



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 10:44 AM BST

PDB ID : 6A5E  
Title : Crystal structure of plant peptide RALF23 in complex with FER and LLG2  
Authors : Xiao, Y.; Chai, J.  
Deposited on : 2018-06-23  
Resolution : 2.77 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

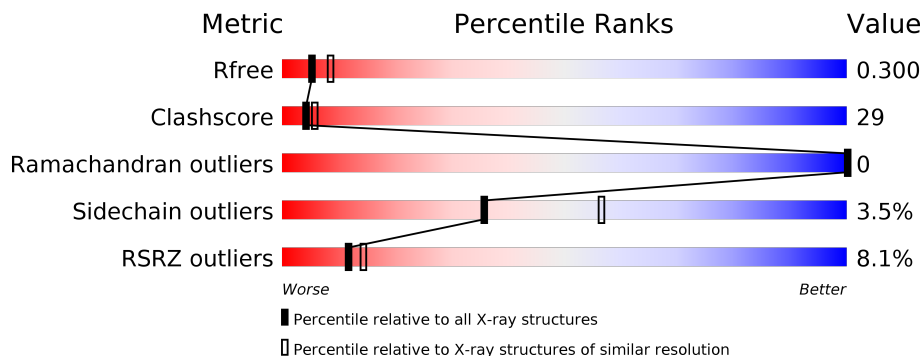
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.77 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.



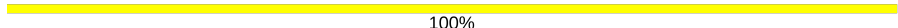


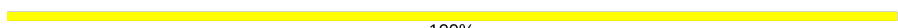
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	396	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">8%      54%      39%      • 5%</p>
1	B	396	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 38%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">12%      55%      38%      • 5%</p>
2	C	84	<div style="display: flex; align-items: center;"> <div style="width: 58%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">58%      40%      •</p>
2	D	84	<div style="display: flex; align-items: center;"> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">60%      39%      •</p>
3	E	15	<div style="display: flex; align-items: center;"> <div style="width: 53%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">53%      40%      7%</p>
3	F	15	<div style="display: flex; align-items: center;"> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">67%      33%</p>

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Mol	Chain	Length	Quality of chain
4	G	2	 100%
4	H	2	 100%
4	I	2	 100%
4	J	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	1004	-	-	-	X
5	NAG	B	1004	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7564 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 Receptor-like protein kinase FERONIA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	375	Total 2924	C 1871	N 466	O 577	S 10	0	0	0
1	B	375	Total 2924	C 1871	N 466	O 577	S 10	0	0	0

- Molecule 2 is a protein called GPI-anchored protein LLG2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	84	Total 650	C 408	N 105	O 127	S 10	0	0	0
2	D	84	Total 650	C 408	N 105	O 127	S 10	0	0	0

- Molecule 3 is a protein called RALF23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	15	Total 124	C 78	N 25	O 20	S 1	0	0	0
3	F	15	Total 124	C 78	N 25	O 20	S 1	0	0	0

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



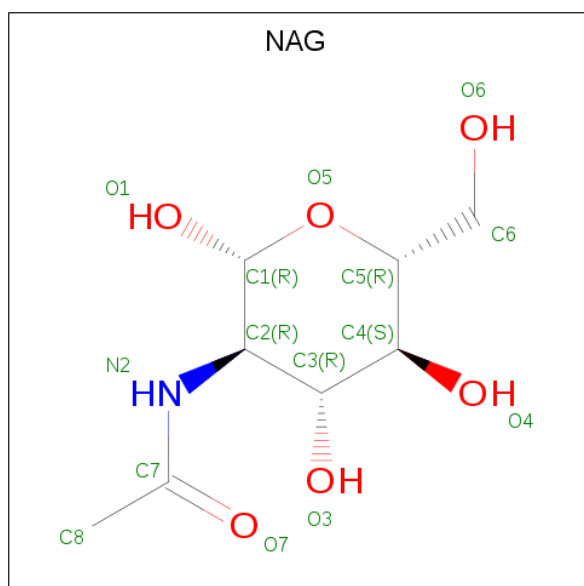
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	2	Total 28	C 16	N 2	O 10	0	0	0

