



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:34 PM BST

PDB ID : 2HLO  
Title : Crystal Structure of Fragment D-dimer from Human Fibrin Complexed with Gly-hydroxyPro-Arg-Pro-amide  
Authors : Doolittle, R.F.; Kollman, J.M.; Chen, A.; Pandi, L.  
Deposited on : 2006-07-08  
Resolution : 2.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

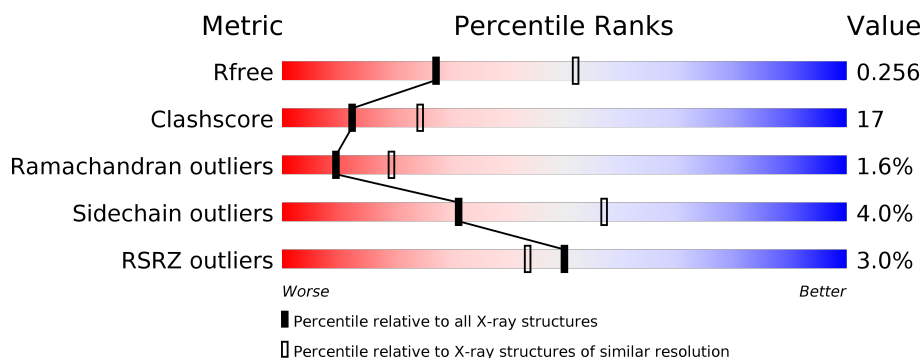
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	87	<div> <div>8%</div> <div> <div>43%</div> <div>32%</div> <div>•</div> <div>23%</div> </div> </div>
1	D	87	<div> <div>5%</div> <div> <div>40%</div> <div>18%</div> <div>•</div> <div>38%</div> </div> </div>
2	B	328	<div> <div>3%</div> <div> <div>64%</div> <div>26%</div> <div>••</div> <div>8%</div> </div> </div>
2	E	328	<div> <div>4%</div> <div> <div>62%</div> <div>27%</div> <div>••</div> <div>10%</div> </div> </div>
3	C	324	<div> <div>%</div> <div> <div>65%</div> <div>23%</div> <div>•</div> <div>10%</div> </div> </div>
3	F	324	<div> <div>%</div> <div> <div>65%</div> <div>21%</div> <div>•</div> <div>12%</div> </div> </div>

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

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
5	NAG	I	1	-	-	-	X
5	NAG	I	2	-	-	-	X
6	NDG	J	2	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10750 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 Fibrin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	67	Total	C	N	O	S	0	0	0
			547	337	103	104	3			
1	D	54	Total	C	N	O	S	0	0	0
			441	269	84	85	3			

- Molecule 2 is a protein called Fibrin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2428	1515	429	462	22			
2	E	296	Total	C	N	O	S	0	0	0
			2377	1484	420	451	22			

- Molecule 3 is a protein called Fibrin, gamma polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	292	Total	C	N	O	S	0	0	0
			2343	1485	396	451	11			
3	F	285	Total	C	N	O	S	0	0	0
			2287	1453	384	439	11			

- Molecule 4 is a protein called GLY-HYP-ARG-PRO-AMIDE PEPTIDE LIGAND.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	5	Total	C	N	O	0	0	1
			31	18	8	5			
4	H	5	Total	C	N	O	0	0	1
			31	18	8	5			

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



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

- Molecule 6 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
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	C	2	Total	Ca	0	0
			2	2		
7	F	1	Total	Ca	0	0
			1	1		
7	E	2	Total	Ca	0	0
			2	2		

- Molecule 8 is water.

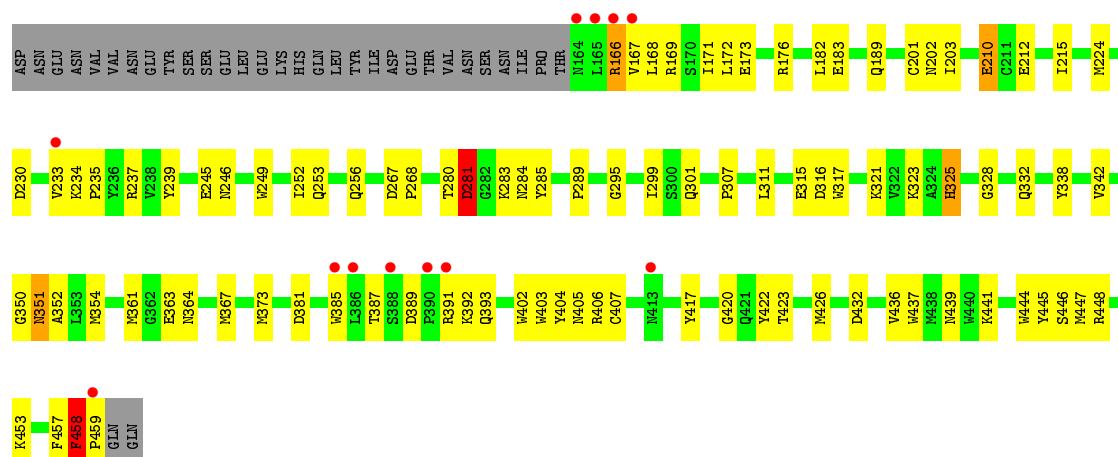
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	8	Total	O	0	0
			8	8		
8	B	55	Total	O	0	0
			55	55		
8	C	44	Total	O	0	0
			44	44		
8	D	13	Total	O	0	0
			13	13		

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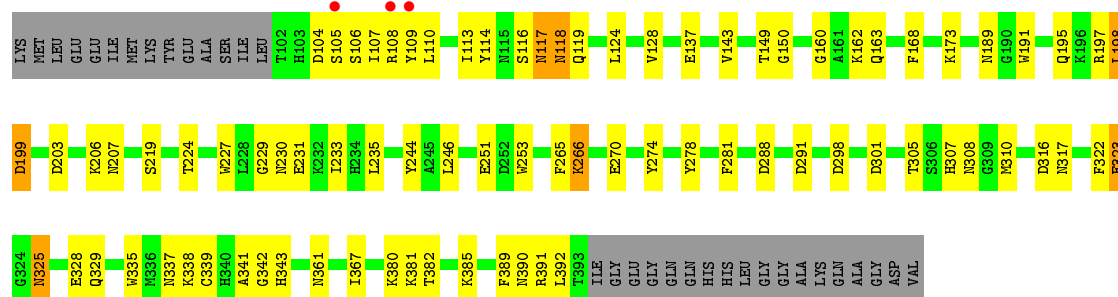
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	46	Total 46	O 46	0	0
8	F	33	Total 33	O 33	0	0
8	G	1	Total 1	O 1	0	0
8	H	2	Total 2	O 2	0	0

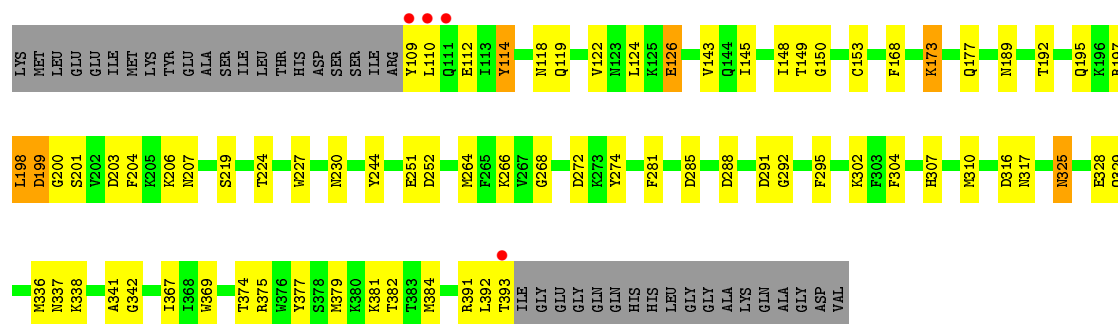




• Molecule 3: Fibrin, gamma polypeptide



• Molecule 3: Fibrin, gamma polypeptide




• Molecule 4: GLY-HYP-ARG-PRO-AMIDE PEPTIDE LIGAND



• Molecule 4: GLY-HYP-ARG-PRO-AMIDE PEPTIDE LIGAND



Chain H:  80% 20%



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

Chain I:  50% 50%



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

Chain J:  50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.69Å 149.48Å 232.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.12 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (30.00-2.60) 93.7 (29.12-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	34.39 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.210 , 0.268 0.200 , 0.256	Depositor DCC
$R_{free}$ test set	2825 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10750	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	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.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: HYP, CA, NAG, NDG, NH2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.29	0/548	0.50	0/731
1	D	0.30	0/441	0.51	0/587
2	B	0.35	0/2490	0.62	0/3364
2	E	0.35	0/2438	0.61	0/3291
3	C	0.37	0/2408	0.60	0/3257
3	F	0.36	0/2351	0.58	0/3180
4	G	0.60	0/21	0.71	0/25
4	H	0.57	0/21	0.60	0/25
All	All	0.35	0/10718	0.60	0/14460

