1:C:49(A):PHE:HE1	1:C:76(A):VAL:HG21	1.65	0.60
1:B:187:ILE:HD11	1:B:263:ILE:HD11	1.83	0.60
1:B:119:THR:HA	1:B:123:ASP:O	2.00	0.60
1:C:99:LEU:HD21	1:C:298:ALA:HA	1.84	0.60
1:C:26:THR:HA	1:C:33:VAL:HG23	1.83	0.59
11:A:429:HOH:O	1:B:274:LYS:HG3	2.02	0.59
1:C:171:GLU:CD	1:C:184:ARG:HH22	2.05	0.59
1:C:125:MET:SD	1:C:279:PHE:CE2	2.96	0.59
1:A:63(A):ASN:OD1	3:E:1:NAG:N2	2.35	0.59
1:C:125:MET:SD	1:C:279:PHE:HE2	2.26	0.59
1:C:84:GLY:O	1:C:87:THR:HG22	2.02	0.59
1:C:19(A):ILE:HG23	11:C:348:HOH:O	2.01	0.58
1:C:150:LYS:HB2	1:C:208:TYR:CE1	2.37	0.58
1:C:210:ARG:HA	1:C:244:SER:HB2	1.84	0.58
1:C:294:LEU:HD13	1:C:294:LEU:O	2.02	0.58
1:C:200:GLN:HG3	1:C:200:GLN:O	2.04	0.58
1:A:26:THR:HG22	1:A:33:VAL:HG23	1.85	0.58
1:A:57(B):ARG:HG3	1:A:58:ALA:N	2.18	0.58
1:C:272:ARG:HB2	1:C:289:THR:CG2	2.33	0.58
1:C:12:TYR:CE2	1:C:286:ILE:HD11	2.39	0.58
1:A:220:SER:O	1:A:224:ARG:HG2	2.03	0.58
1:C:289:THR:O	1:C:292:GLU:HG2	2.04	0.58
1:A:240:HIS:HD2	11:A:390:HOH:O	1.87	0.57
1:C:25:MET:HE1	1:C:87:THR:HG21	1.85	0.57
1:B:69:HIS:HE1	9:B:329:MLI:H12	1.69	0.57
1:B:86(A):ASN:HB3	1:B:89(A):ILE:HG22	1.85	0.57
1:A:242:SER:O	1:A:245:GLU:HG2	2.05	0.57
1:C:129:ASN:O	1:C:140:GLY:HA2	2.05	0.56
1:C:248:TYR:HA	11:C:356:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASN:HB3	1:A:176:VAL:HG21	1.86	0.56
1:C:49(A):PHE:CE1	1:C:76(A):VAL:HG21	2.39	0.56
1:C:2(A):GLN:O	1:C:3(A):ARG:HB2	2.05	0.56
1:B:74:ILE:HD13	1:B:281:LEU:HD23	1.88	0.56
1:C:36:ILE:HG13	1:C:49:VAL:HB	1.88	0.56
1:C:225:GLU:O	1:C:299:LYS:HE2	2.06	0.55
1:C:36(A):ALA:HB3	1:C:39(A):TYR:CD1	2.41	0.55
1:C:68:ILE:HB	1:C:196:HIS:HE1	1.70	0.55
1:C:130:ARG:O	1:C:131:SER:CB	2.54	0.55
1:C:138:CYS:HB2	1:C:160:SER:O	2.06	0.55
1:C:103:MET:CE	1:C:304:VAL:HB	2.37	0.55
1:C:198:TYR:O	1:C:199:SER:HB3	2.07	0.55
1:A:12(A):ARG:HE	1:A:16(A):GLN:HE22	1.54	0.55
1:A:212:ARG:CB	1:A:212:ARG:HH11	2.20	0.55
1:C:17(A):VAL:HG12	11:C:368:HOH:O	2.05	0.55
1:C:222:VAL:HB	11:C:391:HOH:O	2.06	0.55
1:C:73(A):VAL:HG12	1:C:74(A):GLU:O	2.06	0.55
1:A:12(A):ARG:H	1:A:16(A):GLN:NE2	2.04	0.55
1:B:56:GLU:C	1:B:57:GLN:HG3	2.26	0.55
1:C:93:GLU:H	1:C:93:GLU:CD	2.10	0.55
1:C:3(A):ARG:HB3	1:C:52(A):ALA:HB2	1.89	0.55
1:C:130:ARG:HG2	11:C:407:HOH:O	2.05	0.55
1:C:6(A):VAL:O	1:C:72(A):LEU:HB2	2.07	0.55
1:C:28:ARG:HD3	11:C:327:HOH:O	2.05	0.55
1:A:233:ILE:HD11	1:A:292:GLU:CA	2.37	0.54
1:C:134:GLU:O	1:C:135:LYS:HB2	2.07	0.54
1:C:18:ILE:HD13	1:C:80:LEU:HD21	1.89	0.54
1:B:22(A):ASN:HB2	11:B:534:HOH:O	2.06	0.54
1:C:188(B):HIS:HB2	11:C:372:HOH:O	2.07	0.54
1:C:265:TYR:CE2	1:C:304:VAL:HG13	2.43	0.54
1:B:198:TYR:O	1:B:199:SER:CB	2.54	0.54
1:A:19(A):ILE:O	1:A:23(A):VAL:HG23	2.08	0.54
1:A:212:ARG:HH11	1:A:212:ARG:CG	2.20	0.54
1:C:272:ARG:HG3	1:C:292:GLU:OE2	2.08	0.54
1:A:4:ALA:HB3	1:A:28:ARG:NH1	2.23	0.54
1:C:32(A):TRP:HZ3	1:C:278:GLY:HA3	1.73	0.53
1:C:235:ARG:H	1:C:235:ARG:HD3	1.72	0.53
1:B:89(A):ILE:HB	11:B:574:HOH:O	2.06	0.53
1:C:35:LYS:HD3	1:C:48:TYR:CD1	2.43	0.53
1:C:89:TYR:HA	1:C:92:LYS:CD	2.38	0.53
1:C:173:GLU:HB2	1:C:176:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:SER:O	1:B:274:LYS:HE3	2.09	0.53
1:C:18:ILE:CD1	1:C:80:LEU:HD21	2.38	0.53
1:C:219:LEU:HA	1:C:222:VAL:HG12	1.89	0.53
1:C:171:GLU:OE2	1:C:184:ARG:NH2	2.42	0.53
4:F:1:NAG:H61	4:F:2:NAG:HN2	1.74	0.53
1:C:23(A):VAL:HG13	1:C:27(A):TYR:CD2	2.44	0.53
1:C:272:ARG:CB	1:C:273:ASP:HA	2.37	0.53
1:A:70(A):ARG:HG2	1:B:228:PHE:CZ	2.42	0.53
1:C:102:HIS:HB3	1:C:305:VAL:HG21	1.90	0.53
1:C:7:SER:O	1:C:8:TYR:HB3	2.09	0.52
1:C:136:ASN:HB2	1:C:160:SER:CB	2.39	0.52
1:C:221:LEU:HD13	1:C:224:ARG:HH11	1.74	0.52
1:B:60:ASN:HB2	11:B:481:HOH:O	2.09	0.52
1:B:185:ARG:HD3	11:B:423:HOH:O	2.10	0.52
1:A:75(A):ASN:HD21	1:A:78(A):ASP:N	2.06	0.52
1:A:190:LYS:HD2	1:A:308:VAL:CG2	2.40	0.52
1:C:130:ARG:O	1:C:131:SER:HB3	2.10	0.52
1:C:15:LEU:HD21	1:C:113:VAL:HG13	1.92	0.52
1:C:193:ILE:HA	1:C:267:PHE:O	2.08	0.52
1:C:203:VAL:HG12	1:C:204:PHE:N	2.25	0.52
1:B:103:MET:CE	1:B:304:VAL:HB	2.39	0.52
1:A:27:GLU:HB3	11:A:651:HOH:O	2.09	0.52
1:C:145:ARG:HH21	1:C:164:ILE:HG22	1.74	0.52
1:B:263:ILE:N	1:B:263:ILE:HD12	2.25	0.52
1:C:12(A):ARG:NH1	1:C:68(A):PRO:HG2	2.24	0.52
1:C:61(A):HIS:HB2	11:C:366:HOH:O	2.10	0.52
1:C:279:PHE:HB3	1:C:280:LEU:HG	1.92	0.51
1:A:31:ASP:HB2	11:A:379:HOH:O	2.10	0.51
1:C:112:ASN:HD21	1:C:128:LYS:C	2.13	0.51
1:C:19(A):ILE:HG21	1:C:65(A):SER:OG	2.11	0.51
1:C:249:LEU:HD12	1:C:249:LEU:N	2.26	0.51
1:A:171:GLU:HB3	1:A:177:LYS:HE3	1.93	0.51
1:C:65:ASP:OD1	1:C:68:ILE:HD11	2.10	0.51
1:A:190:LYS:HD2	1:A:308:VAL:HG21	1.92	0.51
1:C:212:ARG:NH1	1:C:216:HIS:HB3	2.22	0.51
1:A:245:GLU:HG3	11:A:514:HOH:O	2.11	0.51
1:C:70:ALA:HB3	1:C:126:TRP:O	2.11	0.51
1:A:4:ALA:HB3	1:A:28:ARG:HH12	1.74	0.51
1:C:18:ILE:HD12	1:C:80:LEU:HD11	1.92	0.51
1:C:25:MET:CE	1:C:87:THR:HG21	2.40	0.51
1:C:213:SER:C	1:C:215:ASP:H	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ARG:O	1:B:237:ARG:HG3	2.12	0.50
1:C:81(A):ARG:HA	1:C:84(A):THR:HG22	1.93	0.50
1:B:151:TRP:CH2	1:B:169:TYR:HA	2.46	0.50
1:C:258:ILE:HD11	1:C:263:ILE:HG13	1.92	0.50
1:C:60:ASN:ND2	1:C:190:LYS:HE3	2.26	0.50
1:C:282:PRO:C	1:C:284:SER:N	2.63	0.50
1:B:73:TRP:O	1:B:76:PRO:HD2	2.10	0.50
1:B:75:SER:HB3	1:B:76:PRO:HD3	1.93	0.50
1:B:170:PRO:O	1:B:171:GLU:HB2	2.11	0.50
1:B:212:ARG:HD2	11:B:591:HOH:O	2.11	0.50
1:A:75(A):ASN:ND2	1:A:78(A):ASP:N	2.40	0.50
1:A:302:SER:O	1:A:306:LYS:HD3	2.11	0.50
1:A:227:VAL:HA	1:A:230:MET:CE	2.42	0.50
1:B:19(A):ILE:O	1:B:23(A):VAL:HG23	2.11	0.50
1:B:4:ALA:HB2	1:B:28:ARG:NH2	2.27	0.50
1:A:35:LYS:HD3	1:A:48:TYR:CE1	2.47	0.50
1:C:19:TYR:OH	1:C:45:TYR:HB3	2.12	0.50
1:C:82:PHE:O	1:C:86:VAL:HG22	2.12	0.50
1:C:89:TYR:HB2	1:C:96:HIS:CD2	2.47	0.50
1:C:124:ARG:NH2	1:C:280:LEU:HB3	2.27	0.50
1:A:248:TYR:HA	11:A:543:HOH:O	2.12	0.49
1:A:19(A):ILE:HD13	1:A:65(A):SER:OG	2.13	0.49
1:B:89(A):ILE:HD11	11:B:594:HOH:O	2.12	0.49
1:B:233:ILE:HD11	1:B:292:GLU:CA	2.43	0.49
1:A:72:GLU:HG2	1:A:197:SER:OG	2.12	0.49
1:C:287:ARG:N	1:C:288:PRO:HD2	2.27	0.49
1:B:171:GLU:OE2	1:B:184:ARG:NH2	2.46	0.49
1:C:103:MET:HE3	1:C:304:VAL:HB	1.93	0.49
1:A:92(A):ARG:O	1:A:92(A):ARG:HG3	2.13	0.49
1:C:45(A):GLU:N	11:C:378:HOH:O	2.45	0.49
1:C:273:ASP:CG	1:C:274:LYS:H	2.16	0.49
1:B:233:ILE:HG13	1:B:234:HIS:CD2	2.47	0.49
1:C:73(A):VAL:HG11	1:C:79(A):LEU:HD22	1.95	0.49
1:A:75(A):ASN:HD22	1:A:78(A):ASP:H	1.55	0.49
1:A:75(A):ASN:ND2	1:A:75(A):ASN:C	2.64	0.48
1:B:86(A):ASN:HB3	1:B:89(A):ILE:CG2	2.43	0.48
1:B:51:LYS:HD2	1:B:106:TYR:HE1	1.78	0.48
1:C:148:ALA:HB2	1:C:170:PRO:HB3	1.96	0.48
1:C:221:LEU:CD1	1:C:224:ARG:HH11	2.26	0.48
1:A:15(A):ARG:HD3	11:A:526:HOH:O	2.13	0.48
1:A:25:MET:CE	1:A:87:THR:HG21	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:HIS:HA	8:C:311:SO4:O1	2.13	0.48
1:C:219:LEU:HD22	1:C:267:PHE:CZ	2.48	0.48
1:A:54:LYS:HE3	11:A:608:HOH:O	2.14	0.48
1:A:54:LYS:HD2	1:A:90:TYR:OH	2.13	0.48
1:B:121:LYS:O	1:B:122:LYS:HD2	2.14	0.48
1:C:10:GLU:O	1:C:286:ILE:HD12	2.13	0.48
1:C:136:ASN:ND2	1:C:136:ASN:O	2.47	0.48
1:A:221:LEU:HD22	1:A:221:LEU:O	2.14	0.48
1:A:84:GLY:O	1:A:87:THR:HG22	2.14	0.48
1:A:171:GLU:OE2	1:A:184:ARG:NH2	2.47	0.48
1:C:227:VAL:HA	1:C:230:MET:HE2	1.96	0.48
1:C:256:ASP:O	1:C:259:TYR:HB3	2.14	0.48
1:A:19(A):ILE:HG21	1:A:65(A):SER:OG	2.14	0.48
1:C:62(A):LEU:HD23	1:C:62(A):LEU:C	2.33	0.48
1:C:155:GLY:HA3	1:C:249:LEU:HB2	1.95	0.48
1:C:222:VAL:HA	1:C:225:GLU:HB3	1.96	0.48
1:C:247:LEU:HG	1:C:248:TYR:H	1.79	0.48
1:C:258:ILE:HG13	1:C:263:ILE:HB	1.96	0.48
6:H:2:NAG:H62	6:H:3:BMA:H61	1.94	0.47
1:B:188:LYS:HG3	1:B:188(B):HIS:N	2.29	0.47
1:C:133:HIS:O	1:C:136:ASN:ND2	2.47	0.47
1:A:82(A):GLN:NE2	11:A:417:HOH:O	2.44	0.47
1:B:85(A):SER:OG	4:J:1:NAG:H61	2.14	0.47
1:C:118:TYR:CZ	1:C:122:LYS:HG2	2.50	0.47
1:B:102:HIS:HB3	1:B:305:VAL:HG11	1.96	0.47
1:C:43:GLU:O	1:C:44:LYS:HB2	2.14	0.47
1:A:188:LYS:HG3	11:A:447:HOH:O	2.13	0.47
