



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 28, 2022 – 12:06 PM JST

PDB ID : 7WHU
Title : Human Neutrophil Elastase in-complex with Ecotin Peptide
Authors : Shankar, S.; Jayaraman, S.
Deposited on : 2021-12-31
Resolution : 2.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

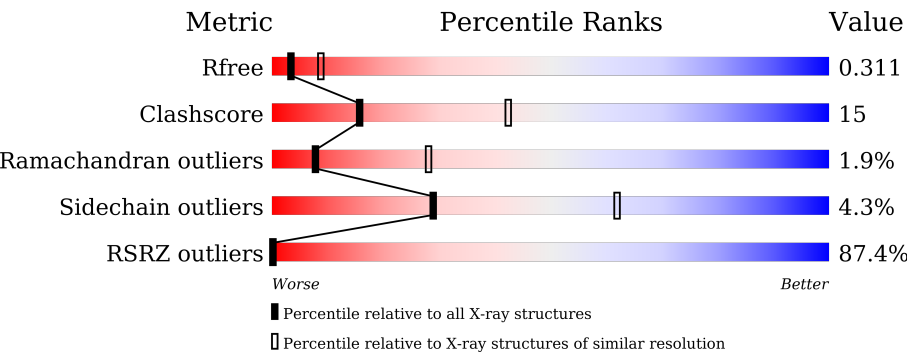
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	267	<div><div>72%</div><div><div>56%</div><div>25%</div><div>•</div><div>18%</div></div></div>
1	B	267	<div><div>66%</div><div><div>55%</div><div>25%</div><div>•</div><div>18%</div></div></div>
1	C	267	<div><div>73%</div><div><div>51%</div><div>29%</div><div>•</div><div>18%</div></div></div>
1	D	267	<div><div>73%</div><div><div>57%</div><div>24%</div><div>•</div><div>18%</div></div></div>
2	E	8	<div><div>88%</div><div><div>62%</div><div>38%</div></div></div>
2	F	8	<div><div>100%</div><div><div>50%</div><div>38%</div><div>12%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	8	
2	H	8	
3	K	3	
3	N	3	
3	O	3	
3	P	3	
4	I	2	
5	J	4	
6	L	2	
7	M	3	

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
3	NAG	K	1	-	-	-	X
3	NAG	K	2	-	-	-	X
3	FUC	K	3	-	-	-	X
3	NAG	N	1	-	-	-	X
3	NAG	N	2	-	-	-	X
3	FUC	N	3	-	-	-	X
3	NAG	O	1	-	-	-	X
3	NAG	O	2	-	-	-	X
3	FUC	O	3	-	-	-	X
3	NAG	P	1	-	-	-	X
3	NAG	P	2	-	-	-	X
3	FUC	P	3	-	-	-	X
4	NAG	I	1	-	-	-	X
4	FUC	I	2	-	-	-	X
5	NAG	J	1	-	-	-	X
5	NAG	J	2	-	-	-	X
5	BMA	J	3	-	-	-	X
5	FUC	J	4	-	-	-	X
6	NAG	L	1	-	-	-	X
6	NAG	L	2	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	M	1	-	-	-	X
7	NAG	M	3	-	-	-	X
8	GOL	A	301	-	-	-	X
8	GOL	B	303	-	-	-	X
8	GOL	B	305	-	-	-	X
8	GOL	C	301	-	-	-	X
8	GOL	D	301	-	-	-	X
9	SO4	B	301	-	-	-	X
9	SO4	B	302	-	-	-	X
9	SO4	C	302	-	-	-	X
9	SO4	C	303	-	-	-	X
9	SO4	D	302	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7019 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.

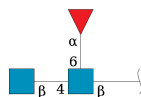
- Molecule 1 is a protein called Neutrophil elastase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	218	Total	C	N	O	S	0	0	0
			1597	1001	306	279	11			
1	A	218	Total	C	N	O	S	0	0	0
			1610	1012	308	279	11			
1	B	218	Total	C	N	O	S	0	0	0
			1610	1012	309	278	11			
1	C	218	Total	C	N	O	S	0	0	0
			1627	1019	316	281	11			

- Molecule 2 is a protein called Ecotin Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	S	0	0	0
			47	29	8	9	1			
2	F	8	Total	C	N	O	S	0	0	0
			51	31	8	11	1			
2	G	8	Total	C	N	O	S	0	0	0
			51	32	8	10	1			
2	H	8	Total	C	N	O	S	0	0	0
			46	27	8	10	1			

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



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

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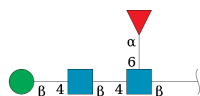
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	N	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	O	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



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

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



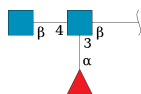
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



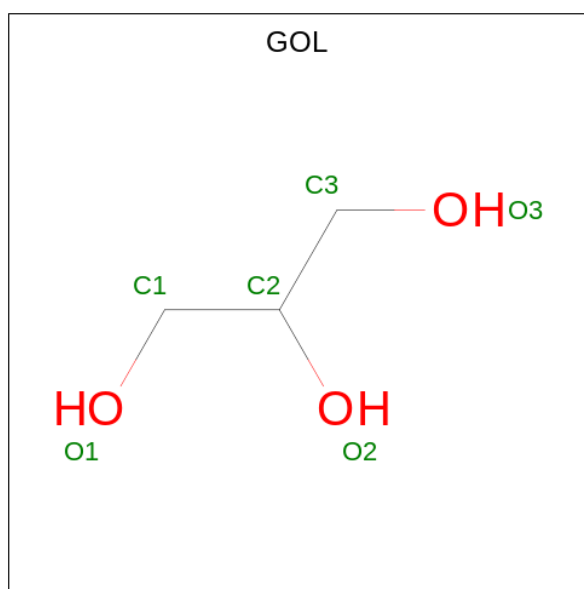
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



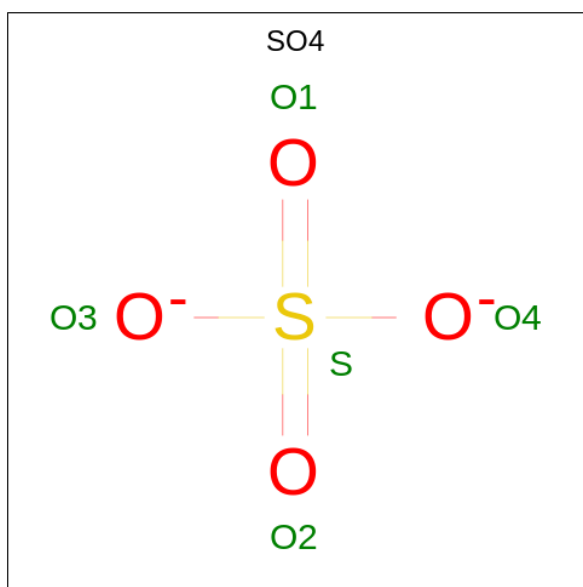
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	M	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

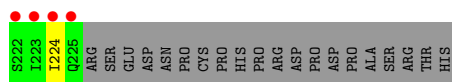
- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



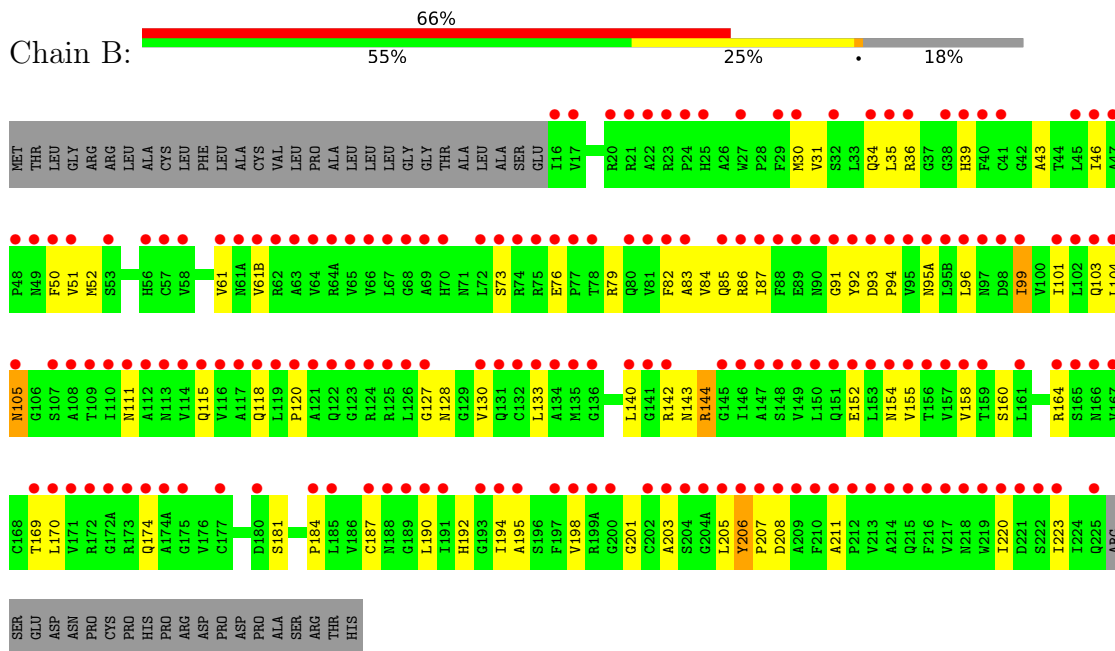
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is water.

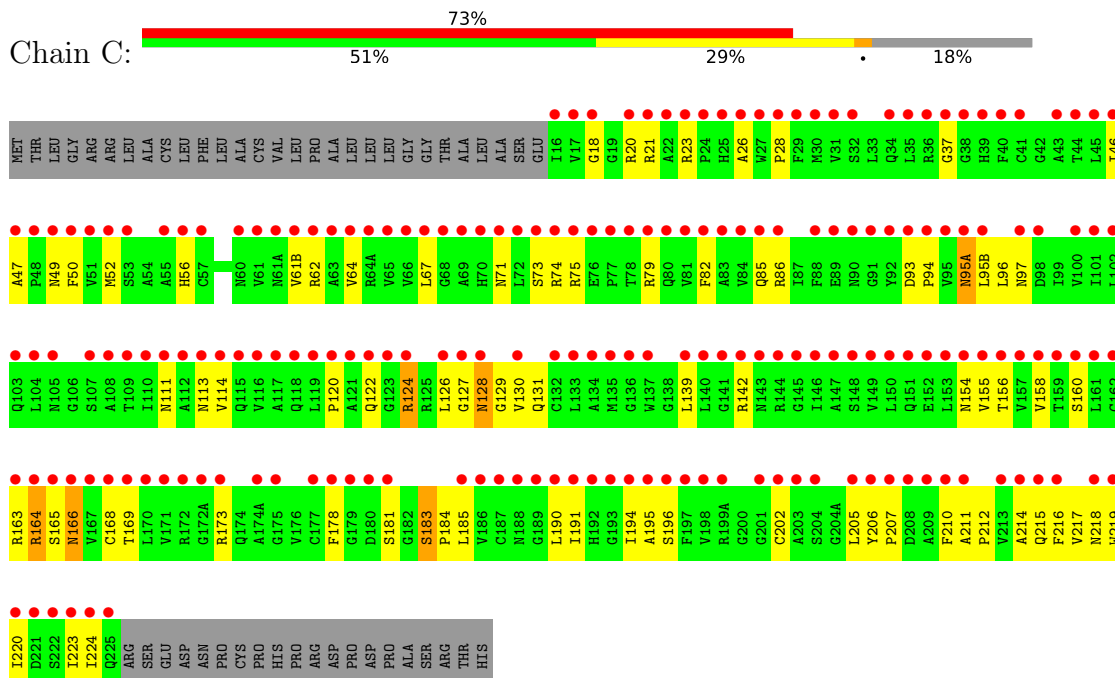
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total	O	0	0
			2	2		
10	A	11	Total	O	0	0
			11	11		
10	B	11	Total	O	0	0
			11	11		
10	C	2	Total	O	0	0
			2	2		
10	F	1	Total	O	0	0
			1	1		
10	G	1	Total	O	0	0
			1	1		



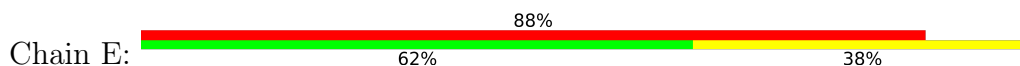
- Molecule 1: Neutrophil elastase

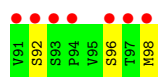


- Molecule 1: Neutrophil elastase

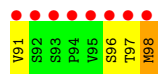


- Molecule 2: Ecotin Peptide

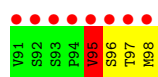




- Molecule 2: Ecotin Peptide



- Molecule 2: Ecotin Peptide



- Molecule 2: Ecotin Peptide



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




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



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



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

Chain O:  67% 33%



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

Chain I:  50% 50%



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

Chain J:  100%



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

Chain L:  100%



- Molecule 7: α -L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 33% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	57.24Å 68.91Å 130.85Å 90.00° 89.90° 90.00°	Depositor
Resolution (Å)	47.45 – 2.89 47.45 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.45-2.89) 99.2 (47.45-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	51.05 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.252 , 0.306 0.253 , 0.311	Depositor DCC
R_{free} test set	2006 reflections (8.78%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 13.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.408 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7019	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6532e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FUC, BMA, NAG, GOL

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	0.47	1/1636 (0.1%)	0.80	7/2227 (0.3%)
1	B	0.34	0/1640	0.59	0/2231
1	C	0.34	0/1657	0.64	0/2252
1	D	0.35	0/1626	0.66	2/2213 (0.1%)
2	E	0.34	0/47	0.70	0/62
2	F	0.37	0/51	0.67	0/69
2	G	0.28	0/51	0.59	0/69
2	H	0.32	0/45	0.69	0/58
All	All	0.38	1/6753 (0.0%)	0.68	9/9181 (0.1%)