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	547	0	573	32	0
1	D	441	0	458	19	0
2	B	2428	0	2295	78	0
2	E	2377	0	2244	103	0
3	C	2343	0	2188	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2287	0	2136	58	0
4	G	31	0	32	4	0
4	H	31	0	32	2	0
5	I	28	0	25	2	0
6	J	28	0	24	3	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	E	2	0	0	0	0
7	F	1	0	0	0	0
8	A	8	0	0	2	0
8	B	55	0	0	2	0
8	C	44	0	0	2	0
8	D	13	0	0	1	0
8	E	46	0	0	4	0
8	F	33	0	0	6	0
8	G	1	0	0	0	0
8	H	2	0	0	0	0
All	All	10750	0	10007	348	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 17.

All (348) 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:141:ARG:HH21	1:A:189:ILE:HD13	1.25	1.02
3:C:338:LYS:N	3:C:339:CYS:HA	1.85	0.89
1:A:136:LEU:HD22	2:B:168:LEU:HD21	1.56	0.85
2:B:160:ASN:HB2	2:B:161:ILE:HD13	1.59	0.84
1:D:175:LEU:H	1:D:175:LEU:HD23	1.46	0.81
2:E:166:ARG:HE	2:E:166:ARG:HA	1.47	0.79
2:B:161:ILE:HD13	2:B:161:ILE:H	1.48	0.78
2:E:230:ASP:O	2:E:233:VAL:HG22	1.84	0.78
2:E:167:VAL:HG23	2:E:168:LEU:HD12	1.65	0.77
2:B:179:ILE:HD12	3:C:117:ASN:HB2	1.66	0.76
2:E:385:TRP:CB	2:E:406:ARG:HD3	2.15	0.76
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.66	0.76
3:C:149:THR:HG22	3:C:150:GLY:H	1.52	0.75
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.68	0.74
2:E:458:PHE:H	2:E:459:PRO:CD	1.99	0.74
2:E:457:PHE:O	2:E:458:PHE:HB3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:325:ASN:HD22	3:F:325:ASN:C	1.90	0.73
3:F:310:MET:HG3	3:F:337:ASN:HB2	1.71	0.72
2:E:183:GLU:HG2	3:F:124:LEU:HD13	1.72	0.72
2:E:423:THR:N	2:E:426:MET:HE3	2.04	0.71
3:C:329:GLN:HE22	4:G:3:ARG:HE	1.35	0.71
3:C:244:TYR:H	3:C:266:LYS:NZ	1.88	0.71
1:A:137:GLN:HA	1:A:140:VAL:HG22	1.71	0.71
2:B:158:ASN:H	2:B:158:ASN:HD22	1.40	0.70
3:C:149:THR:HG22	3:C:150:GLY:N	2.05	0.70
3:C:244:TYR:H	3:C:266:LYS:HZ3	1.39	0.70
1:D:150:LEU:HD21	3:F:124:LEU:HD23	1.74	0.70
2:E:385:TRP:HB2	2:E:406:ARG:HD3	1.72	0.69
2:E:389:ASP:OD2	2:E:392:LYS:HG3	1.93	0.69
3:F:304:PHE:O	3:F:337:ASN:O	2.11	0.69
3:C:329:GLN:NE2	4:G:3:ARG:HH11	1.91	0.69
2:E:423:THR:H	2:E:426:MET:HE3	1.58	0.69
2:E:441:LYS:HD3	2:E:445:TYR:CE1	2.28	0.69
3:F:307:HIS:HE1	3:F:341:ALA:H	1.41	0.68
1:A:144:LEU:HD23	2:B:175:LEU:HD21	1.73	0.68
3:C:329:GLN:HE21	4:G:3:ARG:HH11	1.40	0.68
3:C:338:LYS:H	3:C:339:CYS:HA	1.57	0.68
2:B:183:GLU:HG2	3:C:124:LEU:HD13	1.76	0.67
1:D:140:VAL:HG23	1:D:185:LEU:HD21	1.76	0.67
1:A:128:GLU:C	1:A:131:GLN:HE22	1.97	0.66
2:E:210:GLU:OE2	2:E:212:GLU:HB3	1.96	0.66
6:J:1:NAG:C7	6:J:2:NDG:H8C1	2.26	0.66
2:E:173:GLU:HA	2:E:176:ARG:HH12	1.61	0.65
2:E:315:GLU:HG3	2:E:321:LYS:HG2	1.77	0.65
3:F:195:GLN:OE1	3:F:382:THR:HG22	1.96	0.65
3:F:244:TYR:H	3:F:266:LYS:NZ	1.94	0.65
2:B:282:GLY:C	2:B:283:LYS:HD2	2.17	0.65
3:F:336:MET:HA	8:F:429:HOH:O	1.97	0.65
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.43	0.64
2:B:172:LEU:HB3	3:C:113:ILE:HG21	1.80	0.63
5:I:1:NAG:H61	5:I:2:NAG:O5	1.98	0.63
1:D:175:LEU:H	1:D:175:LEU:CD2	2.11	0.63
2:B:161:ILE:N	2:B:162:PRO:CD	2.62	0.62
3:F:268:GLY:O	3:F:274:TYR:HA	1.99	0.62
2:B:158:ASN:HD22	2:B:158:ASN:N	1.96	0.62
2:E:224:MET:HE2	2:E:237:ARG:HD3	1.82	0.61
2:E:203:ILE:CD1	3:F:145:ILE:HD11	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:307:HIS:CE1	3:F:341:ALA:H	2.17	0.61
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.00	0.61
2:E:458:PHE:N	2:E:459:PRO:CD	2.61	0.61
3:F:392:LEU:HD13	3:F:392:LEU:O	2.01	0.61
3:C:310:MET:SD	3:C:337:ASN:HB2	2.41	0.60
3:F:199:ASP:O	3:F:201:SER:N	2.31	0.60
3:C:149:THR:HG23	3:C:168:PHE:O	2.01	0.60
3:C:329:GLN:O	3:C:361:ASN:ND2	2.33	0.60
2:B:157:VAL:HG22	2:B:158:ASN:H	1.66	0.60
2:B:210:GLU:OE2	2:B:212:GLU:HB3	2.02	0.60
1:D:137:GLN:HA	2:E:168:LEU:HD21	1.84	0.60
3:F:329:GLN:HE22	4:H:3:ARG:HE	1.50	0.60
3:C:163:GLN:CD	3:C:163:GLN:H	2.05	0.59
2:E:252:ILE:HB	8:E:493:HOH:O	2.02	0.59
1:A:153:ASP:O	1:A:157:LYS:HG2	2.02	0.59
2:E:457:PHE:O	2:E:458:PHE:CB	2.51	0.59
1:A:175:LEU:O	1:A:179:GLU:HG2	2.03	0.59
3:C:265:PHE:C	3:C:266:LYS:HD2	2.22	0.59