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

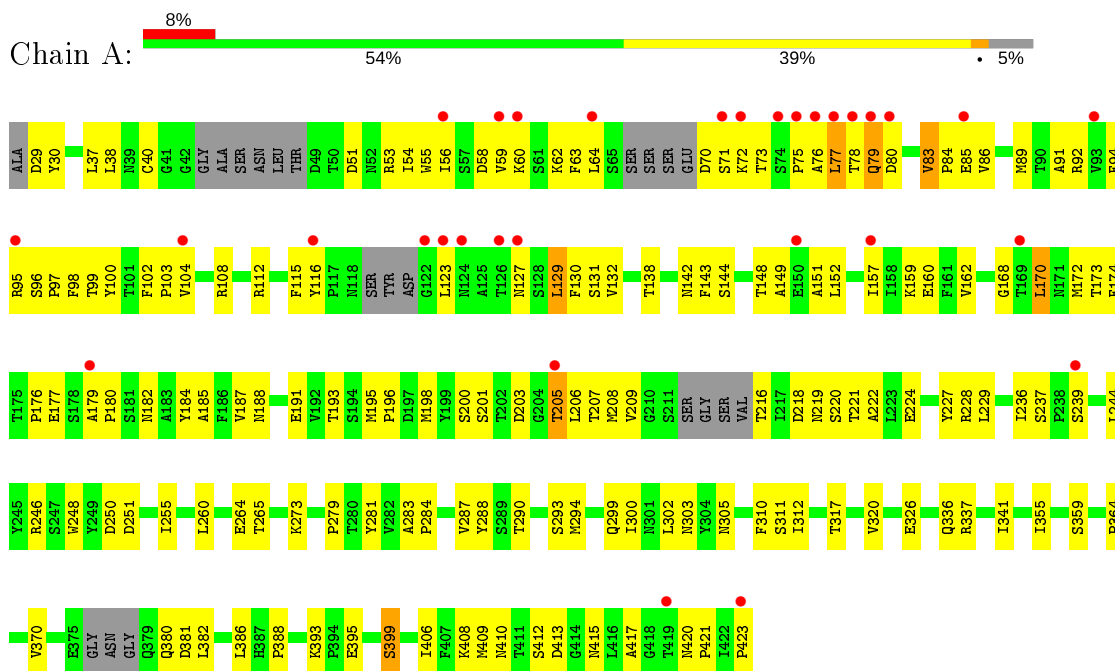


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

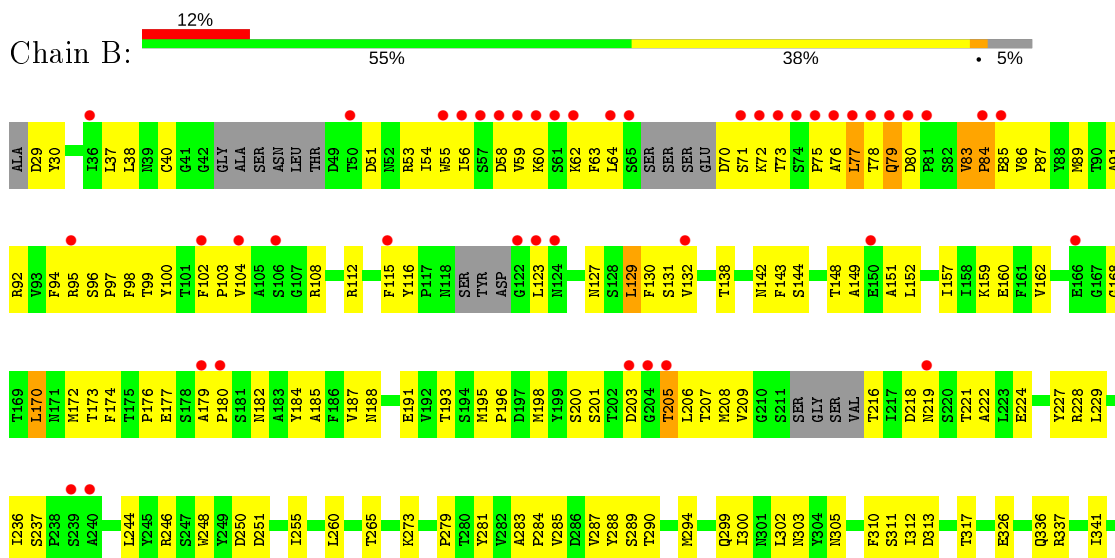
### 3 Residue-property plots

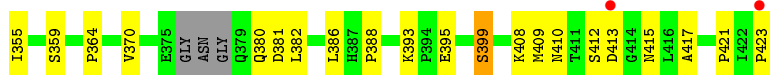
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Receptor-like protein kinase FERONIA



- Molecule 1: Receptor-like protein kinase FERONIA





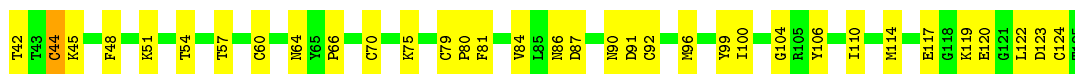
- Molecule 2: GPI-anchored protein LLG2

Chain C: 58% 40%



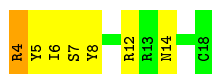
- Molecule 2: GPI-anchored protein LLG2

Chain D: 60% 39%



- Molecule 3: RALF23

Chain E: 53% 40% 7%



- Molecule 3: RALF23

Chain F: 67% 33%



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

Chain G: 100%



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

Chain H: 100%




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

Chain I:  100%

MAG1  
MAG2

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

Chain J:  100%

MAG1  
MAG2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.31Å 62.36Å 97.48Å 105.72° 91.30° 108.48°	Depositor
Resolution (Å)	42.61 – 2.77 42.61 – 2.77	Depositor EDS
% Data completeness (in resolution range)	96.5 (42.61-2.77) 96.6 (42.61-2.77)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.77Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.233 , 0.285 0.264 , 0.300	Depositor DCC
$R_{free}$ test set	1674 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtrriage
Anisotropy	0.307	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 69.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7564	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.27% 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:  
NAG

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	0.74	0/3002	0.79	1/4106 (0.0%)
1	B	0.74	0/3002	0.79	1/4106 (0.0%)
2	C	1.18	2/665 (0.3%)	0.89	1/898 (0.1%)
2	D	1.18	2/665 (0.3%)	0.89	1/898 (0.1%)
3	E	0.57	0/126	0.69	0/169
3	F	0.56	0/126	0.70	0/169
All	All	0.83	4/7586 (0.1%)	0.81	4/10346 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	92	CYS	CB-SG	-18.54	1.50	1.82
2	D	92	CYS	CB-SG	-18.54	1.50	1.82
2	D	44	CYS	CB-SG	-16.87	1.53	1.82
2	C	44	CYS	CB-SG	-16.86	1.53	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	92	CYS	CA-CB-SG	16.34	143.42	114.00
2	C	92	CYS	CA-CB-SG	16.31	143.36	114.00
1	B	83	VAL	C-N-CD	-8.05	102.90	120.60
1	A	83	VAL	C-N-CD	-8.04	102.92	120.60

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	2924	0	2793	191	0
1	B	2924	0	2793	187	0
2	C	650	0	606	28	0
2	D	650	0	606	27	0
3	E	124	0	127	11	0
3	F	124	0	127	6	0
4	G	28	0	25	2	0
4	H	28	0	25	1	0
4	I	28	0	25	1	0
4	J	28	0	25	2	0
5	A	14	0	13	3	0
5	B	14	0	13	3	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
All	All	7564	0	7204	432	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 29.