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
1	D	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	ARG	CG-CD	-7.72	1.32	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ARG	CB-CG-CD	-10.81	83.48	111.60
1	A	23	ARG	NE-CZ-NH1	8.38	124.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ARG	CA-CB-CG	-8.25	95.25	113.40
1	A	23	ARG	CB-CG-CD	7.75	131.74	111.60
1	A	75	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	A	75	ARG	N-CA-CB	-6.18	99.48	110.60
1	D	74	ARG	CB-CG-CD	-6.12	95.69	111.60
1	D	74	ARG	CA-CB-CG	5.93	126.44	113.40
1	A	22	ALA	C-N-CA	-5.20	108.70	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	104	LEU	Peptide
1	D	104	LEU	Peptide
1	D	73	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1610	0	1589	50	0
1	B	1610	0	1604	59	0
1	C	1627	0	1627	54	2
1	D	1597	0	1558	42	2
2	E	47	0	40	4	0
2	F	51	0	45	4	0
2	G	51	0	47	5	0
2	H	46	0	35	3	0
3	K	38	0	34	1	0
3	N	38	0	34	1	0
3	O	38	0	34	0	0
3	P	38	0	34	0	0
4	I	24	0	22	0	0
5	J	49	0	43	0	0
6	L	28	0	25	2	0
7	M	38	0	34	1	0
8	A	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	18	0	23	0	0
8	C	6	0	8	1	0
8	D	6	0	8	0	0
9	B	10	0	0	1	0
9	C	10	0	0	0	0
9	D	5	0	0	0	0
10	A	11	0	0	4	0
10	B	11	0	0	9	0
10	C	2	0	0	2	0
10	D	2	0	0	0	0
10	F	1	0	0	0	0
10	G	1	0	0	1	0
All	All	7019	0	6852	204	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (204) 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:D:178:PHE:HA	2:H:98:MET:HB3	1.59	0.85
1:A:147:ALA:O	10:A:401:HOH:O	1.96	0.82
1:D:194:ILE:HB	1:D:211:ALA:HB3	1.62	0.80
1:C:183:SER:O	10:C:401:HOH:O	2.00	0.79
1:B:61(B):VAL:HG12	1:B:84:VAL:HG21	1.63	0.79
1:A:95:VAL:HG11	7:M:1:NAG:H81	1.64	0.78
1:D:200:GLY:HA2	2:H:92:SER:HB3	1.64	0.77
1:B:194:ILE:HB	1:B:211:ALA:HB3	1.68	0.75
1:A:68:GLY:O	10:A:402:HOH:O	2.03	0.74
1:B:99:ILE:O	10:B:401:HOH:O	2.06	0.73
1:C:20:ARG:NH1	1:C:154:ASN:OD1	2.23	0.71
1:D:221:ASP:HA	1:D:224:ILE:HG22	1.72	0.70
1:B:120:PRO:HG3	1:B:192:HIS:HD2	1.57	0.69
1:C:194:ILE:HB	1:C:211:ALA:HB3	1.75	0.69
1:A:85:GLN:O	1:B:93:ASP:HA	1.94	0.68
1:A:93:ASP:HA	1:B:85:GLN:O	1.93	0.68
1:D:45:LEU:HD22	1:D:67:LEU:HD21	1.76	0.67
1:B:190:LEU:HD11	1:C:190:LEU:HD11	1.76	0.67
1:A:202:CYS:O	10:A:403:HOH:O	2.13	0.67
1:B:101:ILE:HD12	1:B:223:ILE:HD12	1.77	0.66
1:C:163:ARG:HH21	1:C:166:ASN:HD21	1.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ILE:O	1:C:211:ALA:N	2.23	0.66
1:A:194:ILE:HB	1:A:211:ALA:HB3	1.77	0.65
1:B:31:VAL:HB	1:B:43:ALA:HB3	1.79	0.65
1:C:47:ALA:HB3	1:C:50:PHE:HB2	1.80	0.63
1:B:83:ALA:H	1:B:105:ASN:HB2	1.63	0.63
1:B:144:ARG:NH1	9:B:301:SO4:O4	2.32	0.62
1:B:201:GLY:N	10:B:406:HOH:O	2.31	0.62
1:D:155:VAL:HB	1:D:169:THR:HG23	1.80	0.62
1:C:23:ARG:HG3	1:C:26:ALA:HB2	1.80	0.62
1:A:46:ILE:HD13	1:A:52:MET:HB2	1.82	0.61
1:D:128:ASN:HB2	1:D:159:THR:HG23	1.83	0.61
1:C:128:ASN:ND2	1:C:158:VAL:HA	2.16	0.60
1:D:66:VAL:HG22	1:D:81:VAL:HG22	1.84	0.60
1:B:187:CYS:HB2	1:B:192:HIS:CE1	2.37	0.60
2:E:96:SER:O	2:E:98:MET:N	2.30	0.60
1:B:205:LEU:HD23	1:B:205:LEU:H	1.67	0.59
1:C:74:ARG:HE	1:C:75:ARG:H	1.51	0.59
1:D:190:LEU:HD21	1:A:190:LEU:HD11	1.85	0.58
1:A:171:VAL:HG11	1:A:174(A):ALA:HB3	1.85	0.58
1:A:45:LEU:HD11	1:A:67:LEU:HD13	1.86	0.58
1:A:51:VAL:HG23	1:A:102:LEU:HB2	1.85	0.58
1:B:101:ILE:HD11	1:B:220:ILE:HD13	1.87	0.57
1:D:47:ALA:HB3	1:D:50:PHE:HB2	1.87	0.57
1:B:142:ARG:O	10:B:403:HOH:O	2.17	0.57
1:B:120:PRO:HG3	1:B:192:HIS:CD2	2.39	0.57
1:C:46:ILE:HD13	1:C:52:MET:HB2	1.87	0.57
1:D:47:ALA:HB2	1:D:224:ILE:HD11	1.86	0.56
1:B:155:VAL:HB	1:B:169:THR:OG1	2.05	0.56
1:C:131:GLN:OE1	1:C:156:THR:OG1	2.17	0.56
1:D:67:LEU:HD12	1:D:68:GLY:H	1.71	0.56
1:C:195:ALA:HB1	2:G:98:MET:SD	2.46	0.56
1:D:224:ILE:HG23	1:D:225:GLN:HG3	1.87	0.55
1:C:124:ARG:HE	1:C:126:LEU:HD21	1.71	0.55
1:D:133:LEU:HD11	1:D:152:GLU:HG2	1.88	0.55
1:D:56:HIS:HB3	1:D:92:TYR:OH	2.07	0.55
1:A:93:ASP:O	1:A:95(B):LEU:N	2.38	0.55
1:A:86:ARG:HB2	1:A:103:GLN:HB3	1.88	0.55
1:B:50:PHE:CE1	1:B:103:GLN:HG3	2.43	0.54
2:G:96:SER:O	2:G:98:MET:N	2.41	0.54
1:C:128:ASN:HD21	1:C:158:VAL:HG12	1.73	0.54
1:C:185:LEU:HB2	1:C:210:PHE:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:VAL:HG23	2:F:96:SER:HB3	1.91	0.53
1:D:110:ILE:O	1:D:110:ILE:HG13	2.08	0.53
1:A:86:ARG:HB3	1:B:91:GLY:HA2	1.90	0.53
1:B:187:CYS:HB2	1:B:192:HIS:ND1	2.24	0.52
1:A:47:ALA:HB3	1:A:50:PHE:HB2	1.90	0.52
1:C:49:ASN:OD1	1:C:49:ASN:N	2.43	0.52
1:A:101:ILE:HD11	1:A:220:ILE:HG12	1.91	0.52
1:B:128:ASN:ND2	10:B:409:HOH:O	2.43	0.52
1:D:140:LEU:HB2	1:D:145:GLY:O	2.10	0.52
1:A:217:VAL:HA	1:A:220:ILE:HD12	1.93	0.52
1:B:95(A):ASN:HB2	1:B:96:LEU:HD12	1.92	0.52
1:D:86:ARG:H	1:D:103:GLN:HB3	1.75	0.51
1:C:93:ASP:HB3	1:C:96:LEU:H	1.75	0.51
1:D:55:ALA:N	1:D:98:ASP:OD1	2.43	0.51
1:C:220:ILE:O	1:C:224:ILE:HG12	2.09	0.51
1:A:133:LEU:HD12	1:A:134:ALA:N	2.26	0.50
1:C:96:LEU:HB3	1:C:97:ASN:HD22	1.76	0.50
1:D:126:LEU:HD11	1:D:192:HIS:CG	2.46	0.50
1:B:208:ASP:OD2	10:B:404:HOH:O	2.19	0.50
1:D:83:ALA:O	1:D:105:ASN:HB2	2.12	0.50
1:D:89:GLU:HG2	1:D:100:VAL:HG23	1.93	0.50
1:D:71:ASN:HA	1:D:148:SER:O	2.12	0.50
1:B:118:GLN:OE1	10:B:405:HOH:O	2.20	0.50
1:D:62:ARG:HH11	1:D:62:ARG:HG3	1.77	0.50
1:A:25:HIS:H	1:A:70:HIS:CE1	2.30	0.50
1:B:52:MET:SD	1:B:194:ILE:HD11	2.51	0.49
1:B:206:TYR:N	10:B:408:HOH:O	2.35	0.49
1:A:27:TRP:HH2	6:L:2:NAG:H81	1.78	0.49
1:A:181:SER:OG	2:E:98:MET:HG2	2.12	0.49
1:C:93:ASP:CB	1:C:96:LEU:HB2	2.41	0.49
2:E:96:SER:C	2:E:98:MET:H	2.14	0.49
3:N:1:NAG:O3	3:N:2:NAG:O5	2.28	0.49
1:D:53:SER:OG	1:D:54:ALA:N	2.44	0.49
1:B:92:TYR:OH	10:B:402:HOH:O	2.12	0.49
1:C:85:GLN:HG2	1:C:86:ARG:HG3	1.94	0.49
1:A:64(A):ARG:H	1:A:64(A):ARG:HD2	1.76	0.49
1:A:140:LEU:HD21	1:A:147:ALA:HB2	1.94	0.49
1:A:46:ILE:HG21	1:A:52:MET:HE2	1.95	0.48
1:B:111:ASN:O	1:B:115:GLN:NE2	2.46	0.48
1:A:105:ASN:N	1:A:105:ASN:OD1	2.44	0.48
1:A:182:GLY:HA2	1:A:194:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLU:HB2	1:B:79:ARG:HG3	1.96	0.48
1:A:120:PRO:O	1:A:217:VAL:HG11	2.14	0.48
1:C:120:PRO:HA	1:C:190:LEU:HD23	1.95	0.48
1:D:31:VAL:HB	1:D:43:ALA:HB3	1.95	0.48
1:D:118:GLN:HG2	1:A:119:LEU:O	2.13	0.48
1:B:195:ALA:HB1	2:F:98:MET:CE	2.44	0.48
1:C:164:ARG:NH2	8:C:301:GOL:O3	2.46	0.48
1:A:178:PHE:HA	2:E:98:MET:HG3	1.96	0.48
1:C:111:ASN:OD1	1:C:113:ASN:N	2.31	0.48
1:B:205:LEU:HA	10:B:408:HOH:O	2.14	0.47
1:D:164:ARG:HA	1:D:164:ARG:HD3	1.66	0.47
1:C:61(B):VAL:HA	1:C:64:VAL:HG23	1.96	0.47
1:A:133:LEU:HD11	1:A:152:GLU:HB3	1.95	0.47
1:C:128:ASN:HD22	1:C:129:GLY:N	2.13	0.47
1:B:43:ALA:HB1	1:B:51:VAL:HG13	1.96	0.47
1:C:67:LEU:HB3	1:C:114:VAL:HG11	1.96	0.47
1:C:196:SER:C	2:G:98:MET:HG2	2.35	0.47
1:D:62:ARG:HG3	1:D:62:ARG:NH1	2.30	0.47
1:B:206:TYR:HH	2:F:91:VAL:N	2.11	0.47
1:C:185:LEU:HB2	1:C:210:PHE:CE2	2.49	0.47
1:B:30:MET:SD	1:B:184:PRO:HD2	2.55	0.47
1:C:56:HIS:CE1	1:C:181:SER:HB3	2.50	0.47
1:C:18:GLY:O	1:C:173:ARG:NH1	2.43	0.47
1:A:61(B):VAL:HG11	1:A:87:ILE:HD11	1.96	0.47
1:A:81:VAL:O	1:A:82:PHE:HD1	1.98	0.47
2:G:95:VAL:HA	10:G:101:HOH:O	2.15	0.47
1:C:95(A):ASN:HB2	1:C:96:LEU:HD23	1.96	0.46
1:D:43:ALA:HB1	1:D:51:VAL:HG13	1.97	0.46
1:D:185:LEU:HB2	1:D:210:PHE:CE2	2.51	0.46
1:A:161:LEU:H	8:A:301:GOL:H12	1.81	0.46
1:C:155:VAL:HB	1:C:169:THR:HB	1.98	0.46
1:C:71:ASN:OD1	1:C:73:SER:OG	2.30	0.46
1:A:31:VAL:HB	1:A:43:ALA:HB3	1.98	0.45
1:A:32:SER:HB2	1:A:137:TRP:CZ3	2.50	0.45
1:A:81:VAL:C	1:A:82:PHE:HD1	2.19	0.45
1:C:127:GLY:O	1:C:130:VAL:HG23	2.15	0.45
1:A:92:TYR:O	1:B:86:ARG:HA	2.17	0.45
1:D:31:VAL:HG22	1:D:67:LEU:HD13	1.99	0.45
1:C:93:ASP:HB2	1:C:96:LEU:HB2	1.97	0.45
1:B:194:ILE:O	1:B:211:ALA:N	2.36	0.45
1:D:17:VAL:HG13	1:D:141:GLY:HA2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:O	1:A:79:ARG:HA	2.18	0.44
1:B:128:ASN:OD1	1:B:158:VAL:HA	2.17	0.44
2:F:97:THR:O	2:F:97:THR:HG22	2.16	0.44
1:A:30:MET:O	10:A:404:HOH:O	2.21	0.44
1:B:154:ASN:H	1:B:154:ASN:HD22	1.66	0.44
1:C:166:ASN:OD1	10:C:402:HOH:O	2.21	0.44
1:D:155:VAL:HB	1:D:169:THR:CG2	2.46	0.44
1:D:21:ARG:HH11	1:D:149:VAL:HB	1.81	0.44
1:A:83:ALA:HB2	3:K:1:NAG:H62	1.99	0.44
1:C:28:PRO:O	1:C:114:VAL:HA	2.17	0.44
1:C:93:ASP:O	1:C:95(B):LEU:N	2.50	0.43
1:C:205:LEU:HD12	1:C:205:LEU:HA	1.79	0.43
1:D:174:GLN:C	1:D:203:ALA:HB1	2.39	0.43
1:B:92:TYR:CZ	1:B:94:PRO:HA	2.52	0.43
1:B:83:ALA:H	1:B:105:ASN:CB	2.28	0.43
1:B:143:ASN:N	1:B:143:ASN:OD1	2.50	0.43
1:C:212:PRO:HB2	1:C:215:GLN:HG3	2.00	0.43
1:B:170:LEU:HD22	1:B:207:PRO:HG3	1.99	0.43
1:B:174:GLN:HB3	1:B:203:ALA:O	2.19	0.43
1:C:216:PHE:O	1:C:220:ILE:HD12	2.18	0.43
1:D:181:SER:OG	2:H:98:MET:HB2	2.18	0.43
1:B:82:PHE:HD2	1:B:105:ASN:HB3	1.83	0.43
2:G:98:MET:HA	2:G:98:MET:HE2	2.00	0.43
1:A:35:LEU:O	1:A:64(A):ARG:NE	2.51	0.43
1:A:50:PHE:CE2	1:A:224:ILE:HA	2.54	0.43
1:B:99:ILE:HD12	1:B:194:ILE:HD12	2.00	0.42
1:C:214:ALA:HA	1:C:217:VAL:HG23	2.00	0.42
1:C:142:ARG:HH21	1:C:202:CYS:H	1.67	0.42
1:B:61(B):VAL:HG11	1:B:87:ILE:HD11	2.00	0.42
1:B:140:LEU:HB2	1:B:144:ARG:HB2	2.01	0.42
1:C:184:PRO:HB2	1:C:191:ILE:HD12	2.00	0.42
1:D:185:LEU:HB2	1:D:210:PHE:CD2	2.54	0.42
1:A:23:ARG:HH21	1:A:23:ARG:HD3	1.53	0.42
1:B:101:ILE:CD1	1:B:220:ILE:HD13	2.50	0.42
1:C:168:CYS:HB3	1:C:207:PRO:HB2	2.02	0.42
1:D:17:VAL:HA	1:D:141:GLY:HA2	2.01	0.42
1:A:124:ARG:HG2	1:A:192:HIS:NE2	2.34	0.42
1:B:35:LEU:HD23	1:B:35:LEU:HA	1.92	0.42
1:A:35:LEU:HG	1:A:40:PHE:CE2	2.55	0.41
1:D:188:ASN:O	1:A:124:ARG:NH1	2.52	0.41
1:B:34:GLN:HG2	1:B:39:HIS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ILE:HD13	1:B:52:MET:HE2	2.02	0.41
1:C:128:ASN:HD22	1:C:129:GLY:H	1.66	0.41
1:B:46:ILE:HG21	1:B:52:MET:HE3	2.02	0.41
1:C:122:GLN:HG2	1:C:218:ASN:ND2	2.35	0.41
1:B:133:LEU:HD11	1:B:152:GLU:HB2	2.02	0.41
1:A:46:ILE:CG2	1:A:52:MET:HE2	2.51	0.41
1:B:127:GLY:O	1:B:130:VAL:HG23	2.21	0.41
1:C:74:ARG:HG3	1:C:75:ARG:N	2.35	0.41
6:L:1:NAG:H61	6:L:2:NAG:C7	2.50	0.41
1:D:196:SER:OG	1:D:197:PHE:HD1	2.04	0.40
1:A:61(B):VAL:HG12	1:B:94:PRO:HG3	2.03	0.40
1:C:139:LEU:HD12	1:C:178:PHE:HB2	2.02	0.40
1:C:67:LEU:O	1:C:79:ARG:HA	2.21	0.40
1:D:45:LEU:HD13	1:D:67:LEU:HD22	2.03	0.40
1:B:35:LEU:HD11	1:B:61:VAL:HG22	2.04	0.40
1:C:93:ASP:HB3	1:C:96:LEU:HB2	2.03	0.40
1:A:199(A):ARG:HE	1:A:199(A):ARG:HB2	1.74	0.40
1:B:83:ALA:O	1:B:105:ASN:HB2	2.22	0.40
1:C:219:TRP:O	1:C:223:ILE:HD12	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:ARG:NH1	1:C:94:PRO:O[1_655]	1.93	0.27
1:D:94:PRO:O	1:C:62:ARG:NH2[1_655]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	216/267 (81%)	191 (88%)	23 (11%)	2 (1%)	17 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	216/267 (81%)	192 (89%)	19 (9%)	5 (2%)	6	23
1	C	216/267 (81%)	191 (88%)	23 (11%)	2 (1%)	17	48
1	D	216/267 (81%)	192 (89%)	21 (10%)	3 (1%)	11	36
2	E	6/8 (75%)	1 (17%)	4 (67%)	1 (17%)	0	0
2	F	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	G	6/8 (75%)	3 (50%)	1 (17%)	2 (33%)	0	0
2	H	6/8 (75%)	1 (17%)	3 (50%)	2 (33%)	0	0
All	All	888/1100 (81%)	776 (87%)	95 (11%)	17 (2%)	8	28