1:B:171:GLU:CD	1:B:184:ARG:HH22	2.19	0.47
1:C:119:THR:HB	1:C:124:ARG:HA	1.97	0.47
1:C:20:SER:O	1:C:24:VAL:HG23	2.15	0.47
1:C:66:CYS:HB2	1:C:109:PRO:O	2.15	0.47
1:C:32(A):TRP:HB2	1:C:47(A):HIS:HB2	1.97	0.47
1:C:210:ARG:O	1:C:211:SER:HB3	2.14	0.47
1:A:55:LYS:HB2	11:A:652:HOH:O	2.14	0.46
1:C:14(A):SER:O	1:C:17(A):VAL:HG22	2.15	0.46
1:C:123:ASP:O	1:C:124:ARG:HB3	2.15	0.46
1:B:150:LYS:HG3	1:C:262:GLY:HA3	1.97	0.46
1:A:80(A):ILE:O	1:A:84(A):THR:HG22	2.15	0.46
1:B:35:LYS:HD3	1:B:48:TYR:CE1	2.50	0.46
1:C:2(A):GLN:N	1:C:80(A):ILE:HD11	2.29	0.46
1:C:23(A):VAL:O	1:C:29(A):ILE:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32(A):TRP:HE3	1:C:198:TYR:OH	1.98	0.46
1:A:25:MET:HE1	1:A:87:THR:HG21	1.97	0.46
1:C:32(A):TRP:NE1	1:C:279:PHE:CE2	2.83	0.46
1:C:221:LEU:HD13	1:C:224:ARG:HD2	1.98	0.46
1:C:192:TYR:HH	1:C:254:SER:HG	1.59	0.46
1:C:21:TRP:O	1:C:25:MET:HB2	2.16	0.46
1:C:258:ILE:O	1:C:263:ILE:HB	2.16	0.46
1:B:128:LYS:HB3	1:B:141:THR:O	2.16	0.46
1:C:4:ALA:CB	1:C:28:ARG:HH22	2.29	0.46
1:C:129:ASN:ND2	1:C:143:LEU:HD21	2.31	0.46
1:C:283:GLU:H	1:C:283:GLU:HG2	1.56	0.46
1:C:71:ARG:HD2	1:C:279:PHE:CE1	2.51	0.45
1:C:198:TYR:O	1:C:199:SER:CB	2.64	0.45
1:B:209:SER:O	1:B:244:SER:HB3	2.16	0.45
1:A:3(A):ARG:HG2	1:A:77(A):GLU:OE2	2.16	0.45
1:A:237:ARG:CG	1:B:237:ARG:HH21	2.24	0.45
1:B:234:HIS:O	1:B:236:ILE:HG22	2.16	0.45
4:F:1:NAG:H61	4:F:2:NAG:N2	2.30	0.45
1:C:5:SER:HB3	11:C:349:HOH:O	2.17	0.45
1:B:75(A):ASN:ND2	1:B:78(A):ASP:OD2	2.50	0.45
1:A:11(A):PRO:HB2	1:A:17(A):VAL:HG12	1.98	0.45
1:C:5(A):GLN:HE22	1:C:59(A):LYS:HE3	1.82	0.45
1:C:239:THR:O	1:C:240:HIS:HB3	2.17	0.45
1:A:14(A):SER:O	1:A:17(A):VAL:HG22	2.17	0.45
1:A:28:ARG:HG2	1:A:29:TYR:CE2	2.52	0.45
1:A:245:GLU:HG3	1:A:246:SER:N	2.32	0.45
1:B:187:ILE:HD11	1:B:263:ILE:CD1	2.44	0.45
1:C:28:ARG:HB3	11:C:352:HOH:O	2.17	0.45
1:C:272:ARG:HA	1:C:273:ASP:O	2.16	0.45
1:B:184:ARG:HD2	11:C:315:HOH:O	2.17	0.45
1:B:4:ALA:O	1:B:8:TYR:HB3	2.16	0.45
1:B:221:LEU:O	1:B:225:GLU:HG3	2.17	0.45
1:C:195:MET:SD	1:C:269:PHE:HB2	2.57	0.45
1:B:82(A):GLN:NE2	11:B:465:HOH:O	2.49	0.45
1:B:51:LYS:HD2	1:B:106:TYR:CE1	2.52	0.45
1:C:132:LEU:O	1:C:133:HIS:HB2	2.17	0.45
1:B:146:ASN:HB3	1:B:176:VAL:HG21	1.99	0.44
1:A:32:MET:HE3	1:A:100:LEU:HD21	1.99	0.44
1:C:15:LEU:HD11	1:C:113:VAL:CG1	2.48	0.44
1:A:151:TRP:CH2	1:A:169:TYR:HA	2.53	0.44
1:B:230:MET:HG2	1:B:292:GLU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ALA:O	1:C:300:ILE:HG13	2.17	0.44
1:B:198:TYR:O	1:B:199:SER:HB3	2.17	0.44
1:A:8(A):SER:HA	1:A:46(A):VAL:O	2.18	0.44
1:A:47(A):HIS:HD2	1:A:198:TYR:OH	2.00	0.44
1:A:107:ILE:N	1:A:107:ILE:HD12	2.32	0.44
1:B:53:SER:HB2	1:B:104:ASP:OD1	2.17	0.44
1:C:162:SER:OG	1:C:164:ILE:HG12	2.17	0.44
1:C:300:ILE:O	1:C:304:VAL:HG23	2.18	0.44
1:A:105:PHE:HB3	1:A:107:ILE:CD1	2.47	0.44
1:C:94:LYS:O	1:C:95:MET:HB3	2.17	0.44
1:C:173:GLU:O	1:C:176:VAL:HG12	2.17	0.44
1:B:133:HIS:HB2	1:B:136:ASN:ND2	2.32	0.44
1:A:2(A):GLN:HG2	11:A:578:HOH:O	2.18	0.44
1:B:170:PRO:HG2	1:C:187:ILE:HG21	1.99	0.44
1:B:235(B):ASN:HB2	11:B:479:HOH:O	2.16	0.44
1:A:122:LYS:HE3	11:A:583:HOH:O	2.18	0.44
1:C:7:SER:O	1:C:9:TYR:N	2.43	0.44
1:C:33:VAL:HG23	1:C:33:VAL:O	2.17	0.44
1:C:192:TYR:OH	1:C:254:SER:OG	2.34	0.44
6:H:1:NAG:H61	6:H:2:NAG:O5	2.17	0.44
1:B:16:ASN:HB2	11:B:477:HOH:O	2.17	0.43
1:C:31(A):LEU:HD23	1:C:48(A):PHE:HB3	2.00	0.43
1:C:62(A):LEU:HG	1:C:67(A):ILE:HB	1.99	0.43
1:C:4:ALA:HB1	1:C:28:ARG:HH22	1.82	0.43
1:B:160:SER:HA	1:B:165:TYR:CG	2.53	0.43
1:B:171:GLU:HG2	1:B:176:VAL:HG12	2.00	0.43
1:C:21:TRP:CZ3	1:C:80:LEU:HG	2.54	0.43
1:C:71:ARG:HD3	1:C:125:MET:O	2.18	0.43
1:A:75:SER:CB	1:A:76:PRO:HD3	2.41	0.43
10:B:316:NAG:O3	10:B:316:NAG:H83	2.19	0.43
1:B:217:GLU:HG3	11:B:567:HOH:O	2.18	0.43
1:C:38:ILE:HD13	1:C:49:VAL:CG2	2.48	0.43
1:A:212:ARG:CG	1:A:212:ARG:NH1	2.80	0.43
1:C:61:ALA:HB2	1:C:104:ASP:HB2	2.00	0.43
1:B:272:ARG:HA	1:B:273:ASP:HA	1.83	0.43
1:C:148:ALA:O	1:C:257:TRP:HD1	2.01	0.43
1:A:105:PHE:HB3	1:A:107:ILE:HD11	2.00	0.43
1:C:83:VAL:O	1:C:87:THR:HB	2.18	0.43
1:A:188:LYS:NZ	11:A:466:HOH:O	2.52	0.43
1:C:36(A):ALA:C	1:C:38(A):GLU:H	2.21	0.43
1:A:61(A):HIS:O	1:A:65(A):SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ARG:HB2	8:A:327:SO4:O1	2.19	0.43
1:C:42:TYR:CE2	1:C:131:SER:HA	2.54	0.43
1:A:54:LYS:HG3	1:A:90:TYR:CE2	2.53	0.42
1:A:57(B):ARG:HG3	1:A:58:ALA:H	1.84	0.42
11:B:512:HOH:O	4:J:1:NAG:H83	2.17	0.42
1:C:24(A):THR:HB	1:C:31(A):LEU:HD21	2.00	0.42
1:C:62(A):LEU:HD11	1:C:69(A):PHE:CD2	2.54	0.42
1:C:62(A):LEU:HD11	1:C:69(A):PHE:CG	2.54	0.42
1:A:28(A):LYS:HE3	11:A:656:HOH:O	2.19	0.42
1:A:212:ARG:NH1	1:A:212:ARG:HG3	2.34	0.42
1:B:98:ASN:HA	1:B:101:LYS:HB3	2.02	0.42
1:A:3(A):ARG:HG2	11:A:642:HOH:O	2.18	0.42
1:B:293:ALA:O	1:B:297:VAL:HG23	2.20	0.42
1:A:13(A):THR:O	1:A:17(A):VAL:HG13	2.20	0.42
1:C:122:LYS:HD3	11:C:399:HOH:O	2.20	0.42
1:C:123:ASP:C	1:C:125:MET:H	2.23	0.42
1:A:59(A):LYS:O	1:A:63(A):ASN:HB2	2.20	0.42
1:A:5:SER:O	1:A:8:TYR:HB3	2.19	0.42
1:B:65(A):SER:O	1:B:66(A):ARG:HB2	2.20	0.42
1:C:134:GLU:HG3	1:C:135:LYS:HG2	2.01	0.42
1:C:71(A):VAL:HG13	1:C:74(A):GLU:OE1	2.20	0.42
1:C:38:ILE:HD13	1:C:49:VAL:HG23	2.01	0.42
1:A:70(A):ARG:HD2	11:A:475:HOH:O	2.19	0.42
1:C:89:TYR:HD2	1:C:92:LYS:HD3	1.84	0.42
1:B:32:MET:HE3	1:B:100:LEU:CD1	2.50	0.42
1:B:187:ILE:CD1	1:B:263:ILE:HD11	2.47	0.42
1:B:192:TYR:CE2	1:B:194:SER:HB2	2.54	0.42
1:C:12(A):ARG:O	1:C:16(A):GLN:HB2	2.20	0.42
1:C:13:HIS:CD2	1:C:17:GLU:HG2	2.54	0.42
1:A:33:VAL:O	1:A:33:VAL:CG2	2.68	0.41
1:A:88:TYR:HB2	11:A:573:HOH:O	2.20	0.41
1:B:86(A):ASN:O	1:B:87(A):ASP:HB3	2.19	0.41
1:C:72(A):LEU:HD22	1:C:275:GLY:O	2.20	0.41
1:B:85:SER:HA	11:B:543:HOH:O	2.21	0.41
1:B:187:ILE:HG23	1:B:188:LYS:N	2.34	0.41
1:B:4:ALA:C	1:B:6:SER:N	2.68	0.41
1:B:281:LEU:HA	1:B:282:PRO:HD3	1.95	0.41
1:C:173:GLU:O	1:C:176:VAL:CG1	2.68	0.41
1:B:205:PRO:HA	1:B:206:TYR:HA	1.76	0.41
1:C:54(A):ASP:O	1:C:58(A):VAL:HG23	2.19	0.41
1:C:225:GLU:O	1:C:225:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16(A):GLN:HG2	1:A:67(A):ILE:HG12	2.03	0.41
1:B:33(A):GLN:HG2	11:B:452:HOH:O	2.19	0.41
1:B:150:LYS:HE3	1:B:150:LYS:HB2	1.80	0.41
1:B:229:ALA:HB2	1:B:299:LYS:HE3	2.01	0.41
1:C:62(A):LEU:HD11	1:C:69(A):PHE:HB3	2.03	0.41
1:C:15:LEU:HD11	1:C:113:VAL:HG12	2.02	0.41
1:C:42:TYR:CZ	1:C:131:SER:HA	2.56	0.41
1:C:108:MET:HE2	1:C:110:VAL:O	2.21	0.41
1:A:8:TYR:O	1:A:13:HIS:HE1	2.04	0.41
1:C:4(A):GLY:O	1:C:76(A):VAL:HG23	2.21	0.41
1:C:132:LEU:HD12	1:C:132:LEU:HA	1.86	0.41
1:C:226:ALA:O	1:C:230:MET:HG3	2.21	0.41
1:C:62(A):LEU:HD21	1:C:69(A):PHE:CD2	2.56	0.41
1:C:233:ILE:HG23	1:C:234:HIS:HD2	1.85	0.41
1:C:81:TRP:CD1	1:C:290:CYS:HB3	2.56	0.41
1:C:134:GLU:O	1:C:135:LYS:CB	2.69	0.41
1:A:133:HIS:ND1	8:A:323:SO4:O1	2.54	0.40
1:B:20(A):LEU:O	1:B:24(A):THR:HG23	2.21	0.40
1:B:109:PRO:HD2	11:B:357:HOH:O	2.21	0.40
1:C:69(A):PHE:O	1:C:70(A):ARG:HB3	2.20	0.40
1:C:7:SER:C	1:C:9:TYR:H	2.25	0.40
1:C:74:ILE:HD13	1:C:281:LEU:HD23	2.03	0.40
1:C:81:TRP:CG	1:C:290:CYS:HB3	2.56	0.40
1:A:205:PRO:HA	1:A:206:TYR:HA	1.84	0.40
1:A:207:SER:OG	1:A:243:GLY:HA3	2.21	0.40
1:B:197:SER:HA	1:B:198:TYR:HA	1.91	0.40
1:C:91(A):PRO:HB2	1:C:92(A):ARG:H	1.64	0.40
1:C:123:ASP:OD2	1:C:125:MET:HB2	2.22	0.40
1:C:281:LEU:HD11	1:C:285:TYR:CB	2.45	0.40
1:B:292:GLU:O	1:B:295:VAL:HG22	2.21	0.40
1:A:75:SER:HB3	1:A:76:PRO:CD	2.41	0.40
1:A:197:SER:HA	1:A:198:TYR:HA	1.89	0.40
1:B:86(A):ASN:HB2	1:B:87(A):ASP:H	1.68	0.40
1:B:188:LYS:HE2	11:B:597:HOH:O	2.21	0.40
1:C:20(A):LEU:HD23	1:C:20(A):LEU:O	2.21	0.40
1:C:278:GLY:O	1:C:279:PHE:C	2.60	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	399/401 (100%)	386 (97%)	12 (3%)	1 (0%)	41	61
1	B	399/401 (100%)	373 (94%)	20 (5%)	6 (2%)	10	18
1	C	365/401 (91%)	304 (83%)	47 (13%)	14 (4%)	3	4
All	All	1163/1203 (97%)	1063 (91%)	79 (7%)	21 (2%)	8	14