All (432) 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:B:305:ASN:HD21	4:J:1:NAG:C1	1.07	1.60
1:A:305:ASN:HD21	4:G:1:NAG:C1	1.07	1.58
1:A:123:LEU:HD23	1:A:184:TYR:CZ	1.53	1.43
1:B:123:LEU:HD23	1:B:184:TYR:CZ	1.53	1.40
1:A:222:ALA:H	1:A:410:ASN:ND2	1.18	1.38
1:B:222:ALA:H	1:B:410:ASN:ND2	1.18	1.37
1:B:305:ASN:ND2	4:J:1:NAG:C1	1.91	1.34
1:A:305:ASN:ND2	4:G:1:NAG:C1	1.91	1.33
1:A:123:LEU:CD2	1:A:184:TYR:CE1	2.15	1.30
1:B:123:LEU:CD2	1:B:184:TYR:CE1	2.15	1.29
1:B:71:SER:OG	1:B:92:ARG:NH1	1.70	1.24
1:A:71:SER:OG	1:A:92:ARG:NH1	1.70	1.23
1:A:123:LEU:CD2	1:A:184:TYR:CZ	2.23	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:HD21	1:A:184:TYR:CE1	1.76	1.20
1:B:123:LEU:CD2	1:B:184:TYR:CZ	2.23	1.20
1:B:221:THR:HG22	1:B:410:ASN:ND2	1.60	1.17
1:A:221:THR:HG22	1:A:410:ASN:ND2	1.60	1.16
1:B:55:TRP:O	1:B:56:ILE:HD13	1.46	1.15
1:B:123:LEU:HD21	1:B:184:TYR:CE1	1.77	1.15
1:B:123:LEU:HD21	1:B:184:TYR:CD1	1.82	1.14
1:A:55:TRP:O	1:A:56:ILE:HD13	1.46	1.13
1:A:123:LEU:HD21	1:A:184:TYR:CD1	1.82	1.13
1:A:127:ASN:O	1:A:184:TYR:CE1	2.03	1.12
1:B:127:ASN:O	1:B:184:TYR:CE1	2.03	1.11
1:A:72:LYS:HG3	1:A:95:ARG:NE	1.62	1.11
1:B:174:PHE:CE2	1:B:187:VAL:HG11	1.87	1.10
1:B:222:ALA:N	1:B:410:ASN:ND2	1.98	1.10
1:A:174:PHE:CE2	1:A:187:VAL:CG1	2.33	1.10
1:B:174:PHE:CE2	1:B:187:VAL:CG1	2.33	1.10
1:A:222:ALA:N	1:A:410:ASN:ND2	1.98	1.10
1:A:174:PHE:CE2	1:A:187:VAL:HG11	1.87	1.09
1:B:127:ASN:O	1:B:184:TYR:HE1	1.31	1.09
1:A:127:ASN:O	1:A:184:TYR:HE1	1.31	1.08
1:B:72:LYS:HG3	1:B:95:ARG:NE	1.62	1.07
1:A:123:LEU:HD23	1:A:184:TYR:CE1	1.85	1.06
1:B:123:LEU:HD23	1:B:184:TYR:CE1	1.85	1.05
1:B:203:ASP:OD1	1:B:206:LEU:HB2	1.62	0.99
1:B:222:ALA:H	1:B:410:ASN:HD22	0.99	0.98
1:A:203:ASP:OD1	1:A:206:LEU:HB2	1.62	0.98
1:B:174:PHE:HE2	1:B:187:VAL:CG1	1.78	0.96
1:A:94:PHE:CE2	1:A:98:PHE:CG	2.54	0.95
1:B:94:PHE:CE2	1:B:98:PHE:CG	2.54	0.95
1:A:174:PHE:HE2	1:A:187:VAL:CG1	1.78	0.94
1:A:222:ALA:N	1:A:410:ASN:HD22	1.59	0.92
1:B:102:PHE:HD1	1:B:170:LEU:HD11	1.35	0.91
1:A:102:PHE:HD1	1:A:170:LEU:HD11	1.35	0.91
1:B:222:ALA:N	1:B:410:ASN:HD22	1.59	0.90
1:B:129:LEU:HD21	1:B:142:ASN:OD1	1.72	0.90
1:A:79:GLN:HB3	1:A:89:MET:HE3	1.55	0.89
1:A:221:THR:CG2	1:A:410:ASN:ND2	2.36	0.88
1:B:221:THR:CG2	1:B:410:ASN:ND2	2.36	0.88
1:A:222:ALA:H	1:A:410:ASN:HD22	0.99	0.88
1:A:129:LEU:HD21	1:A:142:ASN:OD1	1.72	0.88
1:B:79:GLN:HB3	1:B:89:MET:HE3	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:CD2	1:A:184:TYR:CD1	2.49	0.87
1:B:203:ASP:OD1	1:B:206:LEU:CB	2.22	0.87
1:A:203:ASP:OD1	1:A:206:LEU:CB	2.22	0.86
3:E:4:ARG:HG3	3:E:4:ARG:HH11	1.41	0.86
2:D:119:LYS:NZ	1:B:381:ASP:OD2	2.08	0.85
1:B:94:PHE:CD2	1:B:98:PHE:HB2	2.12	0.85
1:A:381:ASP:OD2	2:C:119:LYS:NZ	2.09	0.85
1:A:94:PHE:CD2	1:A:98:PHE:HB2	2.12	0.85
1:B:123:LEU:CD2	1:B:184:TYR:CD1	2.49	0.84