1:D:169:LEU:H	2:E:189:GLN:HE22	1.50	0.59
2:B:224:MET:HE2	2:B:237:ARG:HD3	1.84	0.59
2:B:158:ASN:H	2:B:158:ASN:ND2	2.00	0.59
2:B:161:ILE:N	2:B:162:PRO:HD3	2.16	0.59
2:B:282:GLY:O	2:B:283:LYS:HD2	2.02	0.59
2:E:385:TRP:CD1	2:E:406:ARG:NH1	2.70	0.59
1:A:140:VAL:HG23	1:A:185:LEU:HD21	1.85	0.59
6:J:1:NAG:HN2	6:J:2:NDG:H8C1	1.68	0.59
6:J:1:NAG:N2	6:J:2:NDG:H8C1	2.17	0.59
1:A:182:GLN:O	1:A:186:GLU:HG3	2.02	0.58
2:B:230:ASP:O	2:B:233:VAL:HG22	2.03	0.58
2:E:224:MET:CE	2:E:237:ARG:HD3	2.34	0.58
3:C:392:LEU:HB2	8:C:450:HOH:O	2.04	0.58
2:B:161:ILE:N	2:B:161:ILE:HD13	2.18	0.58
2:E:363:GLU:O	2:E:367:MET:HG2	2.04	0.58
3:F:219:SER:OG	3:F:224:THR:HG22	2.04	0.58
3:F:198:LEU:HD12	3:F:199:ASP:OD1	2.04	0.57
3:C:105:SER:HA	3:C:108:ARG:HD2	1.85	0.57
1:A:139:ASN:HB3	3:C:114:TYR:CE2	2.40	0.57
2:E:173:GLU:HA	2:E:176:ARG:NH1	2.18	0.57
2:B:406:ARG:N	2:B:407:CYS:HA	2.20	0.57
3:C:278:TYR:CZ	3:C:308:ASN:HB2	2.40	0.57
2:E:391:ARG:HG3	2:E:391:ARG:HH11	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:ILE:H	2:B:162:PRO:HD3	1.70	0.56
3:C:117:ASN:C	3:C:117:ASN:HD22	2.07	0.56
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.87	0.56
1:D:181:GLN:HB3	2:E:171:ILE:HD12	1.87	0.56
3:C:270:GLU:HB2	3:C:274:TYR:CZ	2.40	0.56
3:C:323:GLU:OE1	3:C:323:GLU:N	2.38	0.56
2:B:157:VAL:HG22	2:B:158:ASN:N	2.19	0.56
2:E:230:ASP:HB3	2:E:233:VAL:HG13	1.86	0.56
2:B:157:VAL:HG22	2:B:158:ASN:HD22	1.71	0.56
3:C:219:SER:OG	3:C:224:THR:HG22	2.06	0.56
3:C:337:ASN:O	3:C:337:ASN:CG	2.44	0.56
2:B:332:GLN:O	2:B:338:TYR:HA	2.04	0.56
2:E:387:THR:C	2:E:389:ASP:H	2.08	0.56
3:F:244:TYR:H	3:F:266:LYS:HZ2	1.52	0.56
1:A:138:LYS:HD3	1:A:138:LYS:O	2.06	0.56
3:F:203:ASP:O	3:F:206:LYS:HE2	2.06	0.56
2:B:353:LEU:HD22	8:B:495:HOH:O	2.05	0.55
3:C:203:ASP:O	3:C:206:LYS:HE2	2.06	0.55
2:B:252:ILE:HD13	2:B:454:ILE:HG12	1.89	0.55
3:F:149:THR:HG23	3:F:168:PHE:O	2.05	0.55
2:B:202:ASN:ND2	2:B:284:ASN:O	2.38	0.55
2:B:458:PHE:HB3	2:B:459:PRO:HD3	1.88	0.55
2:E:307:PRO:HD2	2:E:459:PRO:HG3	1.89	0.55
3:F:252:ASP:HB2	3:F:377:TYR:OH	2.05	0.55
3:C:198:LEU:HD12	3:C:199:ASP:OD1	2.06	0.54
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	2.05	0.54
2:E:307:PRO:CG	2:E:459:PRO:HG3	2.37	0.54
2:B:172:LEU:HD12	3:C:113:ILE:HG22	1.89	0.54
2:E:237:ARG:HH11	2:E:237:ARG:HG3	1.70	0.54
2:E:422:TYR:O	2:E:444:TRP:HB3	2.07	0.54
3:F:325:ASN:ND2	3:F:328:GLU:H	2.05	0.54
2:E:351:ASN:C	2:E:351:ASN:HD22	2.11	0.54
3:F:310:MET:CG	3:F:337:ASN:HB2	2.38	0.54
2:B:457:PHE:O	2:B:458:PHE:CB	2.54	0.54
1:A:179:GLU:O	1:A:183:LYS:HG3	2.07	0.54
3:F:189:ASN:OD1	3:F:391:ARG:HG3	2.08	0.54
3:F:272:ASP:HB3	8:F:433:HOH:O	2.08	0.53
2:B:457:PHE:O	2:B:458:PHE:HB2	2.07	0.53
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.43	0.53
2:E:373:MET:HE2	2:E:404:TYR:O	2.09	0.53
1:A:136:LEU:C	1:A:136:LEU:HD23	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ARG:NH2	1:A:189:ILE:HD13	2.09	0.53
2:E:458:PHE:H	2:E:459:PRO:HD3	1.72	0.53
3:F:198:LEU:O	3:F:199:ASP:HB3	2.09	0.53
1:A:136:LEU:HD22	2:B:168:LEU:CD2	2.35	0.52
3:F:149:THR:HG22	3:F:150:GLY:N	2.24	0.52
1:A:137:GLN:CA	1:A:140:VAL:HG22	2.40	0.52
3:C:124:LEU:O	3:C:128:VAL:HG23	2.09	0.52
2:E:166:ARG:HG3	2:E:169:ARG:HB2	1.90	0.52
2:E:406:ARG:N	2:E:407:CYS:HA	2.24	0.52
3:C:149:THR:CG2	3:C:150:GLY:H	2.22	0.52
2:E:212:GLU:O	2:E:215:ILE:HG22	2.09	0.52
2:E:458:PHE:H	2:E:459:PRO:HD2	1.74	0.52
2:E:316:ASP:HB2	2:E:445:TYR:OH	2.09	0.52
3:C:288:ASP:OD2	3:C:291:ASP:HB2	2.10	0.51
2:E:252:ILE:HG23	2:E:299:ILE:HG12	1.92	0.51
2:B:229:PRO:HD2	2:B:233:VAL:HG21	1.92	0.51
3:C:149:THR:CG2	3:C:150:GLY:N	2.74	0.51
2:E:436:VAL:HG12	2:E:437:TRP:N	2.26	0.51
3:C:389:PHE:C	3:C:391:ARG:H	2.14	0.51
3:F:195:GLN:HB3	3:F:384:MET:HB2	1.92	0.51
2:B:373:MET:HE2	2:B:404:TYR:O	2.11	0.51
3:C:231:GLU:HG2	8:C:421:HOH:O	2.10	0.51
3:C:310:MET:HG3	3:C:337:ASN:HB2	1.93	0.51
3:F:325:ASN:ND2	3:F:325:ASN:C	2.62	0.51
1:A:136:LEU:O	1:A:136:LEU:HD23	2.10	0.51
2:E:361:MET:O	2:E:364:ASN:HB2	2.11	0.51