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	SER
1	B	91(A)	PRO
1	B	199	SER
1	C	91(A)	PRO
1	C	131	SER
1	C	199	SER
1	C	211	SER
1	C	13(A)	THR
1	C	92(A)	ARG
1	C	7	SER
1	C	122	LYS
1	C	133	HIS
1	C	274	LYS
1	B	92(A)	ARG
1	B	5	SER
1	B	59	LYS
1	C	214	LYS
1	C	235	ARG
1	B	86(A)	ASN
1	C	60	ASN
1	C	135	LYS

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	358/358 (100%)	328 (92%)	30 (8%)	11	21
1	B	357/358 (100%)	340 (95%)	17 (5%)	25	48
1	C	332/358 (93%)	310 (93%)	22 (7%)	16	32
All	All	1047/1074 (98%)	978 (93%)	69 (7%)	16	32

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20(A)	LEU
1	A	22(A)	ASN
1	A	38(A)	GLU
1	A	42(A)	LYS
1	A	55(A)	VAL
1	A	63(A)	ASN
1	A	65(A)	SER
1	A	75(A)	ASN
1	A	79(A)	LEU
1	A	86(A)	ASN
1	A	5	SER
1	A	11	GLN
1	A	15	LEU
1	A	33	VAL
1	A	47	LEU
1	A	54	LYS
1	A	56	GLU
1	A	57(B)	ARG
1	A	87	THR
1	A	100	LEU
1	A	113	VAL
1	A	145	ARG
1	A	152	CYS
1	A	188	LYS
1	A	210	ARG
1	A	212	ARG

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Mol	Chain	Res	Type
1	A	221	LEU
1	A	224	ARG
1	A	280	LEU
1	A	306	LYS
1	B	3(A)	ARG
1	B	63(A)	ASN
1	B	92(A)	ARG
1	B	25	MET
1	B	27	GLU
1	B	28	ARG
1	B	33	VAL
1	B	47	LEU
1	B	57	GLN
1	B	87	THR
1	B	125	MET
1	B	152	CYS
1	B	177	LYS
1	B	188	LYS
1	B	210	ARG
1	B	247	LEU
1	B	280	LEU
1	C	33(A)	GLN
1	C	38(A)	GLU
1	C	61(A)	HIS
1	C	62(A)	LEU
1	C	63(A)	ASN
1	C	74(A)	GLU
1	C	10	GLU
1	C	15	LEU
1	C	27	GLU
1	C	37	HIS
1	C	93	GLU
1	C	136	ASN
1	C	152	CYS
1	C	188(B)	HIS
1	C	212	ARG
1	C	231	GLU
1	C	235	ARG
1	C	248	TYR
1	C	264	LYS
1	C	279	PHE
1	C	280	LEU

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Mol	Chain	Res	Type
1	C	283	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16(A)	GLN
1	A	18(A)	GLN
1	A	47(A)	HIS
1	A	75(A)	ASN
1	A	82(A)	GLN
1	A	11	GLN
1	A	13	HIS
1	A	60	ASN
1	A	234	HIS
1	A	307	ASN
1	B	18(A)	GLN
1	B	47(A)	HIS
1	B	82(A)	GLN
1	B	83(A)	GLN
1	B	13	HIS
1	B	188(B)	HIS
1	B	234	HIS
1	C	5(A)	GLN
1	C	16(A)	GLN
1	C	18(A)	GLN
1	C	47(A)	HIS
1	C	63(A)	ASN
1	C	82(A)	GLN
1	C	11	GLN
1	C	13	HIS
1	C	102	HIS
1	C	136	ASN
1	C	150(B)	HIS
1	C	216	HIS
1	C	234	HIS
1	C	303	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 ⓘ