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	105	ASN
1	B	105	ASN
2	G	97	THR
2	H	95	VAL
1	B	144	ARG
1	B	160	SER
1	C	206	TYR
2	E	92	SER
2	G	95	VAL
1	D	144	ARG
1	B	36	ARG
1	D	36	ARG
1	A	144	ARG
1	C	37	GLY
1	B	206	TYR
1	A	91	GLY
2	H	93	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	164/212 (77%)	156 (95%)	8 (5%)	25	57
1	B	166/212 (78%)	162 (98%)	4 (2%)	49	79
1	C	169/212 (80%)	159 (94%)	10 (6%)	19	49
1	D	160/212 (76%)	156 (98%)	4 (2%)	47	78
2	E	5/8 (62%)	5 (100%)	0	100	100
2	F	6/8 (75%)	5 (83%)	1 (17%)	2	6
2	G	6/8 (75%)	5 (83%)	1 (17%)	2	6
2	H	5/8 (62%)	4 (80%)	1 (20%)	1	4
All	All	681/880 (77%)	652 (96%)	29 (4%)	29	62

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	124	ARG
1	D	140	LEU
1	D	151	GLN
1	D	173	ARG
1	A	20	ARG
1	A	21	ARG
1	A	36	ARG
1	A	64(A)	ARG
1	A	75	ARG
1	A	143	ASN
1	A	164	ARG
1	A	196	SER
1	B	73	SER
1	B	99	ILE
1	B	164	ARG
1	B	181	SER
1	C	21	ARG
1	C	82	PHE
1	C	95(A)	ASN
1	C	124	ARG
1	C	128	ASN
1	C	160	SER
1	C	164	ARG
1	C	165	SER
1	C	166	ASN
1	C	183	SER
2	F	98	MET

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Mol	Chain	Res	Type
2	G	95	VAL
2	H	93	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	B	128	ASN
1	C	97	ASN
1	C	128	ASN
1	C	166	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 ⓘ

23 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	$\# Z > 2$
4	NAG	I	1	1,4	14,14,15	0.49	0	17,19,21	0.63	0
4	FUC	I	2	4	10,10,11	0.69	0	14,14,16	1.21	2 (14%)
5	NAG	J	1	1,5	14,14,15	0.23	0	17,19,21	0.46	0
5	NAG	J	2	5	14,14,15	0.33	0	17,19,21	0.54	0
5	BMA	J	3	5	11,11,12	0.89	0	15,15,17	0.76	0
5	FUC	J	4	5	10,10,11	0.76	0	14,14,16	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	K	1	1,3	14,14,15	0.46	0	17,19,21	0.54	0
3	NAG	K	2	3	14,14,15	0.28	0	17,19,21	0.66	0
3	FUC	K	3	3	10,10,11	1.53	2 (20%)	14,14,16	1.80	3 (21%)
6	NAG	L	1	1,6	14,14,15	0.37	0	17,19,21	0.55	0
6	NAG	L	2	6	14,14,15	0.31	0	17,19,21	0.67	0
7	NAG	M	1	1,7	14,14,15	1.64	3 (21%)	17,19,21	1.32	2 (11%)
7	FUC	M	2	7	10,10,11	0.99	1 (10%)	14,14,16	1.96	4 (28%)
7	NAG	M	3	7	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	N	1	1,3	14,14,15	0.23	0	17,19,21	0.95	1 (5%)
3	NAG	N	2	3	14,14,15	0.44	0	17,19,21	0.54	0
3	FUC	N	3	3	10,10,11	1.04	1 (10%)	14,14,16	0.63	0
3	NAG	O	1	1,3	14,14,15	0.47	0	17,19,21	0.59	0
3	NAG	O	2	3	14,14,15	0.16	0	17,19,21	0.61	1 (5%)
3	FUC	O	3	3	10,10,11	0.93	0	14,14,16	0.87	0
3	NAG	P	1	3	14,14,15	0.87	1 (7%)	17,19,21	0.78	1 (5%)
3	NAG	P	2	3	14,14,15	0.22	0	17,19,21	0.43	0
3	FUC	P	3	3	10,10,11	0.71	0	14,14,16	0.87	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	FUC	I	2	4	-	-	0/1/1/1
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	FUC	J	4	5	-	-	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	FUC	K	3	3	-	-	0/1/1/1
6	NAG	L	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
7	NAG	M	1	1,7	-	2/6/23/26	0/1/1/1
7	FUC	M	2	7	-	-	0/1/1/1
7	NAG	M	3	7	-	3/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1
3	FUC	N	3	3	-	-	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	4/6/23/26	0/1/1/1
3	FUC	O	3	3	-	-	0/1/1/1
3	NAG	P	1	3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	1/6/23/26	0/1/1/1
3	FUC	P	3	3	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1	NAG	C1-C2	4.37	1.58	1.52
7	M	1	NAG	O5-C1	-3.54	1.38	1.43
3	K	3	FUC	C4-C5	3.42	1.60	1.52
3	P	1	NAG	O5-C1	-3.08	1.38	1.43
3	N	3	FUC	O5-C1	-2.51	1.39	1.43
3	K	3	FUC	O5-C1	-2.49	1.39	1.43
7	M	2	FUC	C1-C2	2.31	1.57	1.52
7	M	1	NAG	C3-C2	2.10	1.57	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	2	FUC	C1-O5-C5	4.74	123.53	112.78
3	K	3	FUC	O5-C5-C4	4.41	117.43	109.52
7	M	1	NAG	C4-C3-C2	4.29	117.30	111.02
3	K	3	FUC	C3-C4-C5	3.48	115.19	109.77
7	M	2	FUC	O5-C1-C2	3.19	115.70	110.77
7	M	2	FUC	O5-C5-C4	2.61	114.21	109.52
7	M	2	FUC	C1-C2-C3	2.58	112.84	109.67
3	K	3	FUC	C1-O5-C5	2.44	118.30	112.78
4	I	2	FUC	C1-O5-C5	2.37	118.15	112.78
3	N	1	NAG	O4-C4-C5	2.20	114.77	109.30
3	P	1	NAG	C1-O5-C5	2.15	115.10	112.19
3	O	2	NAG	C1-O5-C5	2.08	115.01	112.19
7	M	1	NAG	O5-C5-C4	-2.08	105.77	110.83
3	P	3	FUC	O2-C2-C1	2.07	113.39	109.15
4	I	2	FUC	C1-C2-C3	2.01	112.14	109.67

There are no chirality outliers.

All (25) torsion outliers are listed below:

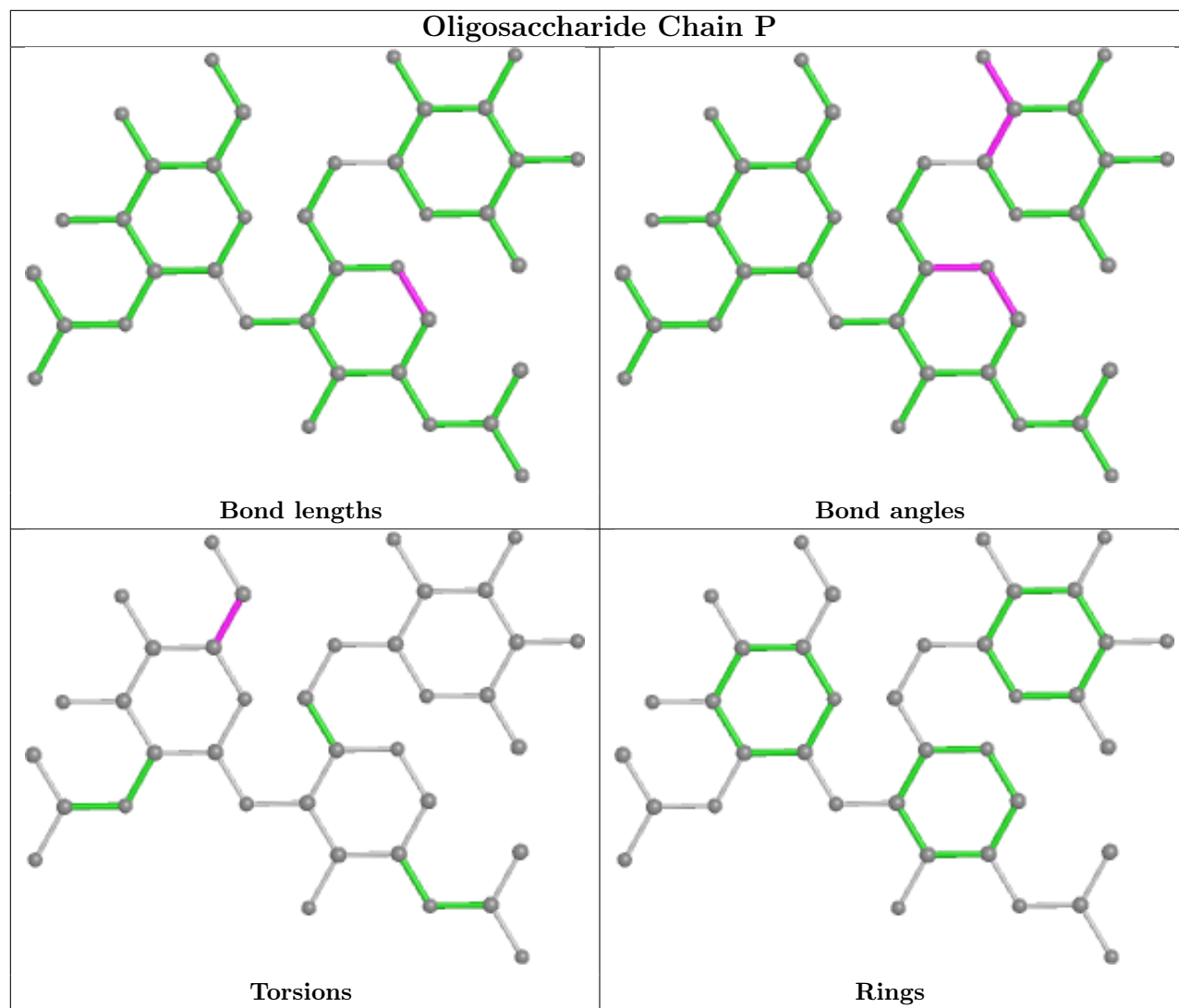
Mol	Chain	Res	Type	Atoms
6	L	2	NAG	C4-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
7	M	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
7	M	3	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
3	O	2	NAG	C8-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
3	K	1	NAG	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
7	M	3	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
7	M	1	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
7	M	3	NAG	C1-C2-N2-C7