1:A:137:GLN:HA	1:A:140:VAL:CG2	2.41	0.51
2:E:436:VAL:CG1	2:E:437:TRP:N	2.74	0.51
2:B:363:GLU:O	2:B:367:MET:HG2	2.12	0.50
3:C:338:LYS:O	3:C:338:LYS:HG2	2.12	0.50
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.60	0.50
1:D:147:MET:HE3	1:D:150:LEU:HD23	1.93	0.50
2:B:280:THR:O	2:B:281:ASP:C	2.51	0.50
3:F:310:MET:SD	3:F:337:ASN:HB2	2.51	0.50
2:B:201:CYS:HB3	2:B:224:MET:HE3	1.94	0.49
1:A:130:VAL:O	1:A:134:GLN:HG2	2.12	0.49
2:E:252:ILE:CG2	2:E:299:ILE:HG12	2.42	0.49
2:B:422:TYR:OH	2:B:432:ASP:HB2	2.12	0.49
2:B:350:GLY:HA3	2:B:439:ASN:HB3	1.95	0.49
1:A:189:ILE:O	1:A:189:ILE:HG22	2.13	0.49
2:E:245:GLU:O	2:E:246:ASN:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:191:TRP:CE3	3:C:385:LYS:HG3	2.48	0.48
2:B:345:TYR:CG	2:B:346:ARG:N	2.81	0.48
3:C:281:PHE:CD2	3:C:288:ASP:HB2	2.49	0.48
3:F:119:GLN:HG2	8:F:440:HOH:O	2.12	0.48
1:D:188:VAL:O	1:D:188:VAL:HG12	2.14	0.48
2:B:165:LEU:HD12	2:B:165:LEU:N	2.28	0.48
3:C:116:SER:C	3:C:118:ASN:H	2.16	0.48
2:E:381:ASP:OD2	2:E:393:GLN:HG2	2.12	0.48
2:E:458:PHE:CG	2:E:458:PHE:O	2.66	0.48
3:C:337:ASN:O	3:C:338:LYS:HB3	2.13	0.48
2:E:385:TRP:CG	2:E:406:ARG:HD3	2.48	0.48
3:C:338:LYS:N	3:C:339:CYS:CA	2.69	0.48
2:B:168:LEU:O	2:B:172:LEU:HD23	2.13	0.48
3:C:163:GLN:NE2	3:C:163:GLN:H	2.12	0.48
1:D:136:LEU:C	1:D:136:LEU:HD13	2.33	0.48
1:A:144:LEU:CD2	2:B:175:LEU:HD21	2.44	0.48
2:B:237:ARG:HH11	2:B:237:ARG:HG3	1.78	0.48
2:E:385:TRP:CH2	2:E:392:LYS:HB3	2.48	0.47
3:C:137:GLU:HA	3:C:137:GLU:OE1	2.14	0.47
2:E:245:GLU:OE2	2:E:323:LYS:NZ	2.47	0.47
2:E:351:ASN:ND2	2:E:354:MET:H	2.13	0.47
2:B:167:VAL:O	2:B:171:ILE:HG12	2.14	0.47
2:E:441:LYS:HD3	2:E:445:TYR:CD1	2.50	0.47
3:C:119:GLN:HA	3:C:119:GLN:NE2	2.29	0.47
2:E:385:TRP:CA	2:E:406:ARG:HD3	2.44	0.47
1:A:191:LYS:HG3	8:A:199:HOH:O	2.15	0.47
3:C:197:ARG:HB2	3:C:382:THR:HB	1.97	0.47
1:D:182:GLN:O	1:D:186:GLU:HG3	2.15	0.47
2:E:169:ARG:HH11	2:E:169:ARG:HG2	1.79	0.47
2:E:311:LEU:HD13	2:E:325:HIS:CD2	2.50	0.47
2:E:332:GLN:O	2:E:338:TYR:HA	2.15	0.47
3:C:265:PHE:O	3:C:266:LYS:HD2	2.14	0.47
3:F:126:GLU:N	3:F:126:GLU:OE2	2.48	0.47
2:B:174:ASN:HD21	2:B:178:LYS:NZ	2.13	0.47
3:C:305:THR:HB	3:C:341:ALA:HB2	1.96	0.47
2:B:169:ARG:O	2:B:173:GLU:HG2	2.15	0.47
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.80	0.47
3:C:307:HIS:HE1	3:C:341:ALA:H	1.63	0.46
1:D:136:LEU:C	1:D:138:LYS:H	2.18	0.46
2:E:387:THR:HG23	2:E:387:THR:O	2.14	0.46
2:E:458:PHE:N	2:E:459:PRO:HD3	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:119:GLN:HA	3:F:119:GLN:NE2	2.30	0.46
1:A:187:GLN:O	1:A:190:ALA:HB3	2.15	0.46
1:A:191:LYS:NZ	2:B:161:ILE:HG13	2.30	0.46
8:A:199:HOH:O	2:B:165:LEU:HD11	2.15	0.46
3:C:343:HIS:O	3:C:367:ILE:HA	2.15	0.46
2:E:239:TYR:CZ	2:E:289:PRO:HD3	2.50	0.46
3:C:143:VAL:O	3:C:143:VAL:HG23	2.14	0.46
1:A:148:LYS:NZ	1:A:182:GLN:HE22	2.13	0.46
3:C:114:TYR:O	3:C:118:ASN:HB2	2.15	0.46
3:C:307:HIS:CE1	3:C:341:ALA:H	2.33	0.46
2:B:363:GLU:HA	2:B:366:THR:OG1	2.16	0.46
2:B:201:CYS:O	3:C:143:VAL:HG21	2.14	0.46
3:C:307:HIS:HE1	3:C:342:GLY:H	1.62	0.46
2:E:295:GLY:O	2:E:299:ILE:HG13	2.16	0.46
2:E:385:TRP:CZ2	2:E:392:LYS:HB3	2.51	0.46
1:D:151:GLU:OE2	2:E:182:LEU:HD21	2.16	0.46
1:D:169:LEU:H	2:E:189:GLN:NE2	2.11	0.46
3:C:229:GLY:O	3:C:233:ILE:HG13	2.16	0.46
2:E:391:ARG:NH1	2:E:391:ARG:HG3	2.31	0.45
3:C:246:LEU:HD22	3:C:265:PHE:CE1	2.51	0.45
2:B:168:LEU:HD23	3:C:110:LEU:HD23	1.99	0.45
3:C:189:ASN:OD1	3:C:391:ARG:HG3	2.16	0.45
4:G:3:ARG:O	4:G:4:PRO:C	2.55	0.45
2:B:203:ILE:HA	2:B:204:PRO:HD3	1.86	0.45
2:E:439:ASN:H	2:E:439:ASN:HD22	1.62	0.45
3:C:253:TRP:CH2	3:C:380:LYS:HG3	2.52	0.45
1:A:176:LYS:O	1:A:176:LYS:HD3	2.16	0.45
2:E:402:TRP:CG	2:E:403:TRP:N	2.85	0.45
3:F:367:ILE:O	3:F:379:MET:HG2	2.17	0.45
2:E:249:TRP:HB3	2:E:453:LYS:HB3	1.99	0.45
2:B:422:TYR:O	2:B:444:TRP:HB3	2.17	0.45
3:C:105:SER:HB3	3:C:109:TYR:CE2	2.52	0.45
2:E:283:LYS:HG2	2:E:285:TYR:CE1	2.52	0.44
2:E:350:GLY:HA3	2:E:439:ASN:HB3	1.99	0.44
3:F:118:ASN:O	3:F:122:VAL:HG23	2.18	0.44