1:A:94:PHE:HE2	1:A:98:PHE:CG	1.95	0.84
1:B:94:PHE:HE2	1:B:98:PHE:CG	1.94	0.84
2:D:84:VAL:O	2:D:90:ASN:ND2	2.10	0.84
1:B:294:MET:SD	1:B:399:SER:OG	2.36	0.84
1:A:100:TYR:HB2	1:A:172:MET:HB3	1.60	0.84
1:A:116:TYR:HB3	1:A:188:ASN:HD21	1.43	0.84
2:C:84:VAL:O	2:C:90:ASN:ND2	2.10	0.84
1:A:294:MET:SD	1:A:399:SER:OG	2.36	0.83
1:B:100:TYR:HB2	1:B:172:MET:HB3	1.60	0.83
1:B:71:SER:CB	1:B:92:ARG:HH11	1.92	0.82
1:A:71:SER:CB	1:A:92:ARG:HH11	1.91	0.82
1:B:116:TYR:HB3	1:B:188:ASN:HD21	1.43	0.82
1:B:174:PHE:CZ	1:B:187:VAL:HG11	2.15	0.82
1:A:123:LEU:CD2	1:A:184:TYR:CE2	2.63	0.81
1:A:174:PHE:CZ	1:A:187:VAL:HG11	2.15	0.81
1:B:222:ALA:H	1:B:410:ASN:HD21	1.25	0.81
1:B:123:LEU:CD2	1:B:184:TYR:CE2	2.63	0.81
1:B:412:SER:OG	1:B:413:ASP:N	2.14	0.81
1:B:102:PHE:CD1	1:B:170:LEU:HD11	2.18	0.79
1:B:116:TYR:HB3	1:B:188:ASN:ND2	1.98	0.79
1:A:116:TYR:HB3	1:A:188:ASN:ND2	1.98	0.78
1:A:72:LYS:HG3	1:A:95:ARG:HE	1.45	0.78
1:B:72:LYS:HG3	1:B:95:ARG:HE	1.45	0.78
1:A:222:ALA:H	1:A:410:ASN:HD21	1.25	0.77
1:A:85:GLU:HA	1:A:89:MET:HG2	1.65	0.77
1:B:85:GLU:HA	1:B:89:MET:HG2	1.65	0.77
1:A:102:PHE:CD1	1:A:170:LEU:HD11	2.18	0.77
1:A:412:SER:OG	1:A:413:ASP:N	2.14	0.77
1:A:94:PHE:CD2	1:A:98:PHE:CB	2.68	0.76
1:A:104:VAL:O	1:A:168:GLY:HA2	1.86	0.76
1:B:130:PHE:HA	1:B:177:GLU:HG2	1.68	0.76
1:B:94:PHE:CD2	1:B:98:PHE:CB	2.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:PHE:CE2	1:A:187:VAL:HG13	2.20	0.75
1:B:174:PHE:CE2	1:B:187:VAL:HG13	2.20	0.75
1:B:104:VAL:O	1:B:168:GLY:HA2	1.86	0.75
1:A:130:PHE:HA	1:A:177:GLU:HG2	1.67	0.74
3:F:4:ARG:O	2:D:123:ASP:O	2.05	0.74
1:A:72:LYS:CG	1:A:95:ARG:NE	2.39	0.73
3:E:4:ARG:HG3	3:E:4:ARG:NH1	1.99	0.73
1:A:162:VAL:HG13	1:A:195:MET:HE1	1.71	0.72
1:B:72:LYS:CG	1:B:95:ARG:NE	2.39	0.71
1:A:221:THR:CG2	1:A:410:ASN:HD21	2.03	0.71
3:F:5:TYR:CD1	2:D:123:ASP:HA	2.25	0.71
1:A:299:GLN:HA	1:A:302:LEU:HD12	1.74	0.70
1:A:170:LEU:O	1:A:170:LEU:HD12	1.91	0.70
1:A:221:THR:HG22	1:A:410:ASN:HD21	1.57	0.70
1:B:162:VAL:HG13	1:B:195:MET:HE1	1.73	0.70
1:B:170:LEU:HD12	1:B:170:LEU:O	1.91	0.70
1:B:299:GLN:HA	1:B:302:LEU:HD12	1.74	0.70
2:C:86:ASN:OD1	3:E:7:SER:OG	2.01	0.70
2:C:123:ASP:O	3:E:4:ARG:O	2.11	0.69
1:A:123:LEU:HD22	1:A:184:TYR:CE2	2.29	0.68
1:B:123:LEU:HD22	1:B:184:TYR:CE2	2.29	0.68
1:A:54:ILE:O	1:A:54:ILE:HD12	1.93	0.68
1:A:77:LEU:CD1	1:A:77:LEU:H	2.07	0.68
1:B:221:THR:CG2	1:B:410:ASN:HD21	2.03	0.68
1:A:200:SER:OG	1:A:218:ASP:O	2.11	0.68
1:B:54:ILE:HD12	1:B:54:ILE:O	1.93	0.68
1:A:123:LEU:HD22	1:A:184:TYR:CD2	2.30	0.67
1:B:200:SER:OG	1:B:218:ASP:O	2.12	0.67
1:B:62:LYS:HE2	1:B:63:PHE:CZ	2.30	0.67
1:B:77:LEU:H	1:B:77:LEU:CD1	2.07	0.67
1:B:123:LEU:HD22	1:B:184:TYR:CD2	2.30	0.67
1:A:85:GLU:HG3	1:A:89:MET:HB2	1.75	0.66
1:B:59:VAL:HG13	1:B:60:LYS:N	2.10	0.66
1:A:62:LYS:HE2	1:A:63:PHE:CZ	2.30	0.66
1:B:94:PHE:CE2	1:B:98:PHE:CD2	2.83	0.66