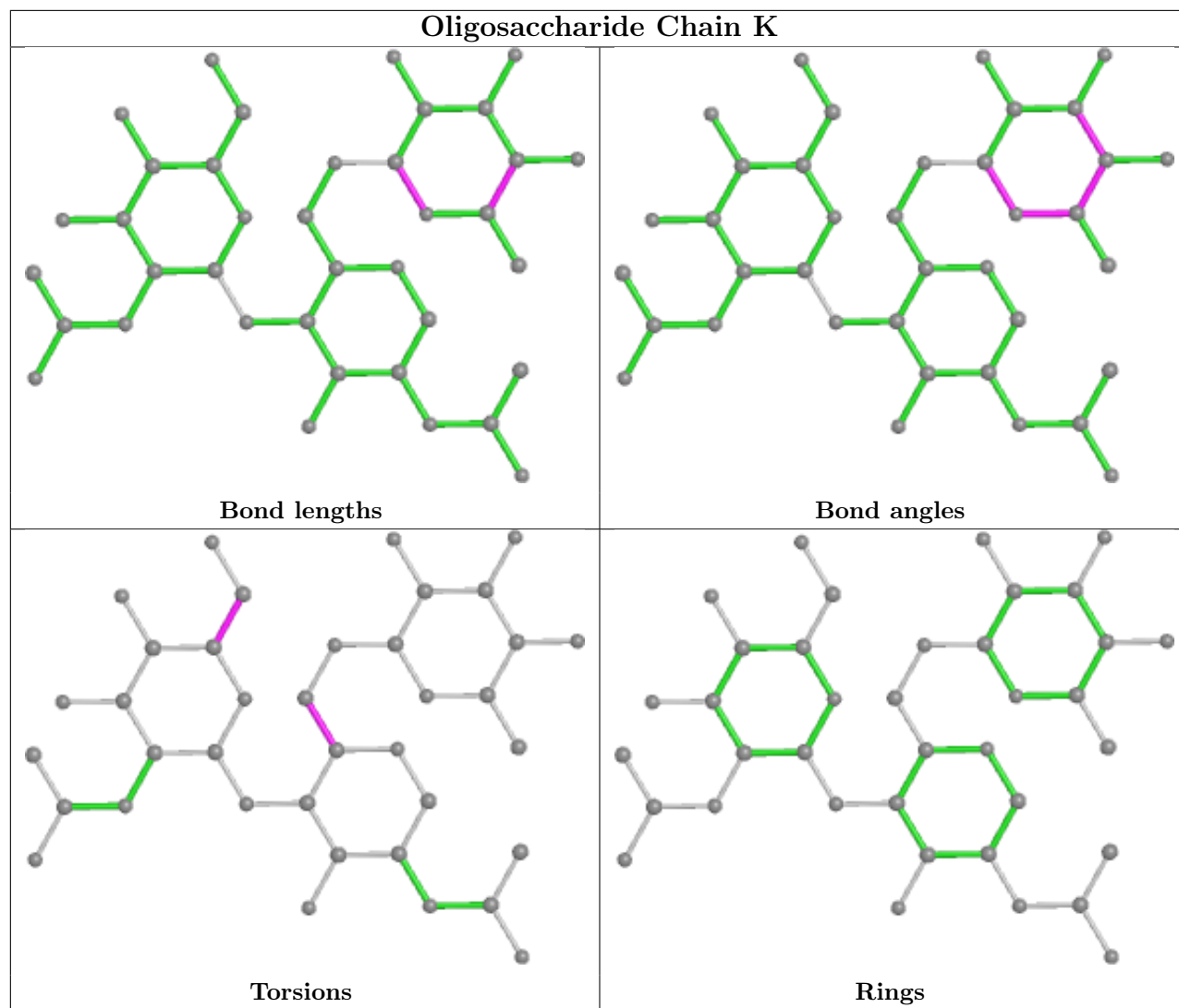
There are no ring outliers.

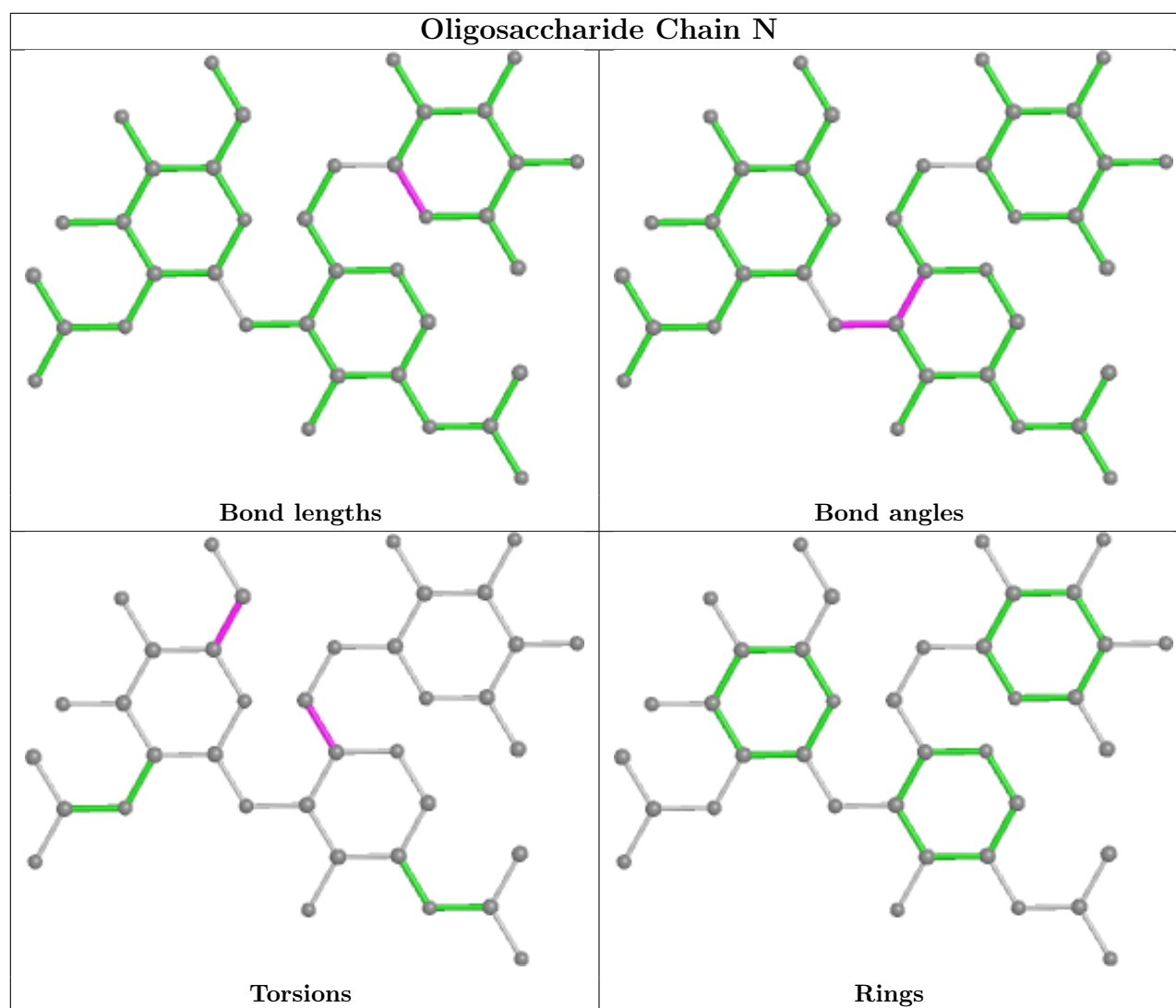
6 monomers are involved in 5 short contacts:

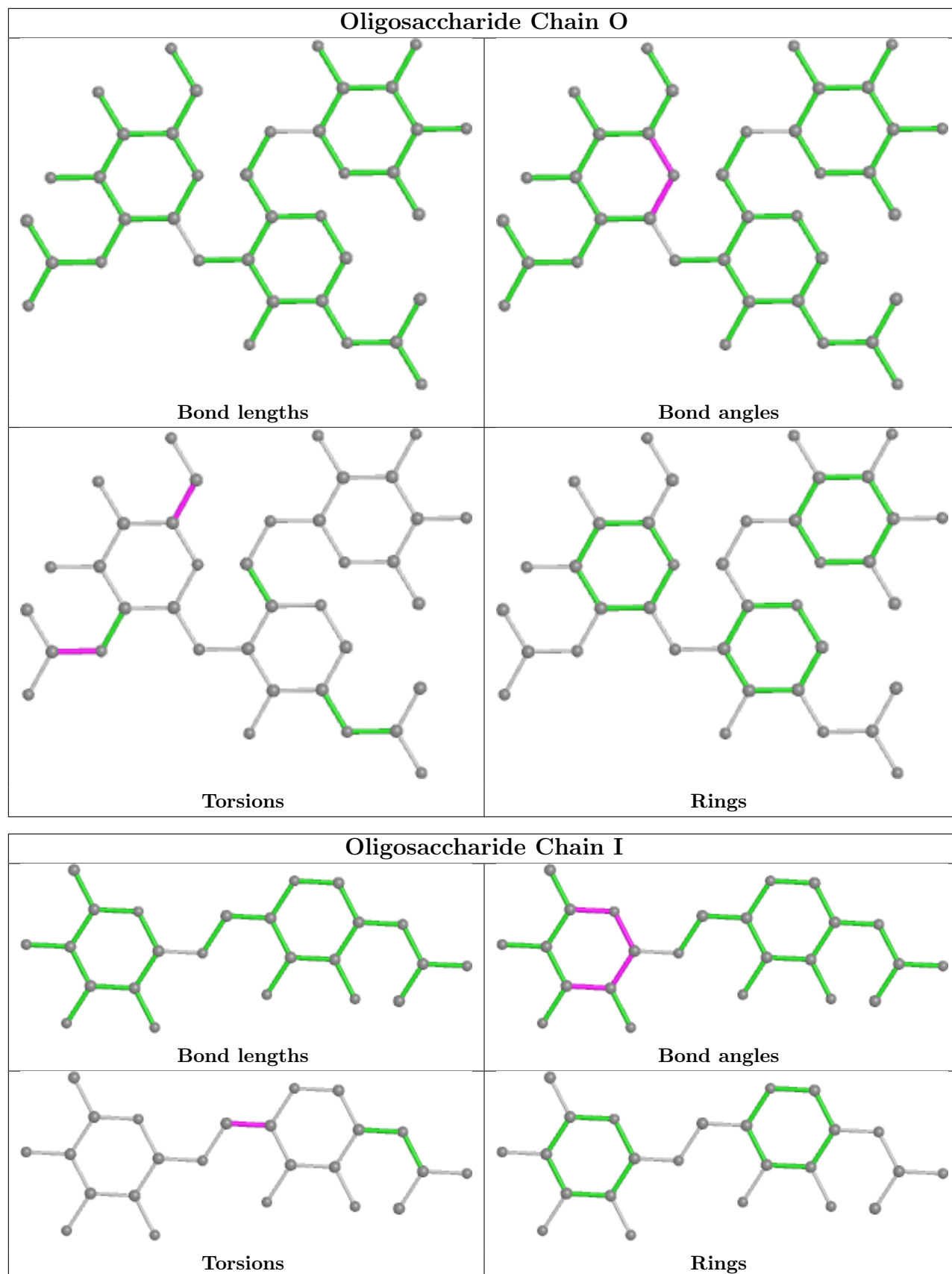
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1	NAG	1	0
7	M	1	NAG	1	0
3	K	1	NAG	1	0
6	L	2	NAG	2	0
6	L	1	NAG	1	0
3	N	2	NAG	1	0

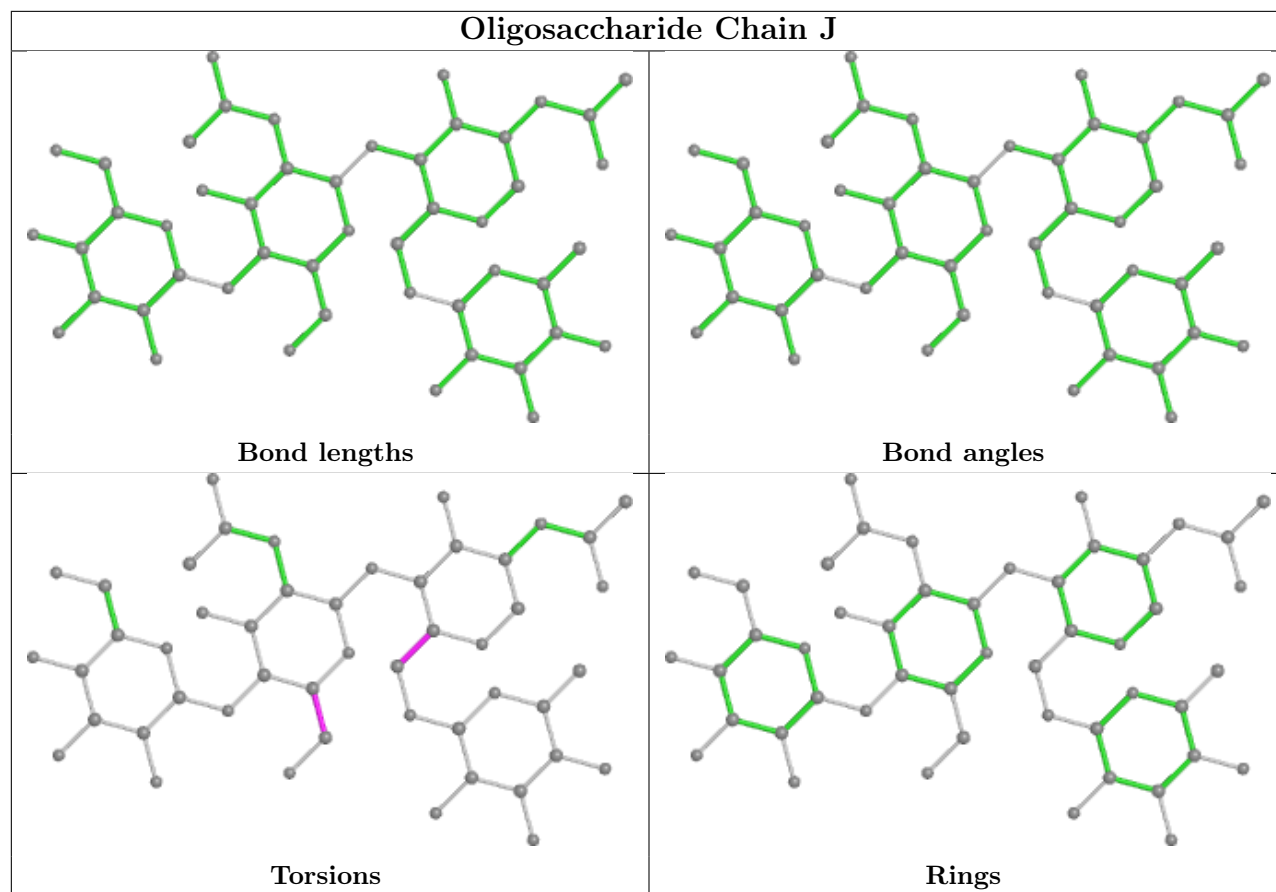
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