2:B:245:GLU:OE2	2:B:323:LYS:NZ	2.50	0.44
2:E:387:THR:C	2:E:389:ASP:N	2.71	0.44
3:F:281:PHE:CD2	3:F:288:ASP:HB2	2.53	0.44
3:F:307:HIS:CE1	3:F:342:GLY:H	2.36	0.44
3:C:163:GLN:N	3:C:163:GLN:CD	2.71	0.44
2:E:252:ILE:CB	8:E:493:HOH:O	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:ARG:CZ	8:D:201:HOH:O	2.66	0.44
2:E:351:ASN:C	2:E:351:ASN:ND2	2.71	0.44
2:E:307:PRO:CD	2:E:459:PRO:HG3	2.46	0.44
3:F:110:LEU:N	3:F:112:GLU:OE2	2.51	0.44
3:F:112:GLU:HB3	8:F:442:HOH:O	2.17	0.44
3:F:168:PHE:HB3	3:F:177:GLN:HE21	1.82	0.44
2:E:280:THR:O	2:E:281:ASP:C	2.57	0.43
2:B:391:ARG:NE	2:B:391:ARG:HA	2.33	0.43
2:B:398:ASP:HB3	8:B:514:HOH:O	2.18	0.43
3:C:298:ASP:HB3	3:C:301:ASP:OD1	2.18	0.43
3:C:307:HIS:CE1	3:C:342:GLY:H	2.36	0.43
1:D:143:GLN:O	1:D:147:MET:HB2	2.19	0.43
5:I:1:NAG:H4	5:I:2:NAG:H2	1.80	0.43
1:D:162:ARG:HB2	1:D:162:ARG:HH11	1.82	0.43
2:E:201:CYS:HB3	2:E:224:MET:HE3	2.00	0.43
3:F:392:LEU:O	3:F:393:THR:HB	2.18	0.43
3:C:278:TYR:CE2	3:C:308:ASN:HB2	2.53	0.43
3:C:143:VAL:O	3:C:143:VAL:CG2	2.67	0.43
2:E:432:ASP:O	2:E:432:ASP:OD2	2.36	0.43
2:B:218:GLY:O	2:B:220:GLU:HG3	2.18	0.43
2:B:245:GLU:O	2:B:246:ASN:HB2	2.19	0.43
2:E:169:ARG:NH1	2:E:169:ARG:HG2	2.33	0.43
2:E:392:LYS:C	2:E:393:GLN:HG3	2.38	0.43
2:E:385:TRP:CD1	2:E:406:ARG:CZ	3.02	0.43
3:C:160:GLY:O	3:C:162:LYS:HG3	2.19	0.42
2:B:316:ASP:HB2	2:B:445:TYR:OH	2.19	0.42
3:F:251:GLU:HB3	3:F:381:LYS:HB2	1.99	0.42
2:B:325:HIS:O	2:B:345:TYR:HA	2.19	0.42
3:F:227:TRP:HZ2	3:F:230:ASN:ND2	2.17	0.42
3:F:369:TRP:HB3	8:F:416:HOH:O	2.19	0.42
1:A:137:GLN:C	1:A:140:VAL:HG22	2.40	0.42
2:B:174:ASN:HD21	2:B:178:LYS:HZ1	1.65	0.42
3:F:173:LYS:HB3	3:F:173:LYS:NZ	2.35	0.42
3:F:292:GLY:C	3:F:302:LYS:HD2	2.39	0.42
3:F:295:PHE:HD2	3:F:375:ARG:NH1	2.17	0.42
1:D:140:VAL:HG12	2:E:172:LEU:HD21	2.01	0.42
2:E:457:PHE:O	2:E:458:PHE:CD1	2.73	0.42
2:E:307:PRO:HG2	2:E:459:PRO:HG3	2.01	0.42
3:C:207:ASN:HB2	3:C:316:ASP:OD2	2.19	0.42
2:E:417:TYR:HB2	2:E:446:SER:HB3	2.02	0.42
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:ASP:OD2	2:B:415:ARG:HD3	2.20	0.42
2:B:435:VAL:O	2:B:446:SER:HA	2.19	0.42
3:F:148:ILE:HG23	8:F:430:HOH:O	2.20	0.42
2:B:436:VAL:CG1	2:B:437:TRP:N	2.82	0.42
2:B:239:TYR:CZ	2:B:289:PRO:HD3	2.55	0.42
3:C:322:PHE:CD2	3:C:323:GLU:N	2.87	0.42
2:E:167:VAL:HG23	2:E:168:LEU:CD1	2.43	0.42
2:E:392:LYS:HG2	8:E:483:HOH:O	2.19	0.42
2:B:402:TRP:CG	2:B:403:TRP:N	2.88	0.41
2:E:237:ARG:HG3	2:E:237:ARG:NH1	2.34	0.41
2:B:337:LYS:HE3	2:B:374:PHE:CE1	2.55	0.41
2:B:181:LYS:HE2	2:B:185:ASP:OD2	2.19	0.41
3:C:310:MET:CG	3:C:337:ASN:HB2	2.51	0.41
3:F:295:PHE:CD2	3:F:375:ARG:NH1	2.88	0.41
2:E:202:ASN:HD22	2:E:284:ASN:HB2	1.86	0.41
2:E:405:ASN:HB3	2:E:406:ARG:H	1.63	0.41
2:B:241:ASP:C	2:B:241:ASP:OD2	2.59	0.41
2:E:352:ALA:HB2	2:E:439:ASN:ND2	2.36	0.41
2:E:317:TRP:CE3	2:E:448:ARG:HD3	2.56	0.41
3:C:107:ILE:HG22	3:C:107:ILE:O	2.21	0.41
3:F:207:ASN:HB2	3:F:316:ASP:OD2	2.20	0.41
1:A:147:MET:HG3	2:B:175:LEU:HD22	2.02	0.41
3:C:231:GLU:O	3:C:235:LEU:HG	2.21	0.41
2:E:166:ARG:NE	2:E:166:ARG:HA	2.27	0.41
2:E:166:ARG:HE	2:E:166:ARG:CA	2.21	0.41
2:E:392:LYS:HA	8:E:483:HOH:O	2.19	0.41
2:E:234:LYS:HA	2:E:235:PRO:HD3	1.94	0.41
2:E:328:GLY:O	2:E:342:VAL:HA	2.21	0.41
3:F:114:TYR:C	3:F:114:TYR:CD1	2.94	0.41
3:F:109:TYR:CD1	3:F:109:TYR:N	2.89	0.41
3:F:122:VAL:O	3:F:126:GLU:OE2	2.39	0.41
3:F:329:GLN:NE2	4:H:3:ARG:HE	2.15	0.41
1:A:140:VAL:HG12	2:B:172:LEU:HD21	2.03	0.40
1:A:181:GLN:HB3	2:B:171:ILE:HD12	2.02	0.40
2:E:406:ARG:HA	2:E:406:ARG:HD2	1.88	0.40
3:F:197:ARG:HD3	3:F:204:PHE:CZ	2.56	0.40
1:A:140:VAL:CG1	2:B:172:LEU:HD21	2.51	0.40
2:B:176:ARG:O	2:B:180:GLN:HG2	2.22	0.40
3:C:325:ASN:OD1	3:C:328:GLU:HB2	2.21	0.40
2:B:314:MET:HA	2:B:449:LYS:O	2.22	0.40
2:B:315:GLU:HG3	2:B:321:LYS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:201:CYS:CB	2:E:224:MET:HE3	2.52	0.40
3:F:153:CYS:SG	3:F:192:THR:HA	2.61	0.40
3:C:307:HIS:HD2	3:C:335:TRP:O	2.05	0.40
2:E:420:GLY:HA2	2:E:446:SER:O	2.21	0.40