1:B:94:PHE:HE2	1:B:98:PHE:CD2	2.12	0.66
2:C:120:GLU:CD	2:C:120:GLU:H	1.99	0.66
1:A:94:PHE:HE2	1:A:98:PHE:CD2	2.13	0.66
1:A:59:VAL:HG13	1:A:60:LYS:N	2.10	0.65
1:B:55:TRP:C	1:B:56:ILE:HD13	2.15	0.65
1:B:85:GLU:HG3	1:B:89:MET:HB2	1.75	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:TRP:C	1:A:56:ILE:HD13	2.15	0.65
2:C:117:GLU:OE2	2:C:123:ASP:HB2	1.97	0.64
1:A:94:PHE:CE2	1:A:98:PHE:CD2	2.83	0.64
2:D:120:GLU:N	2:D:120:GLU:OE1	2.21	0.64
2:D:117:GLU:OE2	2:D:123:ASP:HB2	1.97	0.64
2:D:114:MET:HE2	1:B:303:ASN:HB2	1.80	0.64
2:D:120:GLU:H	2:D:120:GLU:CD	1.99	0.64
2:C:120:GLU:N	2:C:120:GLU:OE1	2.21	0.63
1:A:123:LEU:HD23	1:A:184:TYR:CE2	2.25	0.63
1:B:224:GLU:OE1	1:B:408:LYS:HE3	1.99	0.63
1:A:224:GLU:OE1	1:A:408:LYS:HE3	1.99	0.62
1:B:265:THR:HG22	1:B:290:THR:HG22	1.82	0.62
1:A:176:PRO:HB3	1:A:184:TYR:HA	1.82	0.61
1:A:303:ASN:HB2	2:C:114:MET:HE2	1.81	0.61
1:B:176:PRO:HB3	1:B:184:TYR:HA	1.82	0.61
1:B:159:LYS:NZ	1:B:224:GLU:OE2	2.20	0.61
2:C:54:THR:HA	2:C:57:THR:OG1	2.01	0.61
1:B:209:VAL:HG12	1:B:370:VAL:HG12	1.82	0.61
1:A:94:PHE:CD2	1:A:98:PHE:CG	2.88	0.61
3:E:4:ARG:HH11	3:E:4:ARG:CG	2.14	0.61
2:D:54:THR:HA	2:D:57:THR:OG1	2.01	0.60
1:A:94:PHE:HD2	1:A:98:PHE:HB2	1.66	0.60
1:A:209:VAL:HG12	1:A:370:VAL:HG12	1.82	0.60
1:B:205:THR:HG23	1:B:205:THR:O	2.01	0.60
1:A:127:ASN:O	1:A:184:TYR:CD1	2.55	0.60
1:B:94:PHE:CD2	1:B:98:PHE:CG	2.88	0.60
1:A:265:THR:HG22	1:A:290:THR:HG22	1.82	0.60
1:B:94:PHE:HD2	1:B:98:PHE:HB2	1.66	0.60
1:B:127:ASN:O	1:B:184:TYR:CD1	2.55	0.59
1:A:187:VAL:O	1:A:187:VAL:HG23	2.02	0.59
2:C:124:CYS:SG	3:E:6:ILE:HG13	2.42	0.59
1:A:100:TYR:N	1:A:172:MET:O	2.27	0.59
1:B:236:ILE:HB	1:B:248:TRP:HB2	1.85	0.59
1:A:159:LYS:NZ	1:A:224:GLU:OE2	2.20	0.59
1:B:102:PHE:H	1:B:170:LEU:CD1	2.16	0.59
1:A:102:PHE:N	1:A:170:LEU:HD11	2.18	0.58
1:A:205:THR:O	1:A:205:THR:HG23	2.01	0.58
1:B:94:PHE:CE2	1:B:98:PHE:CB	2.87	0.58
1:A:112:ARG:HD3	1:A:160:GLU:HG3	1.85	0.58
1:A:94:PHE:CE2	1:A:98:PHE:CB	2.87	0.58
1:A:123:LEU:CD2	1:A:184:TYR:CG	2.87	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:PHE:N	1:B:170:LEU:HD11	2.18	0.58
1:A:102:PHE:H	1:A:170:LEU:CD1	2.16	0.57
1:B:123:LEU:CD2	1:B:184:TYR:CG	2.87	0.57
1:B:187:VAL:HG23	1:B:187:VAL:O	2.02	0.57
2:D:110:ILE:O	2:D:114:MET:HG2	2.04	0.57
1:A:236:ILE:HB	1:A:248:TRP:HB2	1.85	0.57
1:B:142:ASN:OD1	5:B:1004:NAG:O5	2.23	0.57
1:B:222:ALA:N	1:B:410:ASN:HD21	1.90	0.57
1:B:112:ARG:HD3	1:B:160:GLU:HG3	1.85	0.57
2:C:110:ILE:O	2:C:114:MET:HG2	2.04	0.57
1:A:209:VAL:HG12	1:A:370:VAL:CG1	2.35	0.57
1:B:71:SER:CB	1:B:92:ARG:NH1	2.56	0.57
1:A:206:LEU:HD23	1:A:206:LEU:C	2.26	0.56
1:B:62:LYS:HE2	1:B:63:PHE:CE1	2.41	0.56
1:B:206:LEU:C	1:B:206:LEU:HD23	2.26	0.56
1:A:80:ASP:HB3	1:A:83:VAL:HG23	1.87	0.56
1:B:209:VAL:HG12	1:B:370:VAL:CG1	2.35	0.56
1:A:142:ASN:OD1	5:A:1004:NAG:O5	2.23	0.56