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	D	1	2,1	14,14,15	0.83	1 (7%)	17,19,21	1.20	2 (11%)
2	NDG	D	2	2	14,14,15	0.75	1 (7%)	17,19,21	0.65	0
3	NAG	E	1	3,1	14,14,15	0.85	1 (7%)	17,19,21	0.73	0
3	FUL	E	2	3	10,10,11	0.56	0	14,14,16	0.47	0
4	NAG	F	1	4,1	14,14,15	0.58	0	17,19,21	0.75	0
4	NAG	F	2	4	14,14,15	0.69	0	17,19,21	0.54	0
5	NAG	G	1	5,1	14,14,15	0.60	0	17,19,21	0.84	1 (5%)
5	NAG	G	2	5	14,14,15	0.59	0	17,19,21	0.65	0
5	FUL	G	3	5	10,10,11	0.65	0	14,14,16	0.61	0
6	NAG	H	1	6,1	14,14,15	0.55	0	17,19,21	0.78	1 (5%)
6	NAG	H	2	6	14,14,15	0.73	0	17,19,21	0.98	0
6	BMA	H	3	6	11,11,12	0.82	0	15,15,17	1.06	2 (13%)
2	NAG	I	1	2,1	14,14,15	0.80	0	17,19,21	1.31	2 (11%)
2	NDG	I	2	2	14,14,15	0.75	0	17,19,21	0.95	2 (11%)
4	NAG	J	1	4,1	14,14,15	0.64	0	17,19,21	0.64	0
4	NAG	J	2	4	14,14,15	0.67	0	17,19,21	0.59	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	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NDG	D	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	6/6/23/26	0/1/1/1
3	FUL	E	2	3	-	-	0/1/1/1
4	NAG	F	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	5/6/23/26	0/1/1/1
5	NAG	G	1	5,1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	4/6/23/26	0/1/1/1
5	FUL	G	3	5	-	-	0/1/1/1
6	NAG	H	1	6,1	-	6/6/23/26	0/1/1/1
6	NAG	H	2	6	-	4/6/23/26	0/1/1/1
6	BMA	H	3	6	-	1/2/19/22	0/1/1/1
2	NAG	I	1	2,1	-	4/6/23/26	0/1/1/1
2	NDG	I	2	2	-	4/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	6/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	C1-C2	2.39	1.55	1.52
2	D	1	NAG	C1-C2	2.20	1.55	1.52
2	D	2	NDG	C1-C2	2.00	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	NAG	C4-C3-C2	3.13	115.60	111.02
2	I	1	NAG	C3-C4-C5	2.95	115.51	110.24
6	H	3	BMA	C1-O5-C5	2.48	115.55	112.19
2	I	2	NDG	O5-C1-C2	-2.36	107.56	111.29
6	H	3	BMA	C1-C2-C3	2.30	112.50	109.67
2	D	1	NAG	C4-C3-C2	-2.30	107.65	111.02
2	I	2	NDG	C2-N2-C7	-2.17	119.82	122.90
5	G	1	NAG	C2-N2-C7	-2.16	119.83	122.90
6	H	1	NAG	C2-N2-C7	-2.11	119.90	122.90
2	D	1	NAG	C3-C4-C5	-2.05	106.58	110.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	1	NAG	C1

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C3-C2-N2-C7
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
6	H	1	NAG	C8-C7-N2-C2
6	H	1	NAG	O7-C7-N2-C2
6	H	2	NAG	C8-C7-N2-C2
6	H	2	NAG	O7-C7-N2-C2
2	D	2	NDG	O5-C5-C6-O6
6	H	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C1-C2-N2-C7
6	H	2	NAG	O5-C5-C6-O6
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O5-C5-C6-O6
6	H	2	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
2	D	2	NDG	C4-C5-C6-O6
6	H	1	NAG	C4-C5-C6-O6
4	J	1	NAG	O7-C7-N2-C2
3	E	1	NAG	O5-C5-C6-O6
6	H	1	NAG	C1-C2-N2-C7
3	E	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	G	2	NAG	C8-C7-N2-C2
4	F	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
6	H	3	BMA	O5-C5-C6-O6

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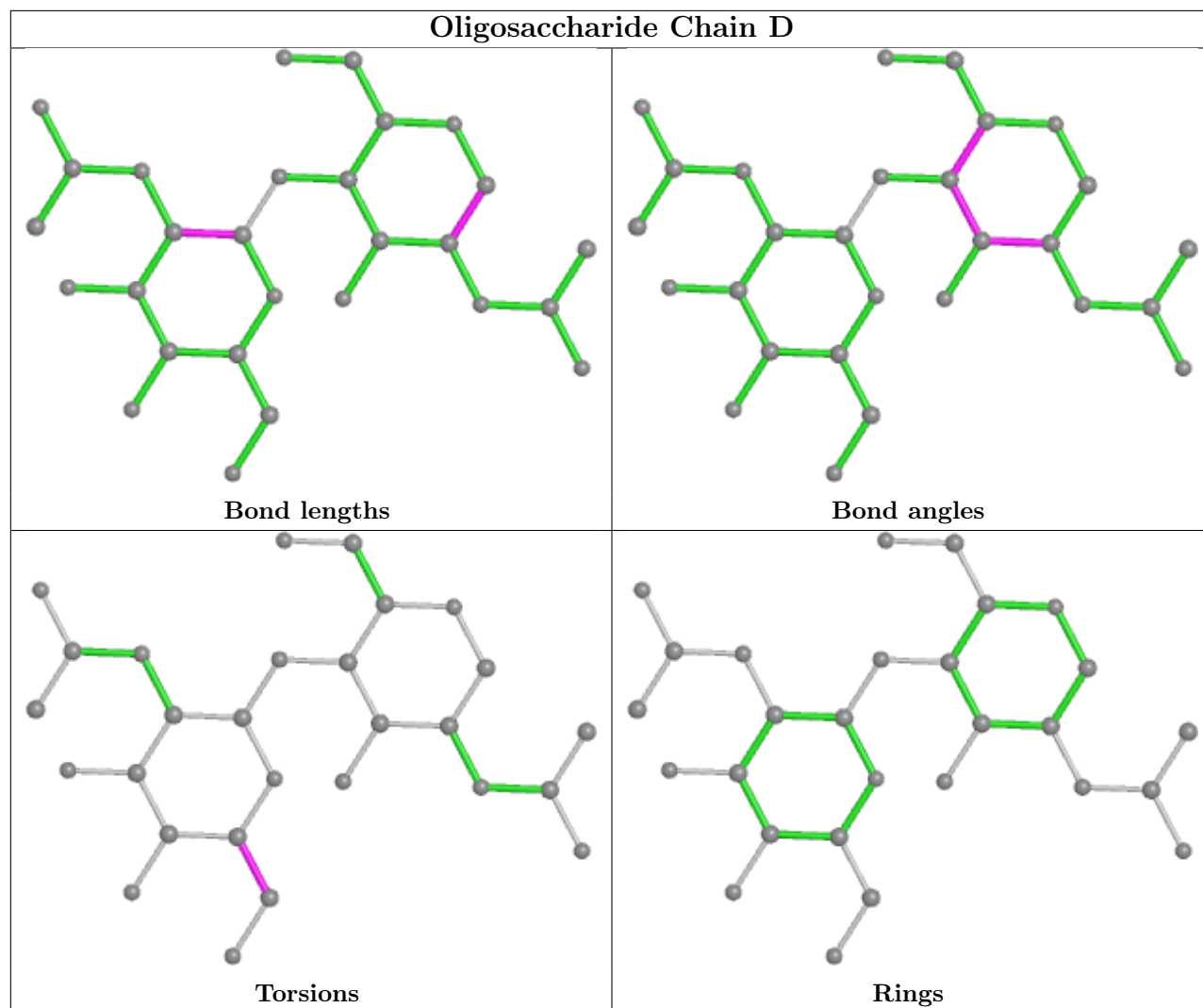
Mol	Chain	Res	Type	Atoms
4	F	1	NAG	C4-C5-C6-O6
2	I	2	NDG	C8-C7-N2-C2
2	I	2	NDG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
5	G	2	NAG	O7-C7-N2-C2
4	J	2	NAG	C1-C2-N2-C7
2	I	2	NDG	O7-C7-N2-C2
3	E	1	NAG	C1-C2-N2-C7
4	F	2	NAG	C4-C5-C6-O6
2	I	2	NDG	O5-C5-C6-O6
4	J	2	NAG	C3-C2-N2-C7
6	H	1	NAG	C3-C2-N2-C7
2	I	1	NAG	C3-C2-N2-C7
3	E	1	NAG	C3-C2-N2-C7

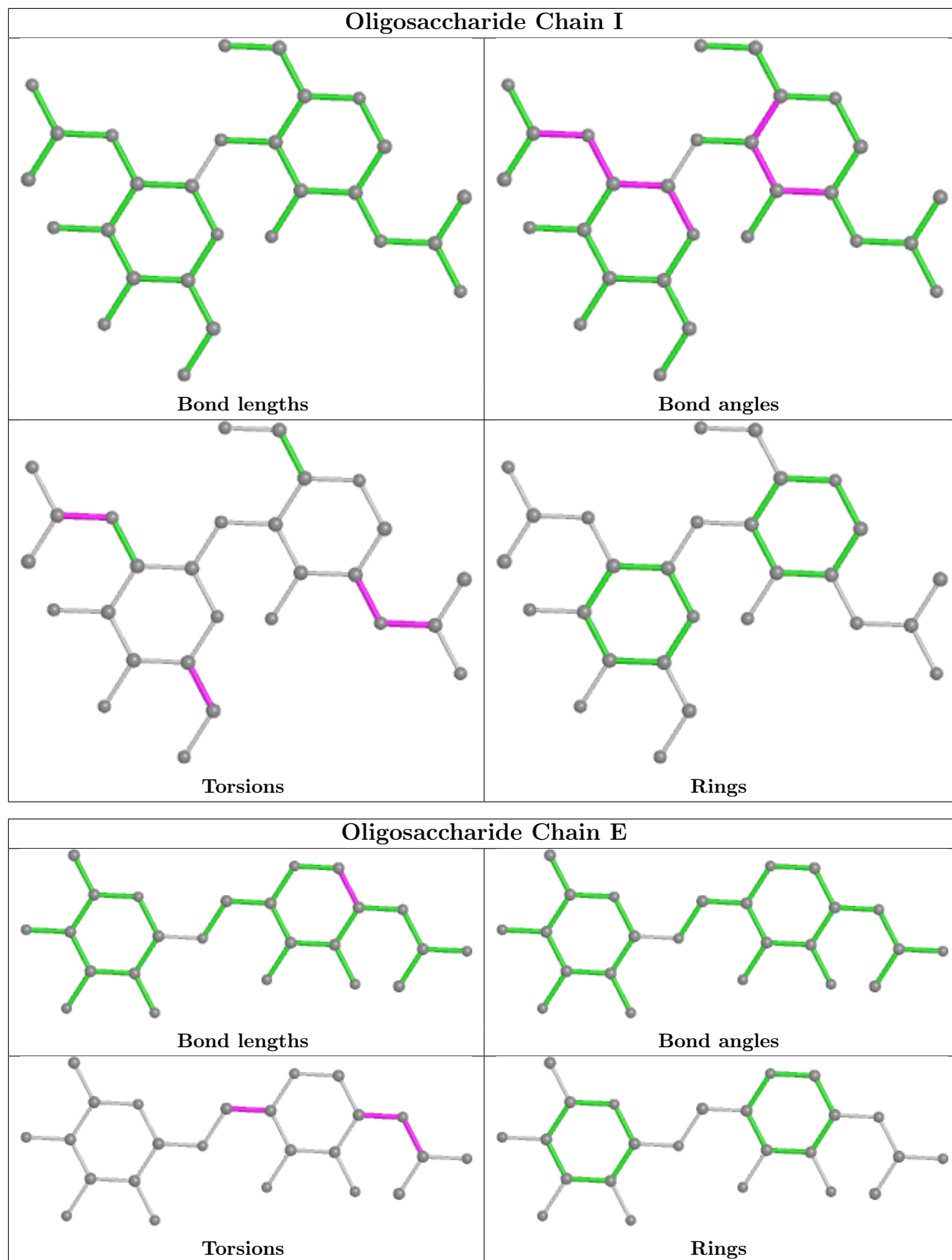
There are no ring outliers.