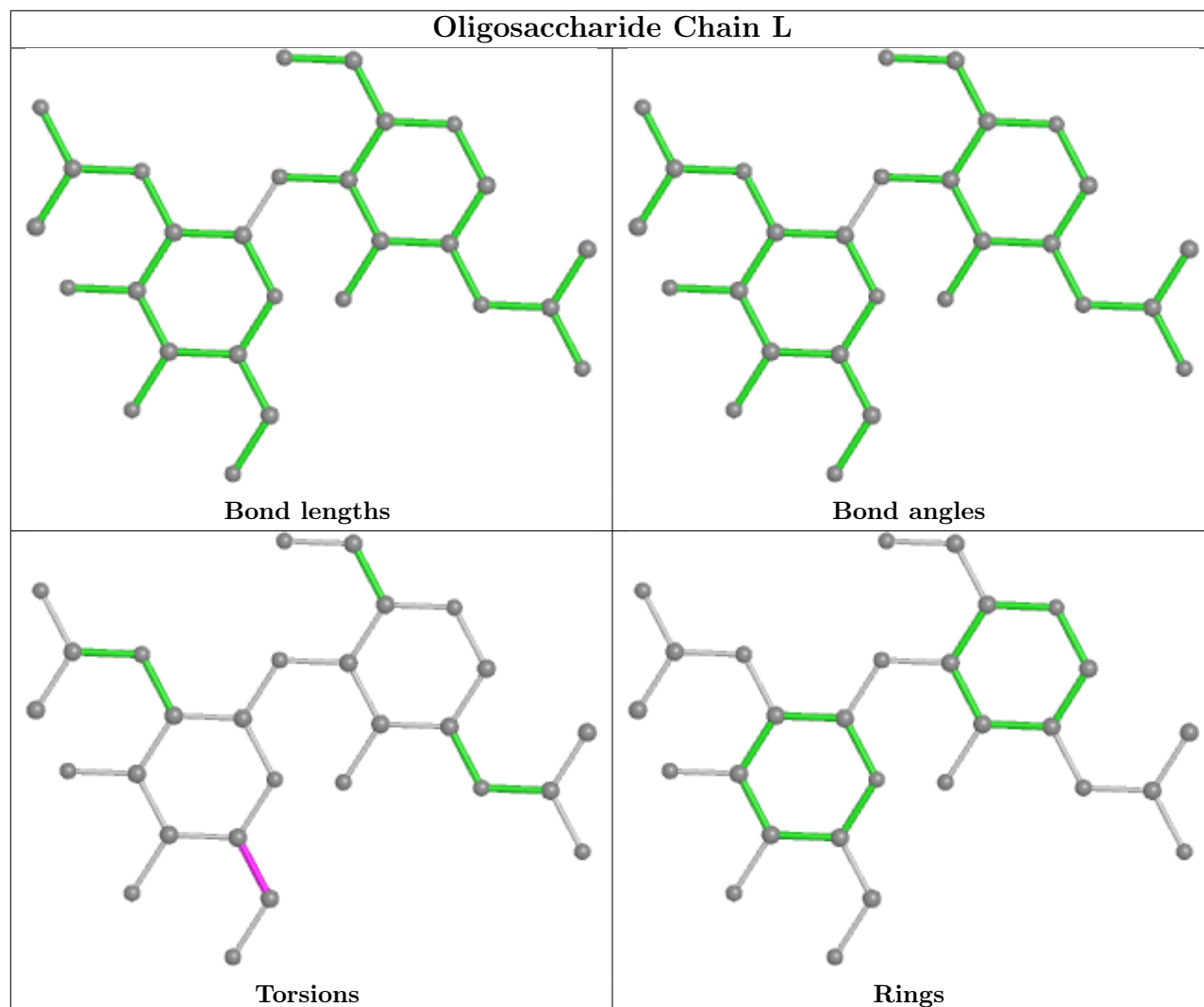


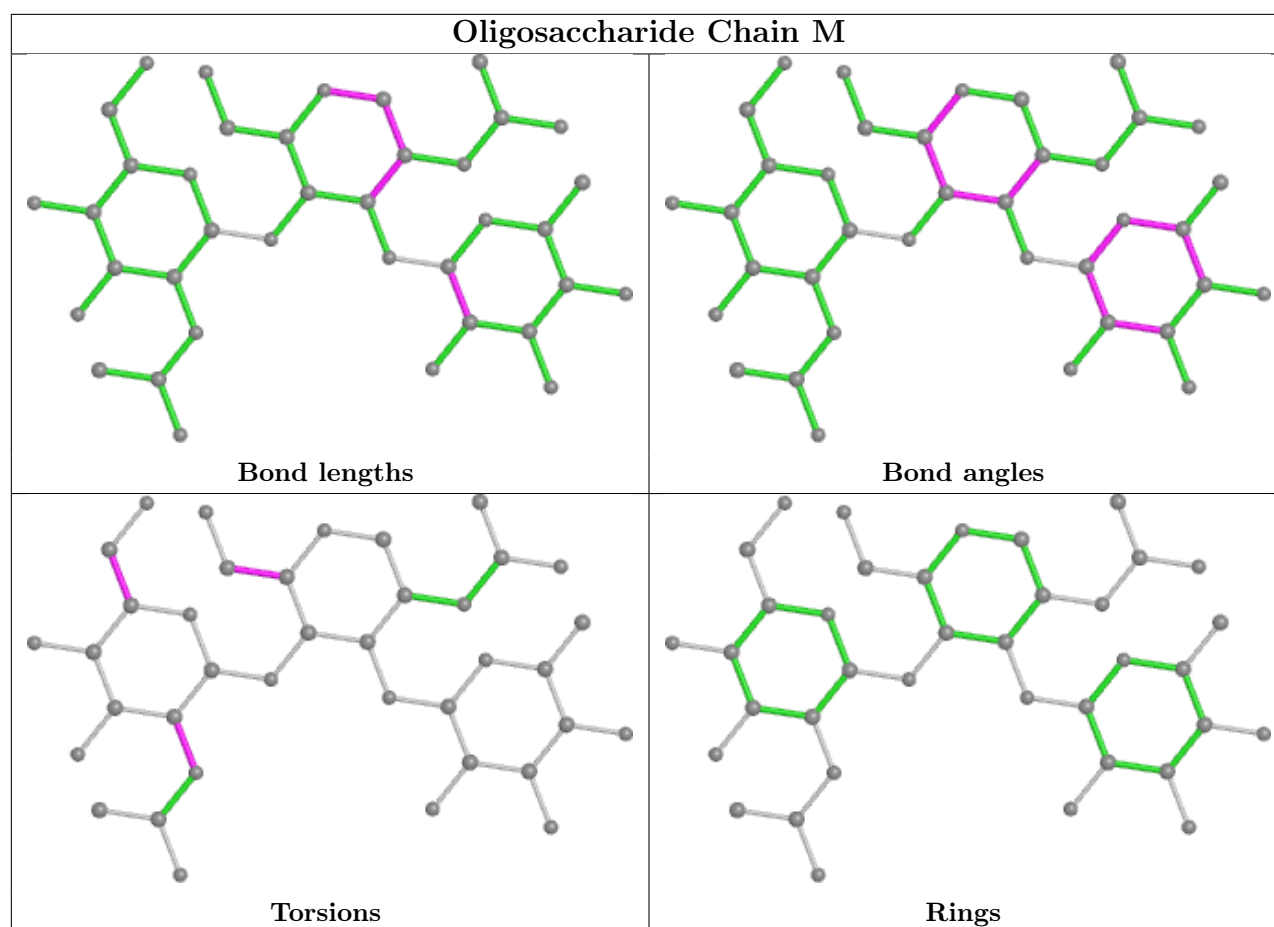












5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	SO4	B	301	-	4,4,4	0.18	0	6,6,6	0.15	0
8	GOL	B	304	-	5,5,5	1.16	0	5,5,5	0.93	0
8	GOL	A	301	-	5,5,5	1.03	0	5,5,5	0.93	0
9	SO4	D	302	-	4,4,4	0.16	0	6,6,6	0.12	0
8	GOL	D	301	-	5,5,5	1.11	0	5,5,5	0.97	0
8	GOL	B	305	-	5,5,5	1.01	0	5,5,5	0.94	0
8	GOL	C	301	-	5,5,5	1.03	0	5,5,5	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	C	302	-	4,4,4	0.16	0	6,6,6	0.08	0
8	GOL	B	303	-	5,5,5	1.03	0	5,5,5	1.00	0
9	SO4	B	302	-	4,4,4	0.18	0	6,6,6	0.17	0
9	SO4	C	303	-	4,4,4	0.18	0	6,6,6	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	B	304	-	-	2/4/4/4	-
8	GOL	A	301	-	-	2/4/4/4	-
8	GOL	D	301	-	-	3/4/4/4	-
8	GOL	B	305	-	-	2/4/4/4	-
8	GOL	C	301	-	-	0/4/4/4	-
8	GOL	B	303	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	301	GOL	O1-C1-C2-C3
8	A	301	GOL	O1-C1-C2-C3
8	B	303	GOL	O1-C1-C2-C3
8	B	304	GOL	O1-C1-C2-C3
8	B	305	GOL	O1-C1-C2-C3
8	B	303	GOL	O1-C1-C2-O2
8	A	301	GOL	O1-C1-C2-O2
8	D	301	GOL	O1-C1-C2-O2
8	D	301	GOL	O2-C2-C3-O3
8	B	304	GOL	O1-C1-C2-O2
8	B	305	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	301	SO4	1	0
8	A	301	GOL	1	0
8	C	301	GOL	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	218/267 (81%)	3.73	193 (88%)  	16, 24, 38, 50	0
1	B	218/267 (81%)	3.39	176 (80%)  	17, 24, 29, 37	0
1	C	218/267 (81%)	3.90	195 (89%)  	19, 27, 38, 56	0
1	D	218/267 (81%)	3.70	195 (89%)  	15, 25, 31, 40	0
2	E	8/8 (100%)	4.03	7 (87%)  	27, 31, 35, 36	0
2	F	8/8 (100%)	4.33	8 (100%)  	22, 28, 32, 32	0
2	G	8/8 (100%)	4.53	8 (100%)  	27, 37, 40, 44	0
2	H	8/8 (100%)	3.73	8 (100%)  	22, 32, 35, 37	0
All	All	904/1100 (82%)	3.70	790 (87%)  	15, 25, 35, 56	0

All (790) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	16.5
1	A	37	GLY	13.6
1	A	141	GLY	11.5
1	D	138	GLY	11.4
1	B	121	ALA	10.9
1	A	106	GLY	10.5
1	C	64	VAL	10.2
1	B	110	ILE	10.1
2	F	97	THR	9.5
1	D	139	LEU	9.4
1	C	117	ALA	9.2
1	D	82	PHE	9.2
1	D	79	ARG	9.2
2	E	92	SER	9.1
1	D	37	GLY	9.0
1	B	175	GLY	8.9