There are no symmetry-related clashes.

## 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	65/87 (75%)	60 (92%)	2 (3%)	3 (5%)	2	3
1	D	52/87 (60%)	50 (96%)	2 (4%)	0	100	100
2	B	301/328 (92%)	274 (91%)	23 (8%)	4 (1%)	12	24
2	E	294/328 (90%)	272 (92%)	19 (6%)	3 (1%)	15	32
3	C	290/324 (90%)	266 (92%)	19 (7%)	5 (2%)	9	18
3	F	283/324 (87%)	262 (93%)	17 (6%)	4 (1%)	11	22
4	G	2/5 (40%)	1 (50%)	0	1 (50%)	0	0
4	H	2/5 (40%)	2 (100%)	0	0	100	100
All	All	1289/1488 (87%)	1187 (92%)	82 (6%)	20 (2%)	9	19

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	ILE
1	A	191	LYS
2	B	281	ASP
2	B	458	PHE
3	C	104	ASP
2	E	281	ASP

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Mol	Chain	Res	Type
2	E	458	PHE
3	F	338	LYS
1	A	128	GLU
2	B	160	ASN
3	C	106	SER
3	F	199	ASP
3	F	200	GLY
2	B	256	GLN
3	C	390	ASN
2	E	256	GLN
3	C	199	ASP
3	F	198	LEU
3	C	198	LEU
4	G	4	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	62/82 (76%)	60 (97%)	2 (3%)	39	65
1	D	50/82 (61%)	46 (92%)	4 (8%)	12	24
2	B	261/286 (91%)	247 (95%)	14 (5%)	22	44
2	E	254/286 (89%)	245 (96%)	9 (4%)	36	62
3	C	246/270 (91%)	239 (97%)	7 (3%)	43	69
3	F	239/270 (88%)	230 (96%)	9 (4%)	33	59
4	G	2/2 (100%)	2 (100%)	0	100	100
4	H	2/2 (100%)	2 (100%)	0	100	100
All	All	1116/1280 (87%)	1071 (96%)	45 (4%)	31	57

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LEU

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Mol	Chain	Res	Type
1	A	172	GLU
2	B	158	ASN
2	B	160	ASN
2	B	161	ILE
2	B	164	ASN
2	B	210	GLU
2	B	253	GLN
2	B	280	THR
2	B	281	ASP
2	B	301	GLN
2	B	325	HIS
2	B	342	VAL
2	B	351	ASN
2	B	363	GLU
2	B	397	GLU
3	C	117	ASN
3	C	118	ASN
3	C	173	LYS
3	C	266	LYS
3	C	317	ASN
3	C	323	GLU
3	C	325	ASN
1	D	135	LEU
1	D	162	ARG
1	D	175	LEU
1	D	182	GLN
2	E	166	ARG
2	E	210	GLU
2	E	253	GLN
2	E	281	ASP
2	E	301	GLN
2	E	325	HIS
2	E	351	ASN
2	E	447	MET
2	E	458	PHE
3	F	114	TYR
3	F	126	GLU
3	F	143	VAL
3	F	173	LYS
3	F	264	MET
3	F	285	ASP
3	F	317	ASN

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Mol	Chain	Res	Type
3	F	325	ASN
3	F	374	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	137	GLN
1	A	182	GLN
2	B	158	ASN
2	B	164	ASN
2	B	174	ASN
2	B	189	GLN
2	B	253	GLN
2	B	256	GLN
2	B	296	ASN
2	B	301	GLN
2	B	325	HIS
2	B	339	GLN
2	B	351	ASN
2	B	439	ASN
3	C	103	HIS
3	C	117	ASN
3	C	118	ASN
3	C	119	GLN
3	C	123	ASN
3	C	134	GLN
3	C	144	GLN
3	C	177	GLN
3	C	230	ASN
3	C	239	GLN
3	C	307	HIS
3	C	317	ASN
3	C	319	ASN
3	C	329	GLN
1	D	143	GLN
1	D	181	GLN
1	D	182	GLN
1	D	187	GLN
2	E	174	ASN
2	E	180	GLN
2	E	189	GLN

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Mol	Chain	Res	Type
2	E	202	ASN
2	E	228	GLN
2	E	253	GLN
2	E	256	GLN
2	E	296	ASN
2	E	301	GLN
2	E	339	GLN
2	E	351	ASN
2	E	408	HIS
2	E	439	ASN
3	F	115	ASN
3	F	118	ASN
3	F	119	GLN
3	F	123	ASN
3	F	130	GLN
3	F	136	GLN
3	F	177	GLN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	329	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	HYP	G	2	4	6,8,9	0.92	0	5,10,12	1.29	1 (20%)
4	HYP	H	2	4	6,8,9	0.71	0	5,10,12	1.10	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
4	HYP	G	2	4	-	0/0/11/13	0/1/1/1
4	HYP	H	2	4	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	HYP	CG-CB-CA	-2.38	100.96	103.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

4 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
5	NAG	I	1	2,5	14,14,15	0.75	0	17,19,21	1.07	1 (5%)
5	NAG	I	2	5	14,14,15	0.61	0	17,19,21	0.61	0
6	NAG	J	1	2,6	14,14,15	0.56	0	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NDG	J	2	6	14,14,15	0.67	0	17,19,21	0.75	1 (5%)

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
5	NAG	I	1	2,5	-	4/6/23/26	0/1/1/1
5	NAG	I	2	5	-	4/6/23/26	0/1/1/1
6	NAG	J	1	2,6	-	2/6/23/26	0/1/1/1
6	NDG	J	2	6	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	NAG	C3-C4-C5	2.19	114.14	110.24
6	J	2	NDG	C2-N2-C7	-2.07	119.95	122.90

There are no chirality outliers.

All (14) torsion outliers are listed below:

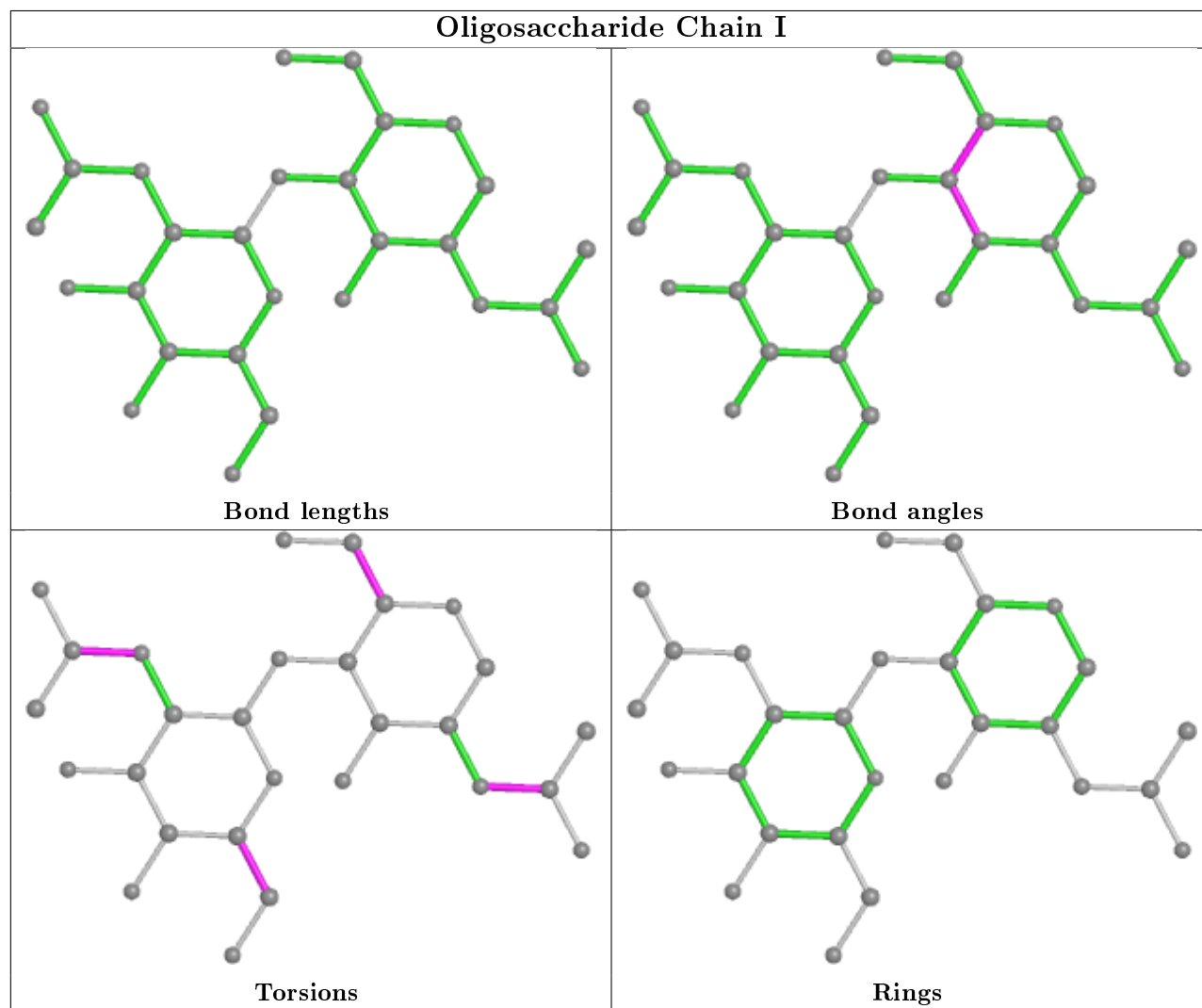
Mol	Chain	Res	Type	Atoms
6	J	2	NDG	C8-C7-N2-C2
6	J	2	NDG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
6	J	1	NAG	C8-C7-N2-C2
6	J	1	NAG	O7-C7-N2-C2
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	I	2	NAG	C4-C5-C6-O6
6	J	2	NDG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
6	J	2	NDG	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6