1:A:71:SER:CB	1:A:92:ARG:NH1	2.56	0.56
1:A:221:THR:CA	1:A:410:ASN:HD21	2.19	0.55
1:B:115:PHE:HE1	1:B:187:VAL:HG12	1.71	0.55
1:B:221:THR:CA	1:B:410:ASN:HD21	2.20	0.55
1:A:130:PHE:HE1	1:A:132:VAL:HG23	1.72	0.55
1:B:80:ASP:HB3	1:B:83:VAL:HG23	1.87	0.55
3:F:6:ILE:HG13	2:D:124:CYS:SG	2.46	0.55
1:B:130:PHE:HE1	1:B:132:VAL:HG23	1.71	0.55
1:A:144:SER:O	1:A:148:THR:HG23	2.07	0.55
1:B:203:ASP:OD1	1:B:206:LEU:HB3	2.05	0.55
2:C:64:ASN:O	2:C:66:PRO:HD3	2.07	0.55
1:B:129:LEU:HD11	5:B:1004:NAG:O6	2.07	0.54
1:A:129:LEU:HD11	5:A:1004:NAG:O6	2.07	0.54
1:B:96:SER:HB2	1:B:97:PRO:CD	2.37	0.54
1:A:62:LYS:HE2	1:A:63:PHE:CE1	2.41	0.54
1:B:144:SER:O	1:B:148:THR:HG23	2.07	0.54
2:C:123:ASP:HA	3:E:5:TYR:CD1	2.42	0.54
1:A:115:PHE:HE1	1:A:187:VAL:HG12	1.71	0.54
1:A:108:ARG:HB3	1:A:195:MET:HE3	1.90	0.54
1:B:100:TYR:N	1:B:172:MET:O	2.27	0.54
1:A:51:ASP:OD2	1:A:237:SER:HB2	2.08	0.54
1:A:222:ALA:N	1:A:410:ASN:HD21	1.90	0.54
2:D:64:ASN:O	2:D:66:PRO:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:SER:HB2	1:A:97:PRO:CD	2.37	0.53
1:B:59:VAL:O	1:B:60:LYS:HD3	2.08	0.53
2:D:104:GLY:HA3	2:D:106:TYR:CE2	2.44	0.53
1:A:77:LEU:HD12	1:A:77:LEU:N	2.23	0.53
1:A:203:ASP:OD1	1:A:206:LEU:HB3	2.05	0.53
1:A:279:PRO:HB3	1:A:281:TYR:CE2	2.44	0.53
1:B:77:LEU:N	1:B:77:LEU:HD12	2.23	0.53
1:A:179:ALA:HB3	1:A:180:PRO:HD3	1.91	0.53
1:A:59:VAL:O	1:A:60:LYS:HD3	2.08	0.53
1:B:77:LEU:N	1:B:77:LEU:CD1	2.72	0.53
1:B:51:ASP:OD2	1:B:237:SER:HB2	2.08	0.53
1:B:96:SER:HB2	1:B:97:PRO:HD2	1.90	0.53
1:A:77:LEU:CD1	1:A:77:LEU:N	2.72	0.53
1:A:96:SER:HB2	1:A:97:PRO:HD2	1.90	0.53
2:C:104:GLY:HA3	2:C:106:TYR:CE2	2.43	0.53
1:B:143:PHE:HE1	1:B:148:THR:HG21	1.74	0.53
1:B:179:ALA:HB3	1:B:180:PRO:HD3	1.91	0.52
1:B:279:PRO:HB3	1:B:281:TYR:CE2	2.43	0.52
1:B:108:ARG:HB3	1:B:195:MET:HE3	1.92	0.52
1:A:326:GLU:OE2	1:A:337:ARG:NH2	2.31	0.52
4:H:1:NAG:O4	4:H:2:NAG:O7	2.28	0.52
1:A:77:LEU:H	1:A:77:LEU:HD12	1.75	0.51
1:B:326:GLU:OE2	1:B:337:ARG:NH2	2.31	0.51
1:A:415:ASN:ND2	1:A:417:ALA:O	2.41	0.51
1:A:143:PHE:HE1	1:A:148:THR:HG21	1.74	0.51
1:A:300:ILE:HG23	2:C:114:MET:HE3	1.92	0.51
1:A:180:PRO:HB2	1:A:182:ASN:OD1	2.10	0.51
1:A:219:ASN:N	1:A:219:ASN:OD1	2.42	0.51
4:I:1:NAG:O4	4:I:2:NAG:O7	2.28	0.51
1:B:180:PRO:HB2	1:B:182:ASN:OD1	2.10	0.51
1:A:103:PRO:HA	1:A:168:GLY:O	2.10	0.51
1:B:59:VAL:CG1	1:B:60:LYS:N	2.74	0.51
1:B:123:LEU:HD23	1:B:184:TYR:OH	2.05	0.51
1:B:227:TYR:CE2	1:B:310:PHE:HB3	2.46	0.51
1:A:138:THR:HG23	1:A:415:ASN:HA	1.93	0.51
1:A:294:MET:SD	1:A:388:PRO:HD3	2.51	0.50
1:B:86:VAL:HG13	1:B:86:VAL:O	2.11	0.50
1:B:219:ASN:N	1:B:219:ASN:OD1	2.42	0.50
1:B:294:MET:SD	1:B:388:PRO:HD3	2.51	0.50
1:A:59:VAL:CG1	1:A:60:LYS:N	2.73	0.50
1:B:103:PRO:HA	1:B:168:GLY:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:CD2	1:A:184:TYR:CD2	2.91	0.50
1:B:138:THR:HG23	1:B:415:ASN:HA	1.93	0.50