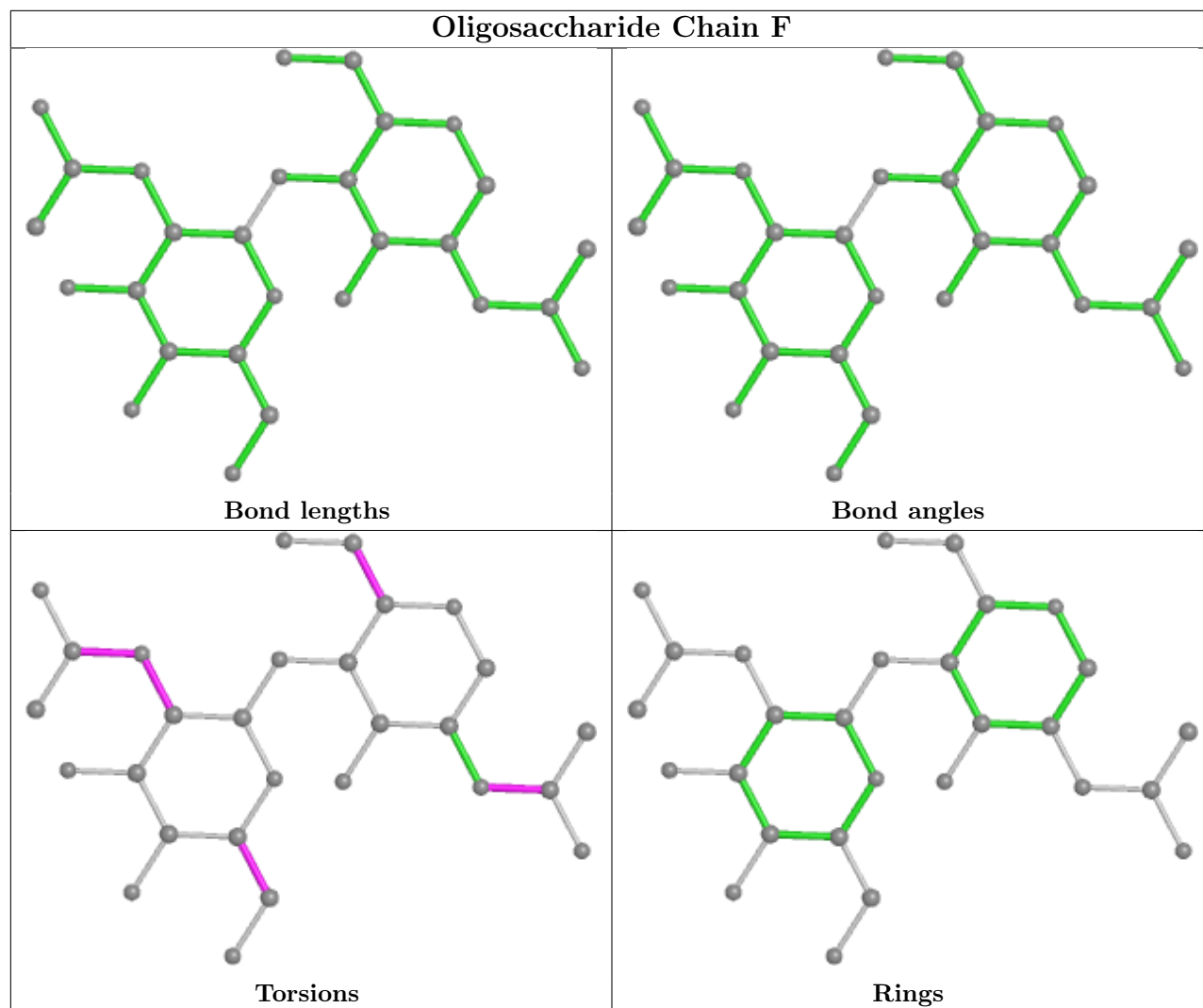
8 monomers are involved in 8 short contacts:

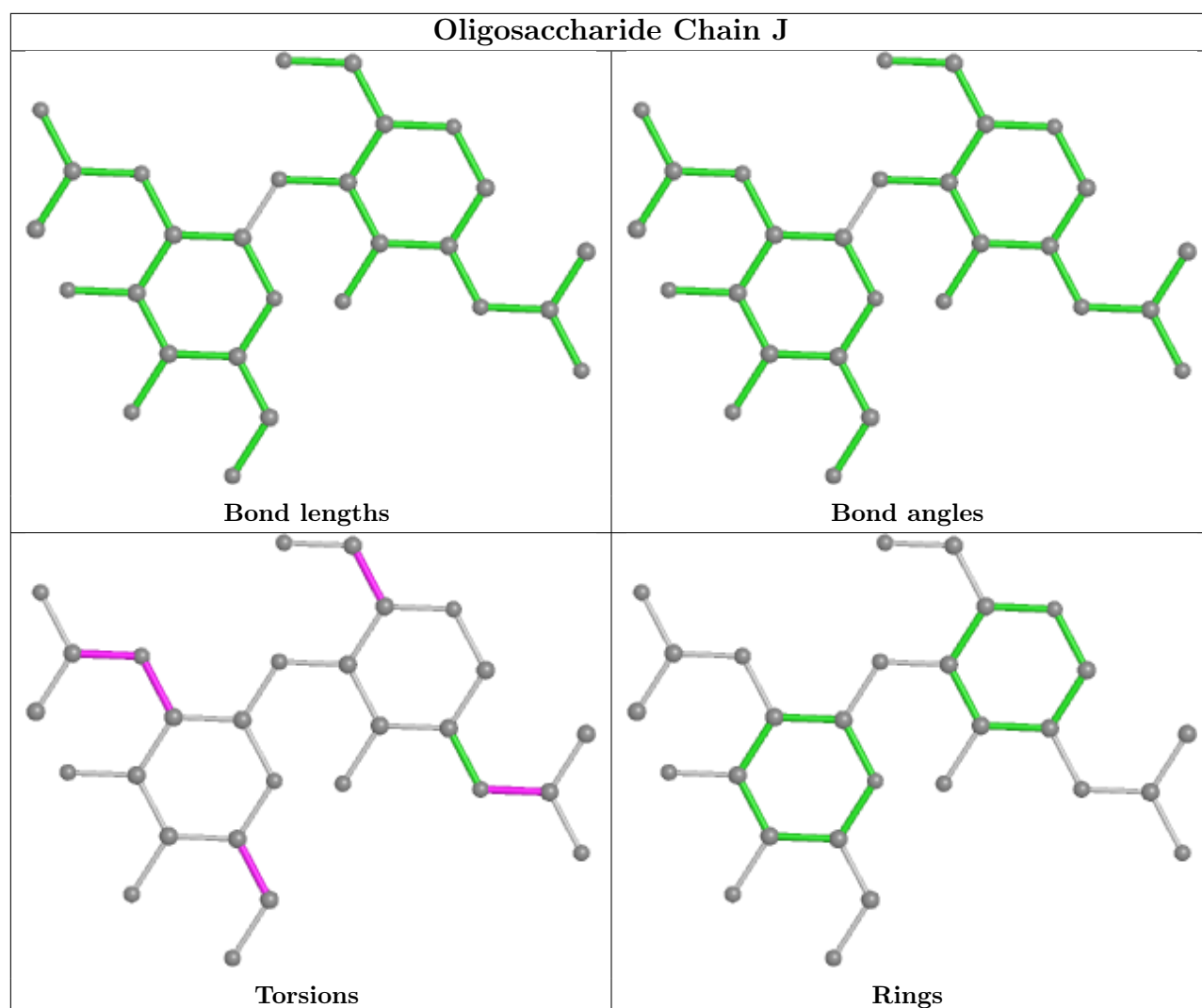
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	2	NAG	2	0
3	E	1	NAG	1	0
6	H	3	BMA	1	0
4	F	1	NAG	2	0
6	H	1	NAG	1	0
2	I	1	NAG	1	0
4	F	2	NAG	2	0
4	J	1	NAG	2	0

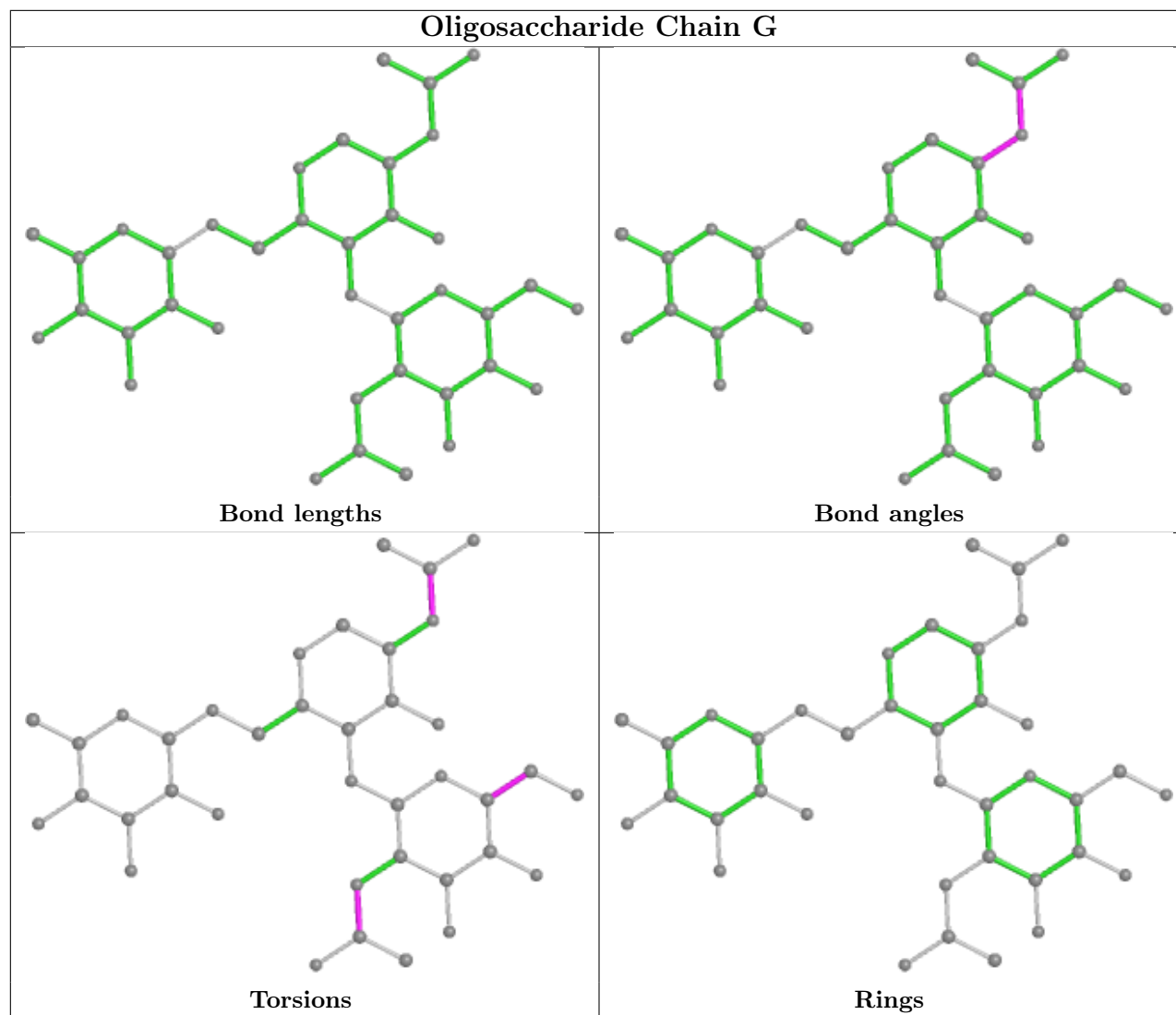
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