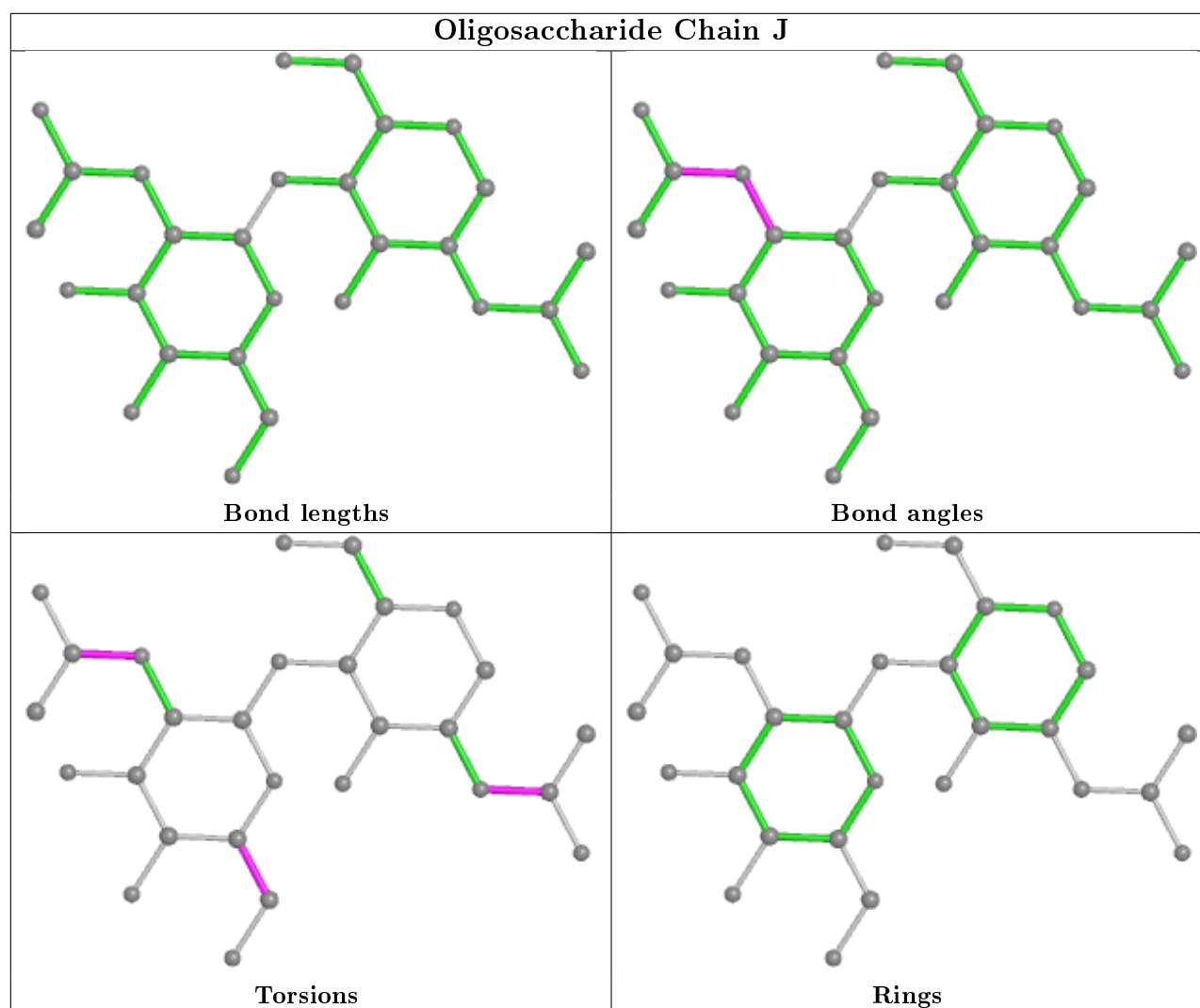
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	2	NDG	3	0
5	I	2	NAG	2	0
6	J	1	NAG	3	0
5	I	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 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	67/87 (77%)	0.17	7 (10%) 6 4	33, 69, 124, 158	0
1	D	54/87 (62%)	-0.12	4 (7%) 14 10	29, 65, 111, 139	0
2	B	303/328 (92%)	-0.26	9 (2%) 50 43	23, 41, 103, 166	0
2	E	296/328 (90%)	-0.25	12 (4%) 37 30	24, 40, 99, 142	0
3	C	292/324 (90%)	-0.36	3 (1%) 82 80	24, 44, 79, 129	0
3	F	285/324 (87%)	-0.39	4 (1%) 75 71	26, 45, 78, 123	0
4	G	3/5 (60%)	-0.64	0 100 100	48, 48, 51, 69	0
4	H	3/5 (60%)	-0.67	0 100 100	42, 42, 46, 61	0
All	All	1303/1488 (87%)	-0.28	39 (2%) 50 43	23, 44, 99, 166	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	459	PRO	9.5
2	E	459	PRO	8.1
2	B	458	PHE	7.1
2	E	390	PRO	6.7
1	A	128	GLU	6.1
2	E	164	ASN	5.3
1	A	129	LYS	4.8
3	F	109	TYR	4.8
2	E	388	SER	4.7
2	E	167	VAL	4.4
1	A	126	VAL	4.1
2	B	161	ILE	3.7
3	F	110	LEU	3.6
1	D	187	GLN	3.4
2	B	390	PRO	3.4
2	E	165	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	385	TRP	3.3
3	F	393	THR	3.2
3	C	109	TYR	3.2
2	E	386	LEU	3.2
1	D	186	GLU	3.1
2	B	163	THR	3.1
3	C	105	SER	3.1
1	D	188	VAL	3.1
2	E	166	ARG	3.0
2	B	391	ARG	3.0
2	E	391	ARG	3.0
2	B	160	ASN	2.8
2	B	158	ASN	2.8
1	A	190	ALA	2.5
2	B	389	ASP	2.5
1	A	183	LYS	2.3
3	F	111	GLN	2.2
1	A	127	ILE	2.2
3	C	108	ARG	2.2
2	E	413	ASN	2.1
1	D	135	LEU	2.1
1	A	191	LYS	2.0
2	E	233	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	HYP	G	2	8/9	0.98	0.11	37,47,50,52	0
4	HYP	H	2	8/9	0.98	0.10	40,46,50,53	0