2:C:122:LEU:O	3:E:5:TYR:HA	2.12	0.50
1:A:130:PHE:C	1:A:130:PHE:CD1	2.86	0.50
3:F:5:TYR:HA	2:D:122:LEU:O	2.11	0.50
1:A:112:ARG:HA	1:A:159:LYS:O	2.12	0.50
1:A:38:LEU:C	1:A:38:LEU:HD23	2.32	0.50
1:A:86:VAL:O	1:A:86:VAL:HG13	2.11	0.50
1:B:38:LEU:HD23	1:B:38:LEU:C	2.32	0.50
1:B:130:PHE:CD1	1:B:130:PHE:C	2.86	0.49
1:A:227:TYR:CE2	1:A:310:PHE:HB3	2.46	0.49
1:A:143:PHE:CE1	1:A:148:THR:HG21	2.48	0.49
1:A:40:CYS:HA	1:A:58:ASP:CG	2.32	0.49
1:A:94:PHE:CE2	1:A:98:PHE:CD1	3.00	0.49
1:B:229:LEU:HD11	1:B:310:PHE:HE1	1.77	0.49
1:B:112:ARG:HA	1:B:159:LYS:O	2.12	0.49
1:B:317:THR:OG1	1:B:409:MET:CE	2.60	0.49
1:A:229:LEU:HD11	1:A:310:PHE:HE1	1.77	0.49
1:A:191:GLU:OE1	1:A:193:THR:OG1	2.30	0.49
1:A:229:LEU:HD11	1:A:310:PHE:CE1	2.47	0.49
3:F:5:TYR:O	2:D:86:ASN:ND2	2.43	0.49
1:B:123:LEU:CD2	1:B:184:TYR:CD2	2.91	0.49
1:B:170:LEU:C	1:B:170:LEU:HD12	2.33	0.49
1:B:91:ALA:HB2	1:B:188:ASN:OD1	2.13	0.49
1:A:142:ASN:O	1:A:420:ASN:ND2	2.36	0.49
1:A:71:SER:HB2	1:A:92:ARG:HG3	1.95	0.49
1:B:40:CYS:HA	1:B:58:ASP:CG	2.32	0.49
1:A:317:THR:OG1	1:A:409:MET:CE	2.60	0.49
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.68	0.48
1:B:148:THR:O	1:B:152:LEU:HG	2.13	0.48
1:B:229:LEU:HD11	1:B:310:PHE:CE1	2.47	0.48
1:B:143:PHE:CE1	1:B:148:THR:HG21	2.48	0.48
1:B:71:SER:HB2	1:B:92:ARG:HG3	1.95	0.48
1:B:94:PHE:CE2	1:B:98:PHE:CD1	3.00	0.48
1:A:91:ALA:HB2	1:A:188:ASN:OD1	2.13	0.48
1:A:170:LEU:C	1:A:170:LEU:HD12	2.33	0.48
1:B:102:PHE:HD1	1:B:170:LEU:CD1	2.18	0.48
1:A:148:THR:O	1:A:152:LEU:HG	2.13	0.48
1:B:123:LEU:HD22	1:B:184:TYR:CG	2.49	0.48
1:B:80:ASP:HB3	1:B:83:VAL:CG2	2.44	0.47
1:B:77:LEU:H	1:B:77:LEU:HD12	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ILE:O	1:B:359:SER:N	2.33	0.47
1:A:85:GLU:HG3	1:A:89:MET:CB	2.43	0.47
1:A:216:THR:HG21	1:A:370:VAL:HG21	1.97	0.47
1:B:54:ILE:HD12	1:B:54:ILE:C	2.35	0.47
1:B:86:VAL:HA	1:B:87:PRO:HA	1.62	0.47
2:C:51:LYS:HE3	2:C:81:PHE:CZ	2.49	0.47
2:D:51:LYS:HE3	2:D:81:PHE:CZ	2.49	0.47
1:B:255:ILE:HG13	1:B:260:LEU:HD23	1.96	0.47
1:B:102:PHE:HB2	1:B:170:LEU:HD21	1.97	0.47
1:B:108:ARG:HB3	1:B:195:MET:CE	2.44	0.47
2:D:48:PHE:HA	2:D:51:LYS:HG3	1.97	0.47
1:B:216:THR:HG21	1:B:370:VAL:HG21	1.97	0.47
1:A:255:ILE:HG13	1:A:260:LEU:HD23	1.96	0.47
1:A:71:SER:HG	1:A:92:ARG:NH1	2.00	0.47
2:D:44:CYS:SG	2:D:45:LYS:N	2.88	0.47
1:A:54:ILE:C	1:A:54:ILE:HD12	2.34	0.46
2:C:48:PHE:HA	2:C:51:LYS:HG3	1.97	0.46
1:A:294:MET:CG	1:A:399:SER:OG	2.64	0.46
1:A:123:LEU:HD23	1:A:184:TYR:OH	2.05	0.46
1:A:58:ASP:OD1	1:A:58:ASP:N	2.31	0.46
1:A:80:ASP:HB3	1:A:83:VAL:CG2	2.45	0.46
1:B:76:ALA:N	1:B:89:MET:O	2.48	0.46
1:B:191:GLU:OE1	1:B:193:THR:OG1	2.30	0.46
1:A:94:PHE:HE2	1:A:98:PHE:CD1	2.32	0.46
1:B:294:MET:CG	1:B:399:SER:OG	2.64	0.46
1:B:273:LYS:O	1:B:364:PRO:HD2	2.16	0.46
2:D:96:MET:O	2:D:100:ILE:HG13	2.16	0.46
1:A:273:LYS:O	1:A:364:PRO:HD2	2.16	0.46