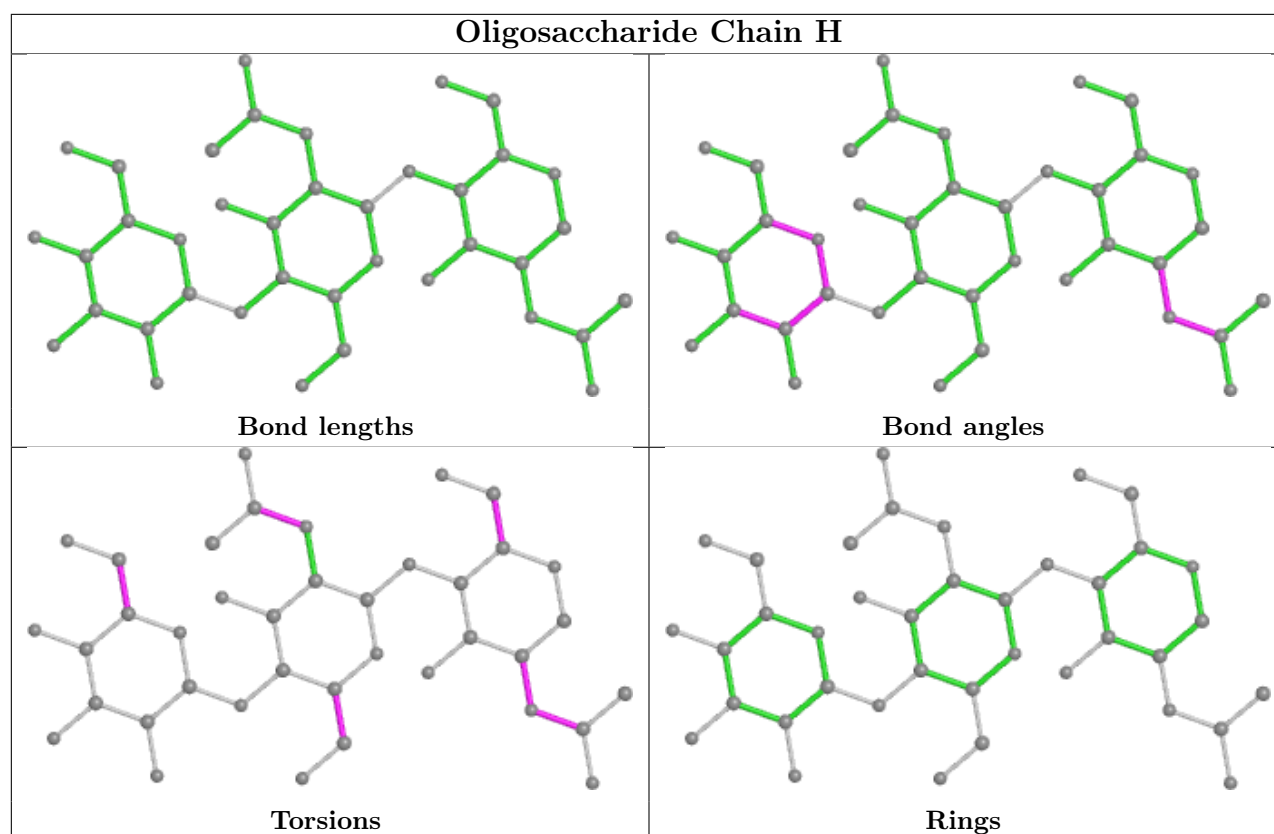












5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 3 are monoatomic - leaving 27 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	$\# Z > 2$
9	MLI	C	313	-	0,6,6	0.00	-	0,7,7	0.00	-
9	MLI	B	329	-	0,6,6	0.00	-	0,7,7	0.00	-
8	SO4	A	327	-	4,4,4	0.22	0	6,6,6	0.16	0
8	SO4	B	328	-	4,4,4	0.26	0	6,6,6	0.07	0
8	SO4	B	323	-	4,4,4	0.27	0	6,6,6	0.09	0
9	MLI	A	328	7	0,6,6	0.00	-	0,7,7	0.00	-
8	SO4	B	319	-	4,4,4	0.23	0	6,6,6	0.12	0
8	SO4	A	322	-	4,4,4	0.31	0	6,6,6	0.13	0
8	SO4	A	325	-	4,4,4	0.24	0	6,6,6	0.04	0
8	SO4	A	324	-	4,4,4	0.22	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	C	312	-	4,4,4	0.25	0	6,6,6	0.17	0
10	NAG	B	316	1	14,14,15	0.58	0	17,19,21	0.76	0
8	SO4	A	323	-	4,4,4	0.23	0	6,6,6	0.17	0
8	SO4	B	324	-	4,4,4	0.27	0	6,6,6	0.10	0
8	SO4	A	321	-	4,4,4	0.27	0	6,6,6	0.08	0
8	SO4	B	325	-	4,4,4	0.26	0	6,6,6	0.07	0
8	SO4	B	322	-	4,4,4	0.28	0	6,6,6	0.07	0
8	SO4	B	327	-	4,4,4	0.24	0	6,6,6	0.10	0
8	SO4	C	311	-	4,4,4	0.26	0	6,6,6	0.10	0
8	SO4	A	326	-	4,4,4	0.24	0	6,6,6	0.07	0
8	SO4	B	318	-	4,4,4	0.23	0	6,6,6	0.14	0
10	NAG	C	309	1	14,14,15	0.50	0	17,19,21	0.70	1 (5%)
8	SO4	A	320	-	4,4,4	0.26	0	6,6,6	0.12	0
8	SO4	B	326	-	4,4,4	0.26	0	6,6,6	0.06	0
8	SO4	B	321	-	4,4,4	0.25	0	6,6,6	0.08	0
8	SO4	A	319	-	4,4,4	0.21	0	6,6,6	0.15	0
8	SO4	B	320	-	4,4,4	0.25	0	6,6,6	0.17	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
10	NAG	B	316	1	-	4/6/23/26	0/1/1/1
9	MLI	C	313	-	-	0/0/4/4	-
9	MLI	B	329	-	-	0/0/4/4	-
10	NAG	C	309	1	1/1/5/7	2/6/23/26	0/1/1/1
9	MLI	A	328	7	-	0/0/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	309	NAG	C2-N2-C7	-2.09	119.93	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	C	309	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	316	NAG	C8-C7-N2-C2
10	B	316	NAG	O7-C7-N2-C2
10	C	309	NAG	C8-C7-N2-C2
10	C	309	NAG	O7-C7-N2-C2
10	B	316	NAG	C4-C5-C6-O6
10	B	316	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	329	MLI	1	0
8	A	327	SO4	1	0
10	B	316	NAG	2	0
8	A	323	SO4	1	0
8	C	311	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	401/401 (100%)	-0.24	6 (1%) 73 75	29, 44, 66, 87	0
1	B	401/401 (100%)	-0.21	9 (2%) 62 65	30, 49, 70, 93	0
1	C	379/401 (94%)	1.47	113 (29%) 0 0	72, 123, 156, 160	0
All	All	1181/1203 (98%)	0.32	128 (10%) 5 5	29, 56, 150, 160	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37(A)	ALA	8.4
1	C	19(A)	ILE	8.2
1	C	228	PHE	8.2
1	C	56(A)	SER	8.2
1	C	60(A)	ALA	7.9
1	C	308	VAL	7.0
1	C	27(A)	TYR	7.0
1	C	15(A)	ARG	6.6
1	A	58	ALA	6.4
1	C	68(A)	PRO	6.2
1	A	57(B)	ARG	5.6
1	C	85(A)	SER	5.6
1	C	82(A)	GLN	5.4
1	C	64(A)	ALA	5.4
1	B	57(B)	ARG	5.3
1	C	232	ASN	5.3
1	C	71(A)	VAL	5.2
1	C	212	ARG	5.1
1	C	6	SER	5.1
1	C	233	ILE	5.1
1	C	6(A)	VAL	5.0
1	C	16(A)	GLN	4.9
1	C	5	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	91(A)	PRO	4.8
1	C	279	PHE	4.8
1	C	70(A)	ARG	4.7
1	C	102	HIS	4.6
1	C	285	TYR	4.6
1	C	55(A)	VAL	4.6
1	C	14(A)	SER	4.6
1	C	5(A)	GLN	4.6
1	C	235	ARG	4.5
1	B	57	GLN	4.5
1	C	12(A)	ARG	4.5
1	C	246	SER	4.4
1	C	221	LEU	4.4
1	C	3(A)	ARG	4.4
1	C	209	SER	4.2
1	C	92(A)	ARG	4.2
1	A	57	GLN	4.2
1	C	153	GLY	4.1
1	B	58	ALA	4.1
1	C	56	GLU	4.0
1	C	206	TYR	3.8
1	C	280	LEU	3.7
1	C	32(A)	TRP	3.6
1	C	26(A)	THR	3.6
1	C	277	TYR	3.6
1	C	89	TYR	3.6
1	C	98	ASN	3.6
1	C	69(A)	PHE	3.5
1	C	248	TYR	3.5
1	C	217	GLU	3.5
1	C	307	ASN	3.4
1	C	245	GLU	3.4
1	C	34(A)	PRO	3.4
1	C	38(A)	GLU	3.4
1	C	304	VAL	3.3
1	C	244	SER	3.3
1	C	75(A)	ASN	3.2
1	C	235(B)	ASN	3.2
1	C	208	TYR	3.1
1	C	78(A)	ASP	3.1
1	C	63(A)	ASN	3.1
1	C	230	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	265	TYR	3.1
1	C	81(A)	ARG	3.0
1	C	204	PHE	3.0
1	C	90	TYR	3.0
1	C	18(A)	GLN	3.0
1	C	13(A)	THR	3.0
1	C	253	GLY	3.0
1	C	55	LYS	2.9
1	C	4	ALA	2.9
1	C	284	SER	2.9
1	C	281	LEU	2.9
1	B	5	SER	2.8
1	B	308	VAL	2.8
1	C	84	GLY	2.8
1	C	74(A)	GLU	2.8
1	C	93	GLU	2.8
1	C	28(A)	LYS	2.7
1	C	127	ARG	2.7
1	B	91(A)	PRO	2.7
1	C	122	LYS	2.7
1	C	21(A)	GLN	2.7
1	C	269	PHE	2.6
1	C	207	SER	2.6
1	C	25(A)	THR	2.6
1	C	95	MET	2.6
1	C	197	SER	2.6
1	C	28	ARG	2.5
1	C	35(A)	VAL	2.5
1	C	267	PHE	2.5
1	C	61(A)	HIS	2.5
1	C	80(A)	ILE	2.5
1	C	266	SER	2.4
1	C	33(A)	GLN	2.4
1	A	89(A)	ILE	2.4
1	C	158	SER	2.4
1	C	154	GLU	2.4
1	C	23(A)	VAL	2.3
1	B	89(A)	ILE	2.3
1	C	48(A)	PHE	2.3
1	C	24	VAL	2.3
1	B	248	TYR	2.3
1	C	83	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	276	LYS	2.3
1	C	91	GLY	2.3
1	C	72(A)	LEU	2.3
1	C	234	HIS	2.2
1	C	7	SER	2.2
1	C	268	THR	2.2
1	A	15(A)	ARG	2.2
1	C	125	MET	2.2
1	C	198	TYR	2.2
1	C	45(A)	GLU	2.2
1	C	252	GLY	2.2
1	C	159	SER	2.2
1	C	59(A)	LYS	2.2
1	A	246	SER	2.1
1	C	132	LEU	2.1
1	C	241	GLY	2.1
1	B	55	LYS	2.1
1	C	12	TYR	2.0
1	C	76(A)	VAL	2.0
1	C	59	LYS	2.0
1	C	131	SER	2.0