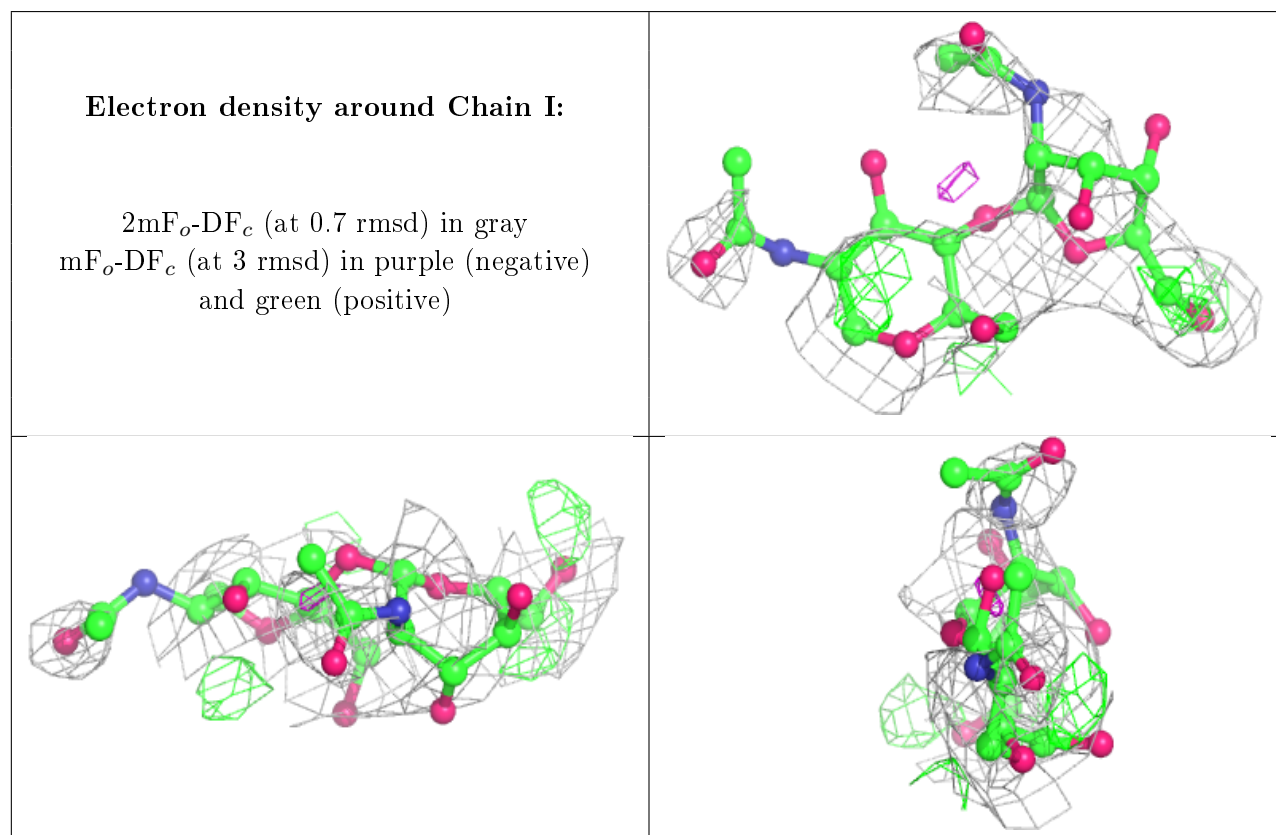
## 6.3 Carbohydrates

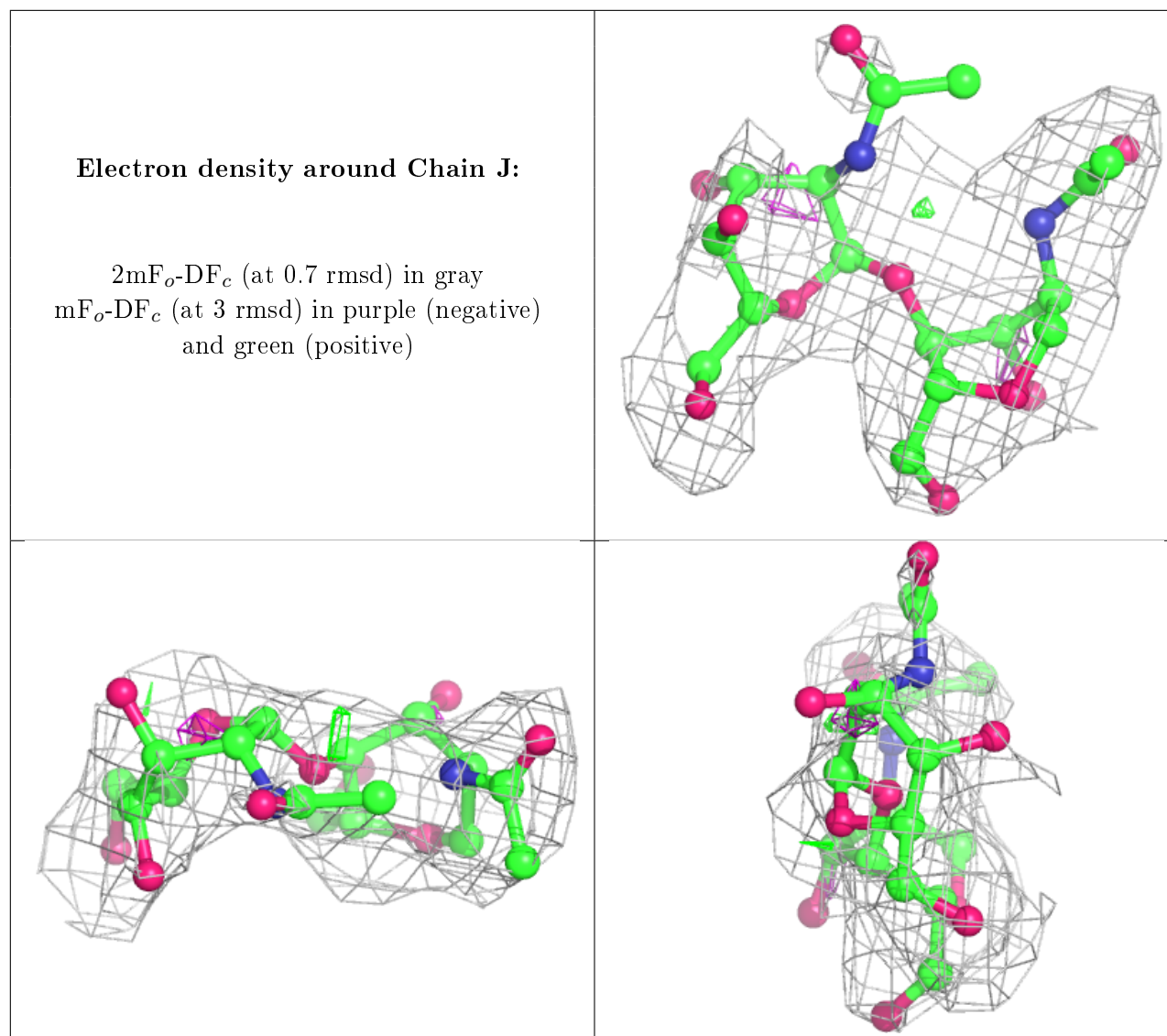
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	I	2	14/15	0.54	0.48	120,154,156,157	0
5	NAG	I	1	14/15	0.62	0.42	121,132,143,154	0
6	NDG	J	2	14/15	0.66	0.41	105,118,126,127	0
6	NAG	J	1	14/15	0.87	0.29	65,85,107,114	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.





## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	CA	C	1	1/1	0.93	0.08	61,61,61,61	0
7	CA	E	2	1/1	0.94	0.06	58,58,58,58	0
7	CA	C	4	1/1	0.95	0.10	55,55,55,55	0
7	CA	B	2	1/1	0.95	0.10	56,56,56,56	0
7	CA	E	3	1/1	0.95	0.14	47,47,47,47	0
7	CA	B	3	1/1	0.96	0.16	53,53,53,53	0
7	CA	F	1	1/1	0.98	0.15	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.