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Mol	Chain	Res	Type	RSRZ
1	C	63	ALA	8.8
1	A	160	SER	8.7
1	C	74	ARG	8.7
1	C	149	VAL	8.5
1	C	61(A)	ASN	8.4
1	D	80	GLN	8.3
1	A	177	CYS	8.2
1	C	211	ALA	8.1
1	B	111	ASN	8.0
1	A	38	GLY	7.7
1	A	48	PRO	7.7
1	A	138	GLY	7.7
1	C	132	CYS	7.7
1	B	132	CYS	7.7
1	C	145	GLY	7.7
2	F	96	SER	7.6
1	D	137	TRP	7.5
1	C	115	GLN	7.4
1	B	219	TRP	7.3
1	D	202	CYS	7.3
1	C	175	GLY	7.3
2	H	94	PRO	7.3
2	G	95	VAL	7.2
1	C	109	THR	7.2
1	A	181	SER	7.1
1	B	120	PRO	7.1
1	D	143	ASN	7.1
1	D	141	GLY	7.0
1	B	203	ALA	7.0
1	C	90	ASN	6.9
1	C	75	ARG	6.8
2	G	98	MET	6.8
1	A	200	GLY	6.8
1	C	165	SER	6.8
1	C	66	VAL	6.8
1	C	210	PHE	6.7
1	D	74	ARG	6.7
1	D	49	ASN	6.7
1	C	118	GLN	6.6
1	D	200	GLY	6.6
1	B	151	GLN	6.6
1	C	222	SER	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	125	ARG	6.6
1	C	147	ALA	6.6
1	D	90	ASN	6.5
1	D	160	SER	6.5
1	C	34	GLN	6.5
1	B	83	ALA	6.5
1	C	47	ALA	6.5
1	B	147	ALA	6.5
1	C	64(A)	ARG	6.5
1	C	116	VAL	6.5
1	C	174(A)	ALA	6.4
1	C	205	LEU	6.4
1	C	39	HIS	6.4
1	A	35	LEU	6.4
1	A	202	CYS	6.3
1	D	58	VAL	6.3
1	A	206	TYR	6.3
1	B	149	VAL	6.3
1	D	25	HIS	6.3
1	B	91	GLY	6.3
1	B	210	PHE	6.3
1	C	95	VAL	6.3
1	B	116	VAL	6.2
1	D	71	ASN	6.2
1	B	64	VAL	6.2
1	C	120	PRO	6.2
1	D	69	ALA	6.1
1	A	176	VAL	6.1
1	B	115	GLN	6.1
1	C	110	ILE	6.1
1	A	179	GLY	6.1
1	B	205	LEU	6.1
1	A	152	GLU	6.1
1	B	150	LEU	6.1
1	A	144	ARG	6.1
1	D	195	ALA	5.9
1	A	137	TRP	5.9
1	C	162	CYS	5.9
1	C	24	PRO	5.8
1	D	76	GLU	5.8
1	C	97	ASN	5.8
1	D	146	ILE	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	70	HIS	5.8
1	D	33	LEU	5.7
1	A	192	HIS	5.7
1	C	219	TRP	5.7
1	B	34	GLN	5.7
1	C	36	ARG	5.7
2	H	91	VAL	5.7
1	C	56	HIS	5.7
1	A	82	PHE	5.7
1	D	178	PHE	5.6
1	D	179	GLY	5.6
1	C	92	TYR	5.6
1	B	131	GLN	5.6
1	C	208	ASP	5.6
1	B	78	THR	5.6
1	D	126	LEU	5.6
1	C	73	SER	5.6
1	D	140	LEU	5.6
1	D	73	SER	5.6
2	G	96	SER	5.6
1	C	79	ARG	5.5
1	C	188	ASN	5.5
1	C	150	LEU	5.5
1	A	55	ALA	5.5
1	A	128	ASN	5.5
2	G	91	VAL	5.5
1	A	194	ILE	5.5
1	A	83	ALA	5.5
1	C	81	VAL	5.5
1	D	113	ASN	5.5
1	C	57	CYS	5.5
1	D	216	PHE	5.5
1	B	189	GLY	5.5
1	D	109	THR	5.4
1	D	206	TYR	5.4
1	C	94	PRO	5.4
2	E	97	THR	5.4
1	D	177	CYS	5.4
1	B	16	ILE	5.4
1	A	182	GLY	5.4
1	C	189	GLY	5.4
1	A	25	HIS	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	159	THR	5.3
1	B	222	SER	5.3
1	A	204(A)	GLY	5.3
1	B	109	THR	5.3
1	D	81	VAL	5.3
1	A	78	THR	5.3
1	C	203	ALA	5.3
1	A	154	ASN	5.2
1	B	75	ARG	5.2
1	C	223	ILE	5.2
1	D	148	SER	5.2
1	D	18	GLY	5.2
1	A	111	ASN	5.2
1	D	75	ARG	5.1
1	C	51	VAL	5.1
1	A	22	ALA	5.1
1	A	209	ALA	5.1
1	A	207	PRO	5.1
1	A	124	ARG	5.1
1	A	148	SER	5.1
1	C	121	ALA	5.1
1	A	33	LEU	5.1
1	D	41	CYS	5.1
1	A	59	ALA	5.1
1	D	119	LEU	5.0
1	C	82	PHE	5.0
1	B	211	ALA	5.0
1	C	76	GLU	5.0
1	C	187	CYS	5.0
1	B	47	ALA	5.0
1	A	184	PRO	5.0
1	B	66	VAL	5.0
1	C	218	ASN	5.0
1	D	112	ALA	5.0
1	D	144	ARG	4.9
1	B	172(A)	GLY	4.9
1	C	32	SER	4.9
1	C	171	VAL	4.9
1	A	46	ILE	4.9
1	C	72	LEU	4.9
1	C	85	GLN	4.9
1	B	39	HIS	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	127	GLY	4.9
1	C	141	GLY	4.9
1	D	59	ALA	4.9
1	C	80	GLN	4.9
1	C	112	ALA	4.9
1	B	95(A)	ASN	4.9
1	A	31	VAL	4.8
1	D	87	ILE	4.8
2	E	93	SER	4.8
1	D	42	GLY	4.8
1	A	27	TRP	4.8
1	C	213	VAL	4.8
1	A	20	ARG	4.8
1	B	154	ASN	4.8
1	C	41	CYS	4.8
1	C	123	GLY	4.7
1	B	65	VAL	4.7
1	B	72	LEU	4.7
1	D	39	HIS	4.7
1	C	155	VAL	4.7
1	B	165	SER	4.7
1	D	142	ARG	4.7
1	B	46	ILE	4.7
1	D	38	GLY	4.7
1	C	151	GLN	4.6
1	D	223	ILE	4.6
1	A	98	ASP	4.6
1	A	159	THR	4.6
1	C	158	VAL	4.6
1	D	62	ARG	4.6
1	B	105	ASN	4.6
1	D	183	SER	4.6
1	C	61(B)	VAL	4.6
1	B	68	GLY	4.6
1	C	154	ASN	4.6
1	B	113	ASN	4.6
1	C	38	GLY	4.6
1	B	62	ARG	4.6
1	C	142	ARG	4.6
1	A	60	ASN	4.6
1	A	105	ASN	4.6
1	D	103	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	114	VAL	4.5
1	B	125	ARG	4.5
1	C	119	LEU	4.5
1	D	224	ILE	4.5
1	C	122	GLN	4.5
1	C	70	HIS	4.5
1	D	28	PRO	4.5
1	D	188	ASN	4.5
1	D	86	ARG	4.5
1	C	135	MET	4.5
2	E	96	SER	4.5
1	D	167	VAL	4.5
1	A	88	PHE	4.5
1	A	23	ARG	4.5
1	A	75	ARG	4.5
1	A	193	GLY	4.5
1	B	23	ARG	4.5
1	D	26	ALA	4.5
1	C	78	THR	4.5
1	D	181	SER	4.5
1	A	183	SER	4.5
1	C	61	VAL	4.4
1	C	191	ILE	4.4
1	C	169	THR	4.4
1	D	48	PRO	4.4
1	C	126	LEU	4.4
1	A	131	GLN	4.4
1	B	80	GLN	4.4
1	B	94	PRO	4.4
1	D	31	VAL	4.4
1	C	84	VAL	4.4
1	A	195	ALA	4.3
1	D	50	PHE	4.3
1	A	118	GLN	4.3
1	C	60	ASN	4.3
1	D	176	VAL	4.3
1	A	185	LEU	4.3
1	A	196	SER	4.3
1	B	81	VAL	4.3
1	B	171	VAL	4.3
1	A	80	GLN	4.3
1	B	218	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	73	SER	4.3
1	D	209	ALA	4.3
1	D	106	GLY	4.3
1	D	217	VAL	4.3
1	A	21	ARG	4.2
1	A	215	GLN	4.2
1	D	35	LEU	4.2
1	A	224	ILE	4.2
1	C	62	ARG	4.2
1	D	56	HIS	4.2
1	B	63	ALA	4.2
1	D	27	TRP	4.2
1	C	144	ARG	4.2
1	C	102	LEU	4.2
1	A	107	SER	4.2
1	B	188	ASN	4.2
1	D	163	ARG	4.2
1	A	39	HIS	4.2
1	D	153	LEU	4.2
1	B	114	VAL	4.1
1	A	71	ASN	4.1
1	A	54	ALA	4.1
1	B	142	ARG	4.1
1	C	173	ARG	4.1
1	C	103	GLN	4.1
1	B	69	ALA	4.1
1	A	41	CYS	4.1
1	A	142	ARG	4.1
1	A	30	MET	4.1
1	A	201	GLY	4.1
1	B	213	VAL	4.1
1	D	172	ARG	4.0
1	C	77	PRO	4.0
1	C	114	VAL	4.0
1	D	60	ASN	4.0
1	D	101	ILE	4.0
1	A	178	PHE	4.0
1	B	40	PHE	4.0
1	C	178	PHE	4.0
1	D	159	THR	4.0
1	B	97	ASN	4.0
1	C	107	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	92	TYR	4.0
1	C	83	ALA	4.0
1	B	21	ARG	4.0
1	B	61(B)	VAL	4.0
1	D	174	GLN	4.0
1	B	118	GLN	4.0
1	A	114	VAL	3.9
1	A	64(A)	ARG	3.9
1	B	56	HIS	3.9
1	B	77	PRO	3.9
1	A	161	LEU	3.9
1	A	188	ASN	3.9
1	D	98	ASP	3.9
1	D	145	GLY	3.9
1	C	89	GLU	3.9
1	A	119	LEU	3.9
1	A	219	TRP	3.9
1	D	108	ALA	3.9
1	D	192	HIS	3.9
1	A	40	PHE	3.9
1	B	45	LEU	3.9
1	B	199(A)	ARG	3.9
1	B	112	ALA	3.9
1	B	89	GLU	3.9
1	B	174	GLN	3.9
1	A	29	PHE	3.9
1	A	153	LEU	3.9
1	C	216	PHE	3.9
1	A	47	ALA	3.9
1	A	113	ASN	3.9
1	B	22	ALA	3.9
1	D	182	GLY	3.9
1	A	146	ILE	3.9
1	C	65	VAL	3.9
1	D	222	SER	3.9
1	C	196	SER	3.9
1	B	208	ASP	3.8
1	C	18	GLY	3.8
1	B	50	PHE	3.8
1	D	61(A)	ASN	3.8
1	C	50	PHE	3.8
2	H	98	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	53	SER	3.8
1	C	206	TYR	3.8
1	D	152	GLU	3.8
1	B	161	LEU	3.8
1	A	120	PRO	3.8
1	A	112	ALA	3.8
1	A	127	GLY	3.8
1	B	155	VAL	3.8
1	A	42	GLY	3.8
1	D	88	PHE	3.8
1	D	194	ILE	3.8
1	B	156	THR	3.8
1	A	147	ALA	3.8
1	A	180	ASP	3.7
1	A	49	ASN	3.7
1	D	66	VAL	3.7
1	D	215	GLN	3.7
1	A	204	SER	3.7
1	A	167	VAL	3.7
1	A	32	SER	3.7
1	B	104	LEU	3.7
1	D	92	TYR	3.7
1	A	50	PHE	3.7
1	D	61(B)	VAL	3.7
1	D	157	VAL	3.7
1	A	17	VAL	3.7
1	A	99	ILE	3.7
1	B	215	GLN	3.7
1	B	169	THR	3.7
1	C	111	ASN	3.7
1	D	99	ILE	3.7
1	A	158	VAL	3.7
1	D	196	SER	3.7
1	C	30	MET	3.6
1	A	187	CYS	3.6
1	B	200	GLY	3.6
1	C	204	SER	3.6
1	D	166	ASN	3.6
1	A	170	LEU	3.6
1	C	86	ARG	3.6
1	D	187	CYS	3.6
1	D	203	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	221	ASP	3.6
1	D	47	ALA	3.6
1	B	184	PRO	3.6
1	C	88	PHE	3.6
1	A	52	MET	3.6
1	C	148	SER	3.6
1	A	172(A)	GLY	3.5
1	B	127	GLY	3.5
1	A	191	ILE	3.5
1	A	61(A)	ASN	3.5
1	D	201	GLY	3.5
1	B	204(A)	GLY	3.5
1	B	117	ALA	3.5
1	C	214	ALA	3.5
2	G	97	THR	3.5
1	C	140	LEU	3.5
1	D	118	GLN	3.5
1	C	168	CYS	3.5
1	B	32	SER	3.5
1	A	174	GLN	3.5
1	B	17	VAL	3.5
1	A	45	LEU	3.5
1	A	135	MET	3.5
1	B	135	MET	3.5
1	C	197	PHE	3.5
1	D	123	GLY	3.4
1	C	25	HIS	3.4
1	D	128	ASN	3.4
1	D	133	LEU	3.4
1	A	101	ILE	3.4
2	F	91	VAL	3.4
1	B	67	LEU	3.4
1	D	151	GLN	3.4
1	B	82	PHE	3.4
1	C	180	ASP	3.4
1	D	77	PRO	3.4
1	D	147	ALA	3.4
1	C	20	ARG	3.4
1	B	204	SER	3.4
1	B	172	ARG	3.4
1	C	136	GLY	3.4
1	A	86	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	185	LEU	3.4
1	D	184	PRO	3.4
1	A	163	ARG	3.4
1	A	168	CYS	3.4
1	B	25	HIS	3.4
1	B	61	VAL	3.4
1	D	135	MET	3.4
1	A	217	VAL	3.4
1	A	81	VAL	3.3
1	B	158	VAL	3.3
1	B	86	ARG	3.3
1	C	166	ASN	3.3
1	A	61	VAL	3.3
1	B	92	TYR	3.3
1	A	66	VAL	3.3
2	F	94	PRO	3.3
1	B	64(A)	ARG	3.3
1	C	55	ALA	3.3
1	D	218	ASN	3.3
1	D	124	ARG	3.3
1	C	46	ILE	3.3
1	C	130	VAL	3.3
1	B	107	SER	3.3
1	A	218	ASN	3.3
1	C	95(A)	ASN	3.3
1	C	153	LEU	3.3
1	C	68	GLY	3.3
1	D	83	ALA	3.3
1	B	51	VAL	3.3
1	D	193	GLY	3.3
1	A	216	PHE	3.3
1	A	26	ALA	3.3
1	C	198	VAL	3.3
1	A	190	LEU	3.3
1	B	29	PHE	3.2
1	A	108	ALA	3.2
1	B	35	LEU	3.2
1	B	126	LEU	3.2
1	D	130	VAL	3.2
1	A	77	PRO	3.2
1	D	34	GLN	3.2
1	B	174(A)	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	43	ALA	3.2
1	A	28	PRO	3.2
1	B	122	GLN	3.2
1	C	104	LEU	3.2
1	B	217	VAL	3.2
1	C	26	ALA	3.2
1	B	193	GLY	3.2
1	D	205	LEU	3.2
1	B	185	LEU	3.2
1	A	69	ALA	3.2
1	D	115	GLN	3.2
1	B	57	CYS	3.2
1	B	177	CYS	3.2
1	A	126	LEU	3.2
1	B	123	GLY	3.2
1	C	37	GLY	3.2
1	D	161	LEU	3.2
2	F	98	MET	3.2
1	D	116	VAL	3.2
1	A	70	HIS	3.2
1	B	49	ASN	3.2
1	B	30	MET	3.2
1	D	221	ASP	3.1
1	D	95(B)	LEU	3.1
1	B	90	ASN	3.1
1	D	220	ILE	3.1
1	D	63	ALA	3.1
1	A	186	VAL	3.1
1	A	95(A)	ASN	3.1
1	B	202	CYS	3.1
1	D	186	VAL	3.1
1	B	141	GLY	3.1
1	D	44	THR	3.1
1	D	156	THR	3.1
1	D	169	THR	3.1
1	A	205	LEU	3.1
1	C	152	GLU	3.1
1	A	210	PHE	3.1
1	D	117	ALA	3.1
1	B	130	VAL	3.1
1	B	124	ARG	3.1
1	B	206	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	105	ASN	3.1
1	C	40	PHE	3.1
2	H	97	THR	3.1
1	D	105	ASN	3.1
1	A	58	VAL	3.1
1	C	52	MET	3.1
1	A	172	ARG	3.1
1	B	225	GLN	3.1
1	D	170	LEU	3.1
1	B	170	LEU	3.1
1	B	102	LEU	3.0
1	A	18	GLY	3.0
1	D	131	GLN	3.0
1	C	202	CYS	3.0
1	D	21	ARG	3.0
1	B	216	PHE	3.0
1	D	17	VAL	3.0
1	B	167	VAL	3.0
1	B	119	LEU	3.0
1	A	123	GLY	3.0
1	A	90	ASN	3.0
1	A	149	VAL	3.0
1	D	19	GLY	3.0
1	D	111	ASN	3.0
1	C	49	ASN	3.0
2	E	98	MET	3.0
1	D	45	LEU	3.0
1	A	102	LEU	3.0
1	B	159	THR	3.0
1	D	53	SER	3.0
1	D	68	GLY	3.0
1	B	136	GLY	3.0
1	D	30	MET	3.0
2	G	94	PRO	3.0
1	C	53	SER	3.0
1	B	134	ALA	3.0
1	C	91	GLY	3.0
1	B	197	PHE	2.9
1	C	28	PRO	2.9
1	D	110	ILE	2.9
1	D	29	PHE	2.9
1	B	214	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	172	ARG	2.9
1	B	166	ASN	2.9
1	B	85	GLN	2.9
1	C	69	ALA	2.9
1	D	136	GLY	2.9
1	B	153	LEU	2.9
1	C	139	LEU	2.9
2	H	95	VAL	2.9
1	D	204(A)	GLY	2.9
1	D	57	CYS	2.9
1	D	154	ASN	2.9
1	C	143	ASN	2.9
1	A	87	ILE	2.9
1	D	171	VAL	2.9
1	B	53	SER	2.9
1	C	124	ARG	2.9
1	C	194	ILE	2.9
1	D	64	VAL	2.9
1	D	52	MET	2.9
1	A	222	SER	2.9
1	A	44	THR	2.9
1	B	146	ILE	2.9
1	D	155	VAL	2.9
1	A	51	VAL	2.9
1	D	174(A)	ALA	2.9
1	C	209	ALA	2.9
1	C	16	ILE	2.9
1	C	195	ALA	2.9
1	B	36	ARG	2.8
1	D	132	CYS	2.8
1	C	27	TRP	2.8
1	A	67	LEU	2.8
1	C	134	ALA	2.8
1	A	56	HIS	2.8
1	C	35	LEU	2.8
1	D	51	VAL	2.8
1	B	157	VAL	2.8
1	C	45	LEU	2.8
1	A	143	ASN	2.8
1	B	76	GLU	2.8
1	B	152	GLU	2.8
1	C	93	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	158	VAL	2.8
1	B	61(A)	ASN	2.8
1	B	87	ILE	2.8
1	C	207	PRO	2.8
1	C	215	GLN	2.8
1	A	136	GLY	2.8
1	D	208	ASP	2.8
1	A	72	LEU	2.8
1	B	95	VAL	2.8
1	C	100	VAL	2.8
1	A	225	GLN	2.8
1	A	155	VAL	2.7
1	A	115	GLN	2.7
1	D	225	GLN	2.7
2	F	92	SER	2.7
2	E	91	VAL	2.7
1	D	89	GLU	2.7
1	D	61	VAL	2.7
1	B	190	LEU	2.7
1	C	67	LEU	2.7
1	C	108	ALA	2.7
1	B	191	ILE	2.7
1	C	190	LEU	2.7
1	A	76	GLU	2.7
1	A	223	ILE	2.7
1	D	120	PRO	2.7
1	D	207	PRO	2.7
1	B	101	ILE	2.7
1	D	43	ALA	2.7
1	D	210	PHE	2.7
1	A	199(A)	ARG	2.7
1	A	84	VAL	2.7
1	C	48	PRO	2.7
1	B	93	ASP	2.6
1	A	166	ASN	2.6
1	A	162	CYS	2.6
1	B	133	LEU	2.6
1	D	180	ASP	2.6
1	D	191	ILE	2.6
1	D	104	LEU	2.6
2	F	95	VAL	2.6
1	C	161	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	219	TRP	2.6
1	C	199(A)	ARG	2.6
1	A	16	ILE	2.6
1	C	181	SER	2.6
1	C	23	ARG	2.6
1	C	95(B)	LEU	2.6
1	C	172(A)	GLY	2.6
1	D	65	VAL	2.6
1	B	195	ALA	2.6
1	C	22	ALA	2.6
1	D	204	SER	2.5
1	C	128	ASN	2.5
1	A	145	GLY	2.5
1	D	36	ARG	2.5
1	D	168	CYS	2.5
1	A	65	VAL	2.5
1	C	160	SER	2.5
1	A	97	ASN	2.5
1	D	185	LEU	2.5
1	B	140	LEU	2.5
1	A	165	SER	2.5
1	D	212	PRO	2.5
1	D	190	LEU	2.5
1	A	100	VAL	2.5
1	C	98	ASP	2.5
1	A	121	ALA	2.5
1	B	74	ARG	2.5
2	H	92	SER	2.5
2	H	93	SER	2.5
1	C	157	VAL	2.5
1	A	197	PHE	2.5
1	D	85	GLN	2.5
1	C	179	GLY	2.5
1	A	61(B)	VAL	2.5
1	B	145	GLY	2.5
1	B	212	PRO	2.5
1	A	104	LEU	2.5
1	A	212	PRO	2.5
2	G	92	SER	2.5
1	A	93	ASP	2.5
1	A	91	GLY	2.5
1	B	221	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	165	SER	2.4
1	A	73	SER	2.4
1	A	198	VAL	2.4
1	C	31	VAL	2.4
1	D	78	THR	2.4
1	A	116	VAL	2.4
1	D	102	LEU	2.4
1	D	23	ARG	2.4
1	D	122	GLN	2.4
1	A	74	ARG	2.4
1	A	164	ARG	2.4
1	B	164	ARG	2.4
1	B	187	CYS	2.4
1	B	194	ILE	2.4
1	C	21	ARG	2.4
1	A	36	ARG	2.4
1	B	198	VAL	2.4
1	C	170	LEU	2.4
1	C	164	ARG	2.4
1	A	64	VAL	2.4
1	C	224	ILE	2.4
1	C	201	GLY	2.4
1	B	27	TRP	2.4
1	D	20	ARG	2.4
1	D	164	ARG	2.4
1	C	163	ARG	2.3
1	C	29	PHE	2.3
2	E	94	PRO	2.3
1	A	132	CYS	2.3
1	A	140	LEU	2.3
1	A	171	VAL	2.3
1	C	225	GLN	2.3
1	D	32	SER	2.3
1	D	197	PHE	2.3
1	B	207	PRO	2.3
1	C	177	CYS	2.3
1	A	43	ALA	2.3
1	A	174(A)	ALA	2.3
1	D	40	PHE	2.3
1	B	38	GLY	2.3
1	B	88	PHE	2.3
2	F	93	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	96	LEU	2.3
1	D	91	GLY	2.3
1	D	97	ASN	2.3
1	A	169	THR	2.3
1	A	95	VAL	2.3
1	B	95(B)	LEU	2.3
1	A	122	GLN	2.3
1	C	44	THR	2.2
1	C	133	LEU	2.2
1	B	99	ILE	2.2
1	D	22	ALA	2.2
1	A	95(B)	LEU	2.2
1	C	113	ASN	2.2
1	C	221	ASP	2.2
1	A	134	ALA	2.2
1	D	173	ARG	2.2
1	A	62	ARG	2.2
1	D	72	LEU	2.2
1	B	220	ILE	2.2
1	A	103	GLN	2.2
1	D	149	VAL	2.2
1	A	150	LEU	2.2
1	B	108	ALA	2.2
1	B	48	PRO	2.2
1	A	157	VAL	2.2
1	D	127	GLY	2.2
1	C	220	ILE	2.2
1	C	192	HIS	2.2
1	B	58	VAL	2.2
1	C	186	VAL	2.2
1	D	175	GLY	2.1
1	D	96	LEU	2.1
1	D	100	VAL	2.1
1	B	209	ALA	2.1
1	D	94	PRO	2.1
1	B	24	PRO	2.1
1	B	148	SER	2.1
2	G	93	SER	2.1
2	H	96	SER	2.1
1	B	173	ARG	2.1
1	B	20	ARG	2.1
1	C	167	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	98	ASP	2.1
1	A	203	ALA	2.1
1	B	223	ILE	2.1
1	C	146	ILE	2.1
1	C	17	VAL	2.1
1	C	193	GLY	2.1
1	B	180	ASP	2.1
1	C	71	ASN	2.1
1	D	125	ARG	2.0
1	D	214	ALA	2.0
1	C	101	ILE	2.0
1	B	41	CYS	2.0
1	A	19	GLY	2.0
1	D	16	ILE	2.0
1	A	96	LEU	2.0
1	B	103	GLN	2.0
1	C	137	TRP	2.0
1	C	156	THR	2.0