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

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

6.3 Carbohydrates [i](#)

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

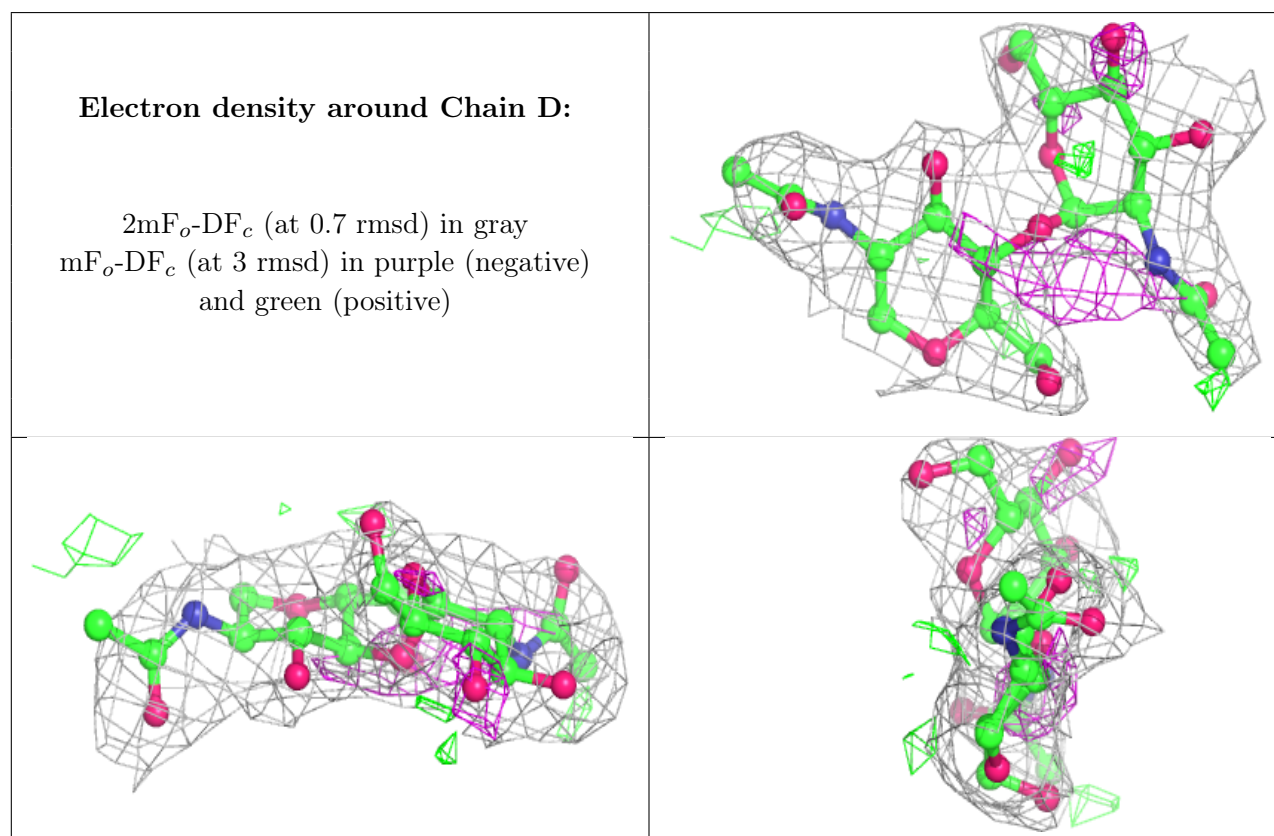
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	BMA	H	3	11/12	0.35	0.63	102,103,104,104	0
4	NAG	J	2	14/15	0.59	0.58	106,107,108,108	0
4	NAG	F	2	14/15	0.62	0.54	103,104,105,105	0
2	NDG	I	2	14/15	0.67	0.64	96,98,99,99	0
2	NAG	I	1	14/15	0.73	0.39	84,86,89,93	0
3	FUL	E	2	10/11	0.74	0.60	100,101,102,102	0
4	NAG	F	1	14/15	0.75	0.31	95,97,99,101	0

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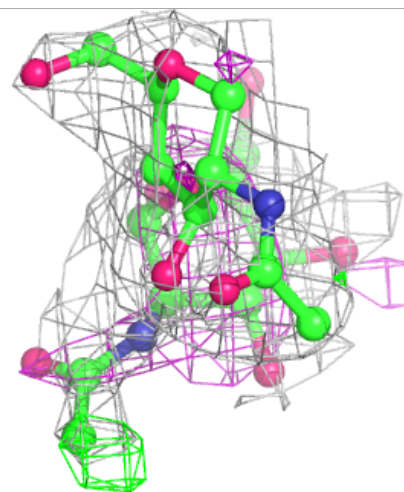
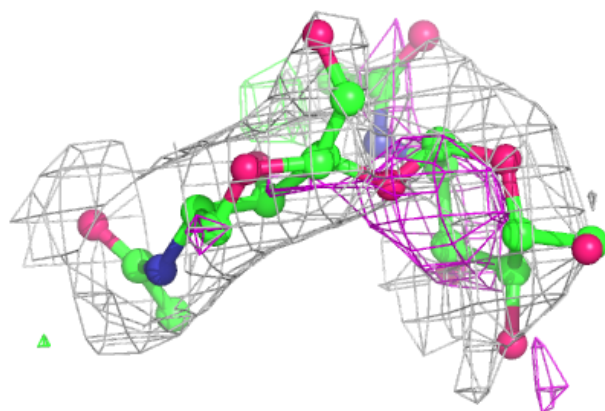
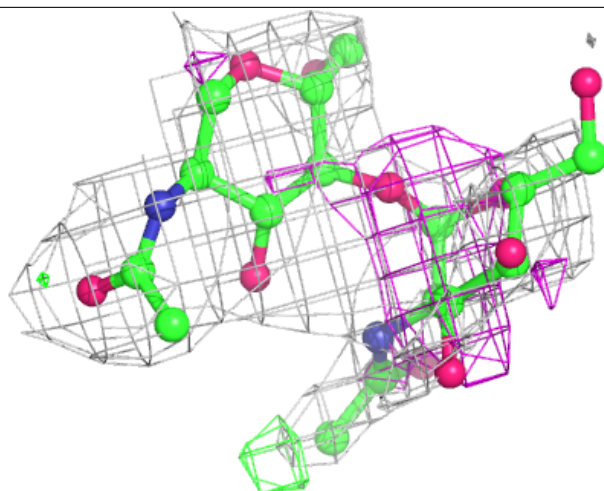
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	G	2	14/15	0.75	0.75	102,103,104,105	0
5	FUL	G	3	10/11	0.75	0.47	100,101,101,102	0
3	NAG	E	1	14/15	0.75	0.45	88,92,94,98	0
4	NAG	J	1	14/15	0.77	0.40	97,99,101,104	0
6	NAG	H	2	14/15	0.79	0.54	90,94,95,99	0
5	NAG	G	1	14/15	0.82	0.35	90,93,99,99	0
2	NDG	D	2	14/15	0.86	0.45	82,84,85,86	0
2	NAG	D	1	14/15	0.89	0.28	69,71,75,79	0
6	NAG	H	1	14/15	0.92	0.20	72,74,79,85	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.



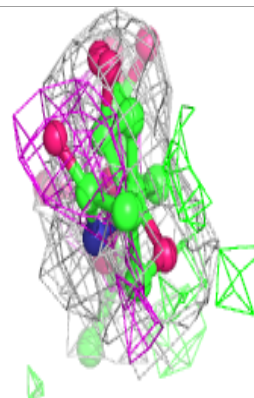
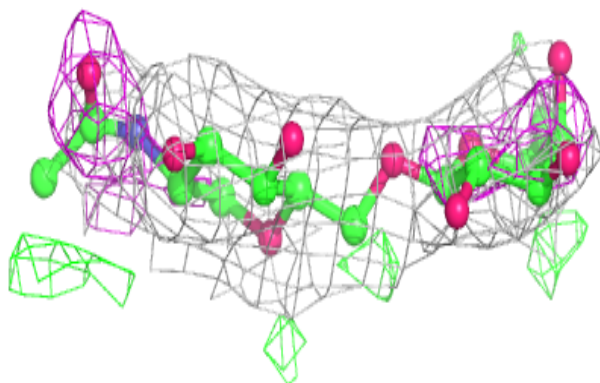
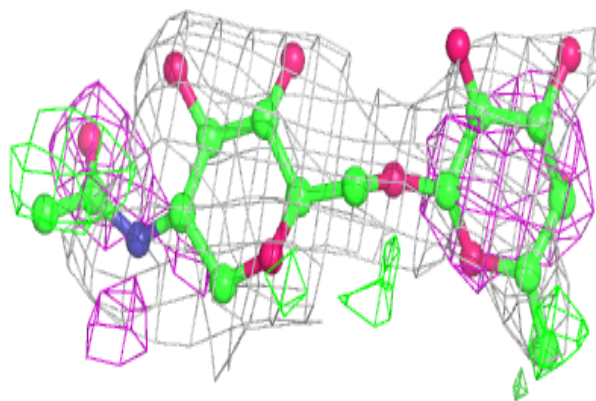
Electron density around Chain I:

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

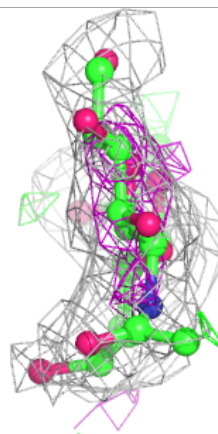
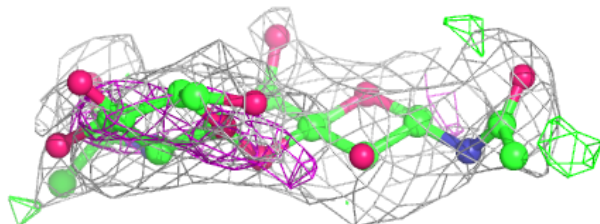
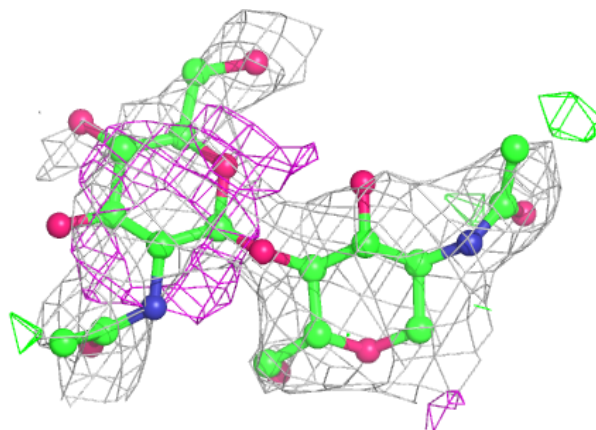


Electron density around Chain E:

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

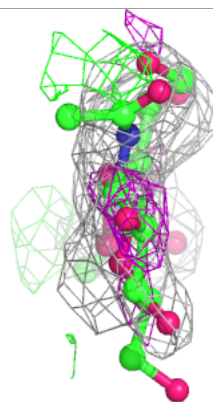
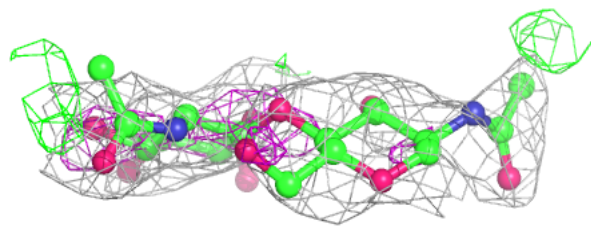
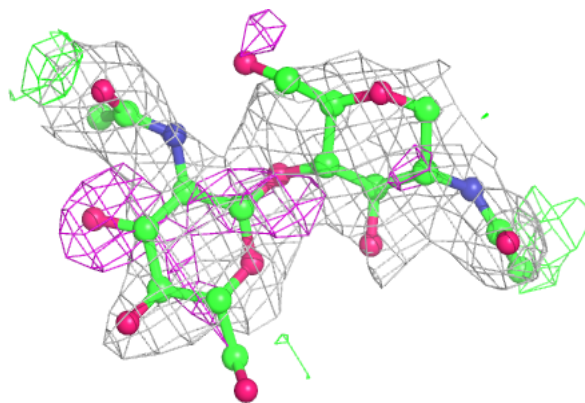
**Electron density around Chain F:**

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



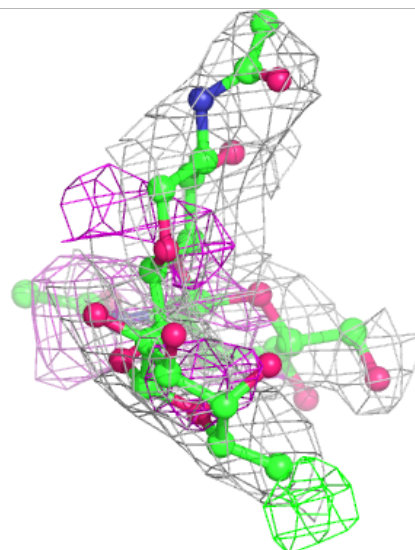
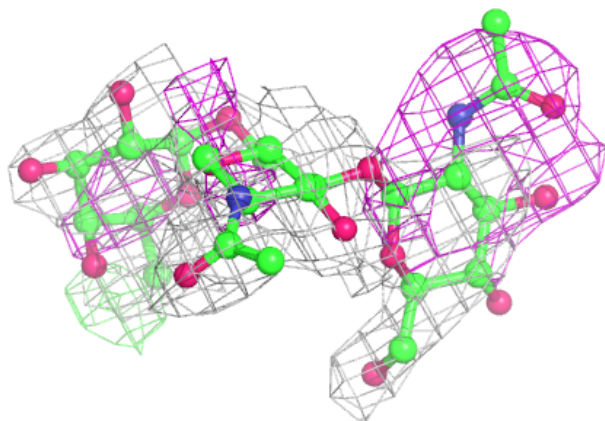
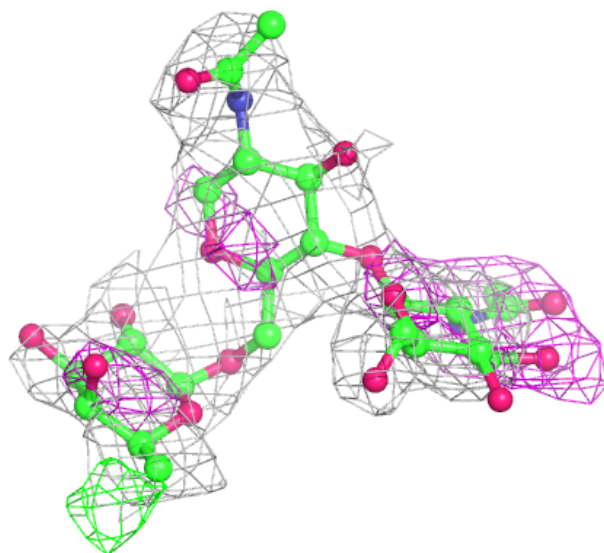
Electron density around Chain J:

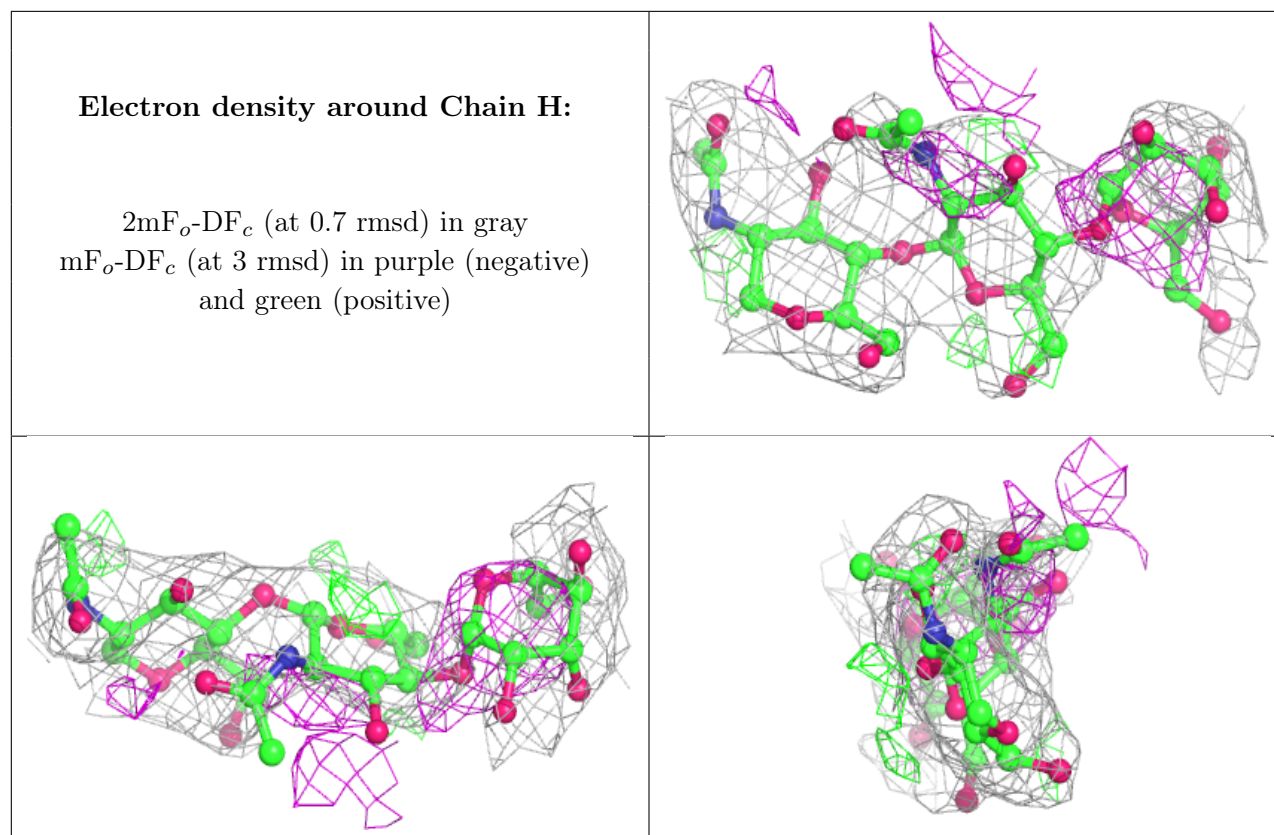
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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 ⓘ

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
10	NAG	C	309	14/15	0.53	0.46	151,152,152,152	0
10	NAG	B	316	14/15	0.78	0.48	85,88,89,90	0
8	SO4	A	327	5/5	0.78	0.21	98,99,99,99	0
8	SO4	C	312	5/5	0.79	0.23	136,136,136,136	0
8	SO4	B	328	5/5	0.84	0.17	140,140,140,140	0
9	MLI	A	328	7/7	0.86	0.34	72,73,74,74	0
9	MLI	B	329	7/7	0.87	0.27	66,67,68,68	0
7	ZN	C	310	1/1	0.90	0.09	110,110,110,110	0
8	SO4	B	322	5/5	0.91	0.26	127,127,127,127	0
8	SO4	B	324	5/5	0.92	0.14	103,103,104,104	0
9	MLI	C	313	7/7	0.94	0.21	109,109,109,109	0
8	SO4	B	326	5/5	0.94	0.12	129,129,129,129	0
8	SO4	B	327	5/5	0.94	0.20	94,94,95,95	0
8	SO4	A	323	5/5	0.95	0.15	92,92,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	SO4	A	325	5/5	0.95	0.17	114,114,114,114	0
8	SO4	A	326	5/5	0.95	0.32	147,147,147,147	0
8	SO4	A	324	5/5	0.96	0.15	80,80,81,81	0
8	SO4	B	323	5/5	0.96	0.12	105,105,105,105	0
8	SO4	C	311	5/5	0.96	0.16	110,110,110,110	0
8	SO4	A	320	5/5	0.97	0.08	71,72,72,72	0
8	SO4	A	321	5/5	0.97	0.09	80,81,81,81	0
8	SO4	A	322	5/5	0.97	0.13	86,86,86,87	0
8	SO4	B	320	5/5	0.98	0.11	73,73,74,74	0
8	SO4	B	325	5/5	0.98	0.15	118,118,118,118	0
8	SO4	B	321	5/5	0.98	0.19	100,100,100,100	0
7	ZN	B	317	1/1	0.99	0.10	39,39,39,39	0
7	ZN	A	318	1/1	0.99	0.10	39,39,39,39	0
8	SO4	B	318	5/5	0.99	0.07	58,58,59,60	0
8	SO4	B	319	5/5	0.99	0.14	73,74,74,75	0
8	SO4	A	319	5/5	0.99	0.09	51,52,52,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.