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

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

6.3 Carbohydrates [i](#)

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

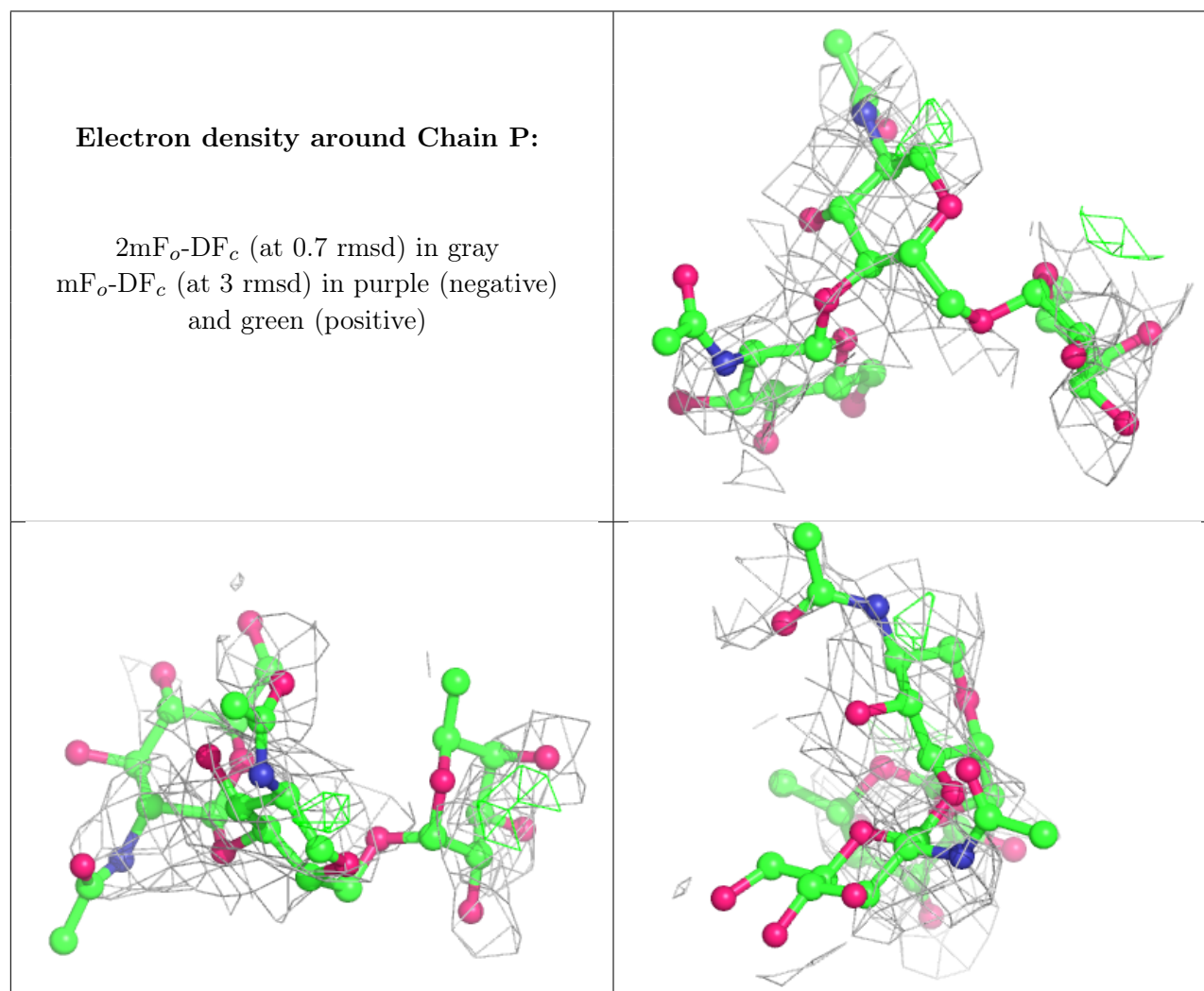
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FUC	P	3	10/11	0.11	0.74	28,33,35,37	0
4	NAG	I	1	14/15	0.11	0.83	31,38,50,53	0
3	FUC	K	3	10/11	0.12	0.76	35,39,42,44	0
6	NAG	L	1	14/15	0.12	0.59	32,35,39,39	0
5	NAG	J	1	14/15	0.19	0.56	38,41,47,48	0
5	BMA	J	3	11/12	0.23	0.49	65,69,72,72	0
7	NAG	M	3	14/15	0.25	1.03	46,48,50,50	0
4	FUC	I	2	10/11	0.27	0.76	44,47,49,50	0
3	NAG	N	2	14/15	0.33	0.52	38,39,42,42	0
3	NAG	P	2	14/15	0.34	0.76	45,47,49,49	0

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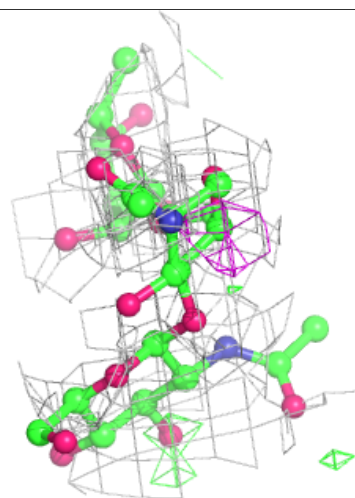
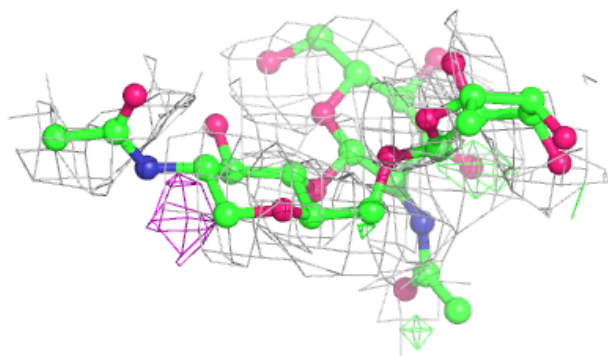
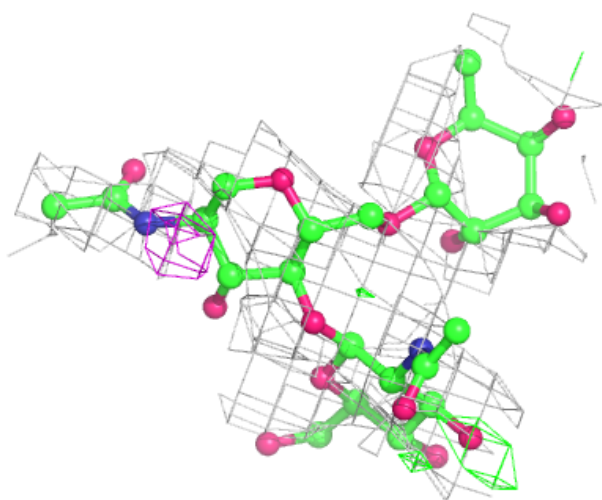
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	K	1	14/15	0.34	0.58	31,35,39,46	0
3	FUC	O	3	10/11	0.35	0.73	26,31,33,34	0
7	NAG	M	1	14/15	0.39	0.42	35,41,45,46	0
6	NAG	L	2	14/15	0.40	0.55	37,41,45,48	0
5	NAG	J	2	14/15	0.41	0.58	45,55,61,65	0
3	NAG	P	1	14/15	0.42	0.46	38,42,45,46	0
3	NAG	N	1	14/15	0.43	0.44	37,40,42,48	0
3	NAG	K	2	14/15	0.43	0.56	38,41,42,43	0
7	FUC	M	2	10/11	0.44	0.39	44,47,51,65	0
3	NAG	O	2	14/15	0.47	0.74	50,54,58,58	0
3	FUC	N	3	10/11	0.53	0.44	36,39,42,45	0
3	NAG	O	1	14/15	0.53	0.54	36,41,45,47	0
5	FUC	J	4	10/11	0.64	0.45	27,33,38,39	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.



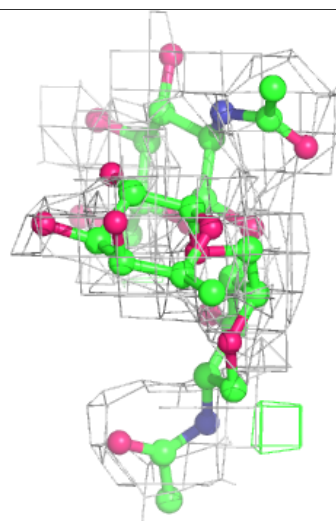
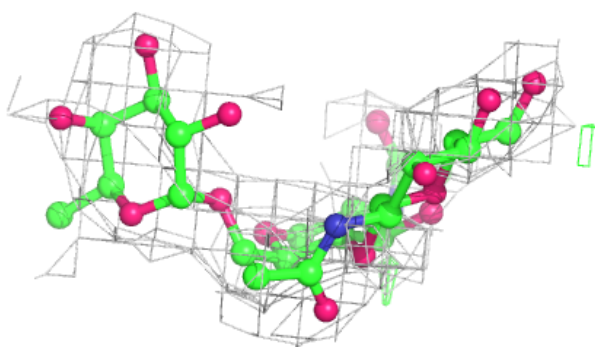
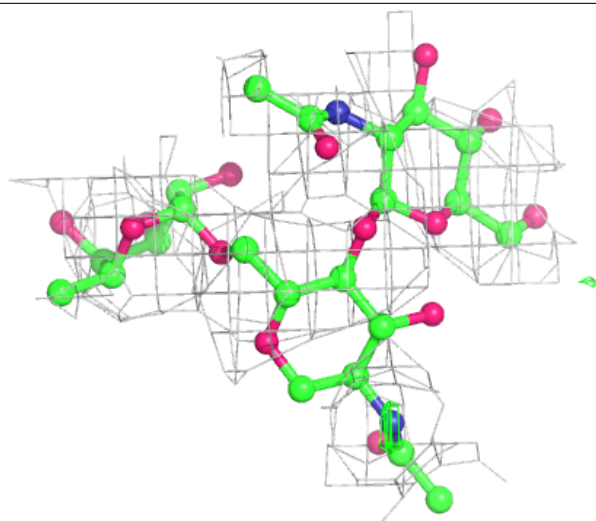
Electron density around Chain K:

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



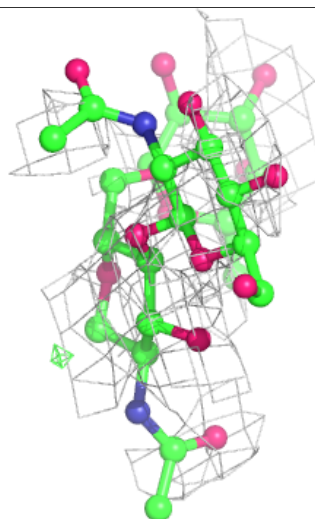
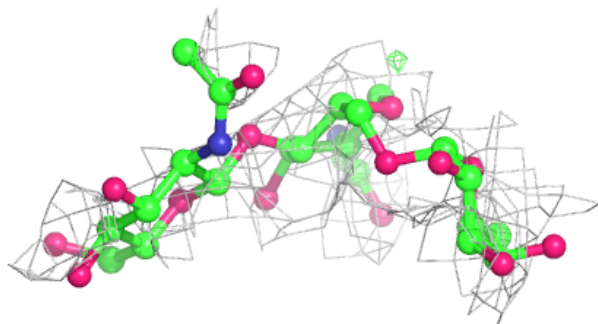
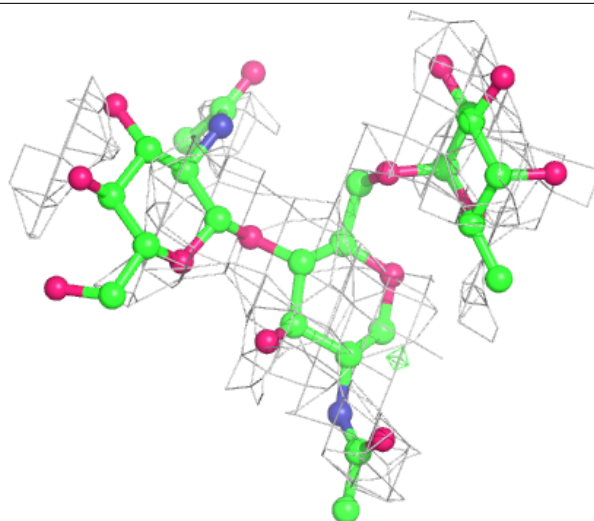
Electron density around Chain N:

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



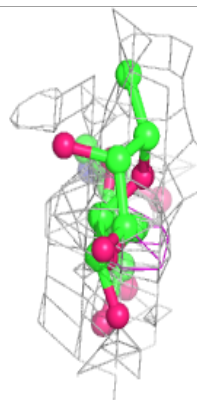
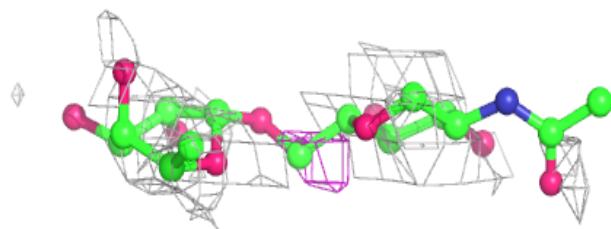
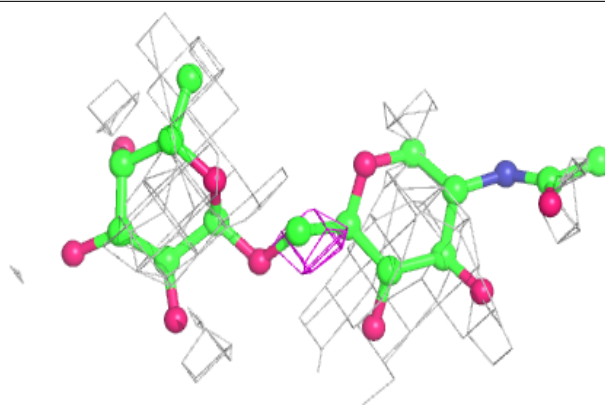
Electron density around Chain O:

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



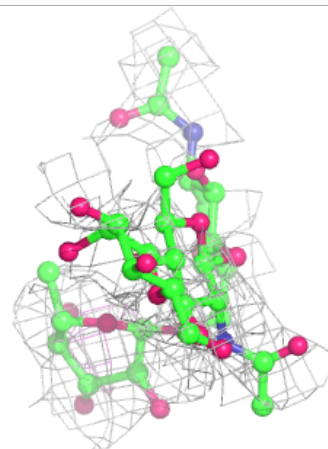
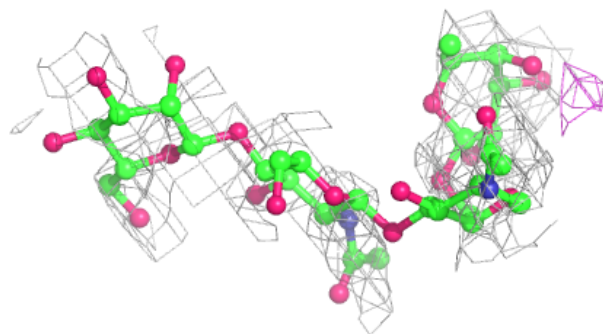
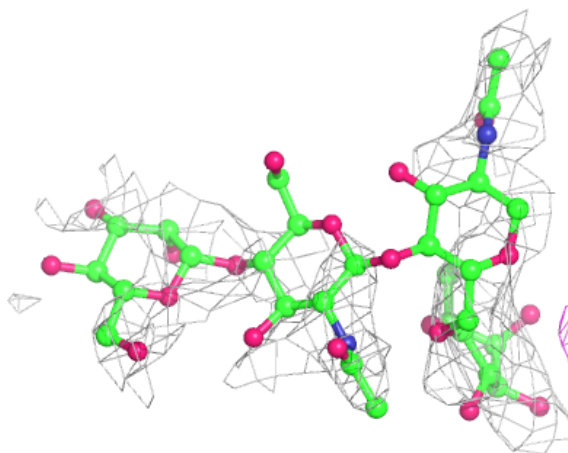
Electron density around Chain I:

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



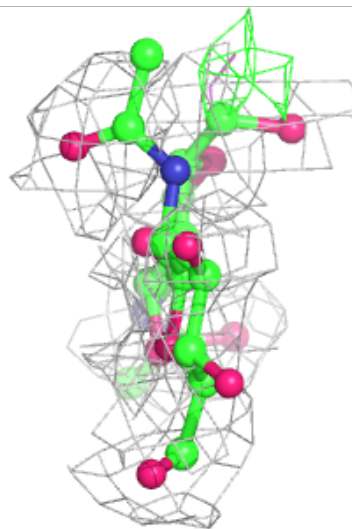
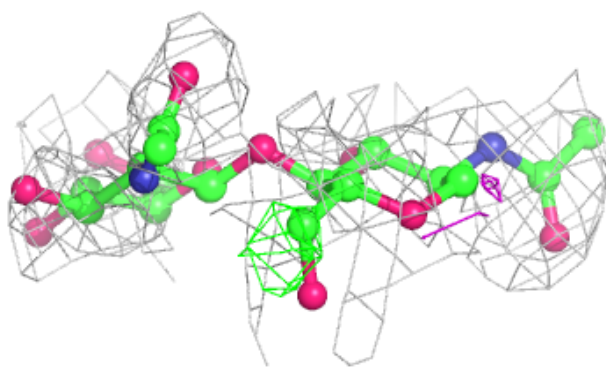
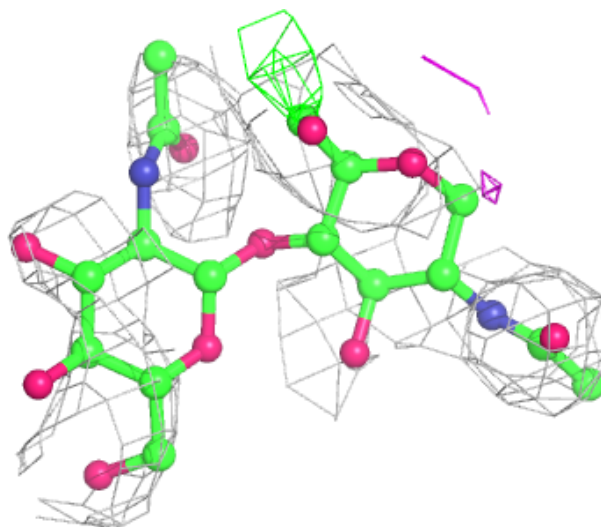
Electron density around Chain J:

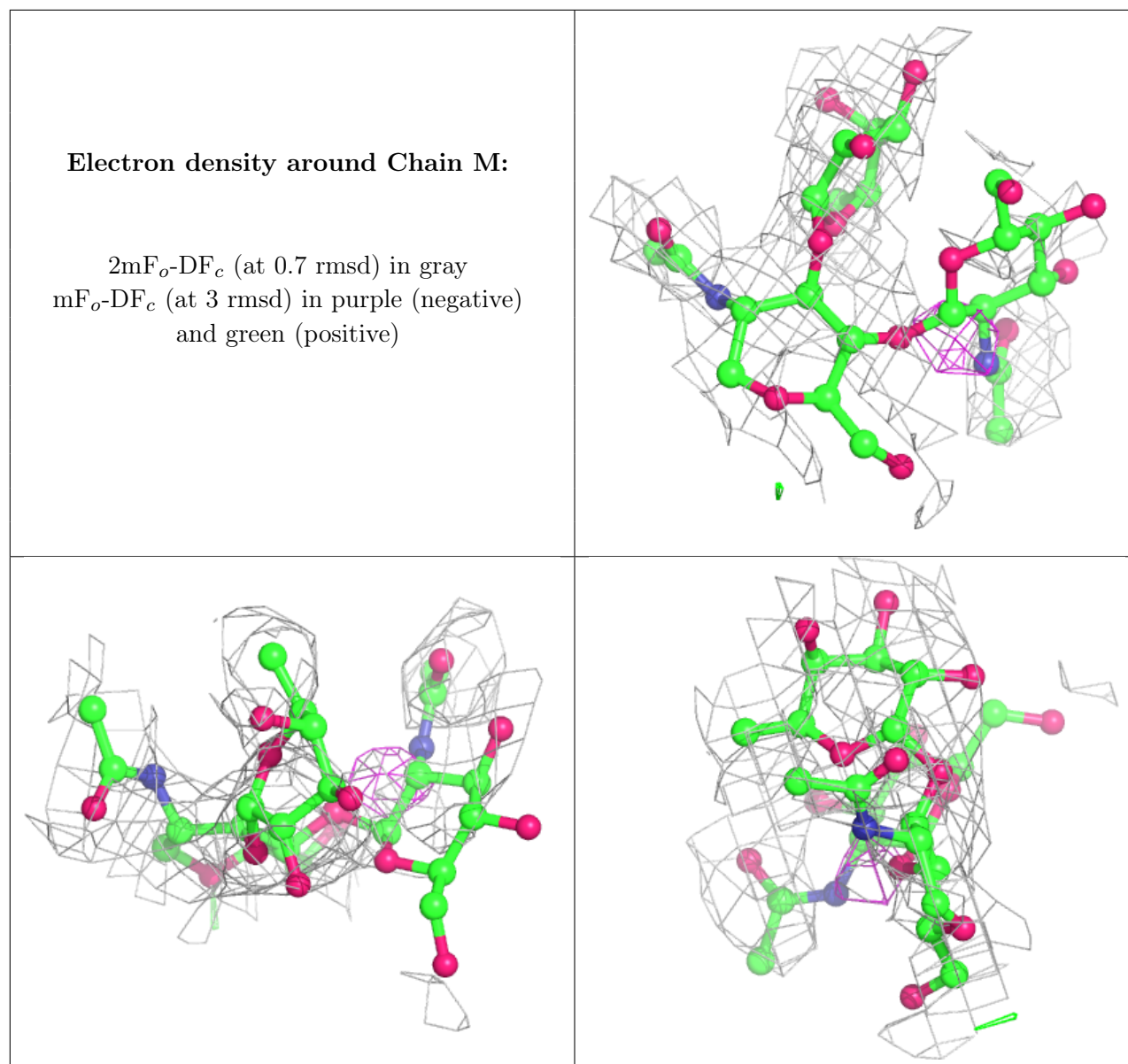
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SO4	C	302	5/5	0.21	0.89	58,58,67,70	0
8	GOL	C	301	6/6	0.26	0.77	31,33,33,34	0
8	GOL	B	305	6/6	0.30	0.44	14,15,15,15	0
9	SO4	B	302	5/5	0.34	0.67	31,31,37,40	0
9	SO4	D	302	5/5	0.42	0.77	40,53,54,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	GOL	B	303	6/6	0.47	0.49	20,22,26,33	0
8	GOL	A	301	6/6	0.50	0.54	24,26,28,28	0
8	GOL	D	301	6/6	0.56	0.55	17,20,20,21	0
8	GOL	B	304	6/6	0.57	0.34	12,13,15,15	0
9	SO4	B	301	5/5	0.66	0.50	39,42,44,56	0
9	SO4	C	303	5/5	0.67	0.45	41,43,46,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.