2:C:96:MET:O	2:C:100:ILE:HG13	2.16	0.46
1:A:108:ARG:HB3	1:A:195:MET:CE	2.44	0.46
2:C:44:CYS:SG	2:C:45:LYS:N	2.88	0.46
1:A:102:PHE:HB2	1:A:170:LEU:HD21	1.97	0.46
1:B:283:ALA:HB3	1:B:288:TYR:CE2	2.51	0.46
1:B:94:PHE:HE2	1:B:98:PHE:CD1	2.32	0.46
1:A:51:ASP:O	1:A:53:ARG:HG3	2.16	0.46
1:B:51:ASP:O	1:B:53:ARG:HG3	2.16	0.46
1:A:58:ASP:O	1:A:64:LEU:HD11	2.16	0.45
1:A:283:ALA:HB3	1:A:288:TYR:CE2	2.51	0.45
1:B:100:TYR:CB	1:B:172:MET:HB3	2.39	0.45
1:A:221:THR:HA	1:A:410:ASN:HD21	1.82	0.45
1:A:264:GLU:OE1	1:A:293:SER:OG	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ILE:HG12	1:A:386:LEU:HD22	1.99	0.45
1:A:123:LEU:HD22	1:A:184:TYR:CG	2.49	0.45
1:A:170:LEU:C	1:A:170:LEU:CD1	2.85	0.45
2:C:112:ALA:HB2	3:E:14:ASN:HB3	1.98	0.45
2:D:79:CYS:HB3	2:D:124:CYS:HB3	1.86	0.45
1:A:148:THR:HG22	1:A:421:PRO:HD2	1.98	0.45
1:A:393:LYS:HG3	1:A:393:LYS:O	2.17	0.45
1:A:100:TYR:CB	1:A:172:MET:HB3	2.39	0.45
1:B:129:LEU:CD1	5:B:1004:NAG:O6	2.65	0.45
3:E:8:TYR:O	3:E:12:ARG:HG3	2.17	0.45
1:A:149:ALA:HB2	1:A:157:ILE:HD11	1.98	0.45
1:B:170:LEU:C	1:B:170:LEU:CD1	2.85	0.45
2:C:86:ASN:ND2	3:E:5:TYR:O	2.44	0.45
1:A:129:LEU:CD1	5:A:1004:NAG:O6	2.65	0.45
1:A:130:PHE:CD2	1:A:185:ALA:HA	2.52	0.45
3:F:8:TYR:O	3:F:12:ARG:HG3	2.17	0.45
1:B:30:TYR:CE1	1:B:196:PRO:HG3	2.52	0.45
1:B:393:LYS:HG3	1:B:393:LYS:O	2.17	0.45
1:B:250:ASP:OD1	1:B:251:ASP:N	2.50	0.44
1:B:222:ALA:CA	1:B:410:ASN:HD22	2.29	0.44
1:B:58:ASP:O	1:B:64:LEU:HD11	2.16	0.44
1:A:250:ASP:OD1	1:A:251:ASP:N	2.50	0.44
1:A:273:LYS:HB2	1:A:273:LYS:HE2	1.88	0.44
1:A:76:ALA:N	1:A:89:MET:O	2.48	0.44
2:D:114:MET:CE	1:B:303:ASN:HB2	2.46	0.44
1:B:221:THR:HA	1:B:410:ASN:HD21	1.82	0.44
1:B:415:ASN:ND2	1:B:417:ALA:O	2.41	0.44
1:B:341:ILE:HG12	1:B:386:LEU:HD22	1.99	0.44
1:A:102:PHE:HD1	1:A:170:LEU:CD1	2.18	0.44
1:A:130:PHE:HD1	1:A:131:SER:N	2.16	0.44
1:B:149:ALA:HB2	1:B:157:ILE:HD11	1.98	0.44
1:A:30:TYR:CE1	1:A:196:PRO:HG3	2.52	0.44
1:A:415:ASN:CG	1:A:417:ALA:H	2.21	0.44
1:B:29:ASP:HB3	1:B:30:TYR:H	1.69	0.44
2:D:79:CYS:N	2:D:80:PRO:HD2	2.33	0.44
1:B:313:ASP:OD2	1:B:408:LYS:NZ	2.32	0.44
1:B:148:THR:HG22	1:B:421:PRO:HD2	1.98	0.44
1:B:130:PHE:CD2	1:B:185:ALA:HA	2.52	0.44
1:B:85:GLU:HG3	1:B:89:MET:CB	2.44	0.44
1:B:130:PHE:HD1	1:B:131:SER:N	2.16	0.43
1:B:37:LEU:HD23	1:B:37:LEU:HA	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ASN:CG	1:B:417:ALA:H	2.21	0.43
2:D:114:MET:HE3	1:B:300:ILE:HG23	2.00	0.43
1:A:151:ALA:HB2	1:A:423:PRO:HG3	2.00	0.43
1:B:311:SER:HA	1:B:380:GLN:O	2.18	0.43
1:A:198:MET:HE1	1:A:244:LEU:CD1	2.48	0.43
1:A:311:SER:HA	1:A:380:GLN:O	2.18	0.43
1:B:336:GLN:HG2	1:B:395:GLU:OE1	2.19	0.43
1:B:79:GLN:HA	1:B:89:MET:HE1	2.00	0.43
1:A:130:PHE:HE1	1:A:132:VAL:CG2	2.31	0.43
2:C:60:CYS:CB	2:C:70:CYS:HG	2.25	0.43
1:A:112:ARG:HG2	1:A:160:GLU:HG3	2.01	0.43
2:C:79:CYS:N	2:C:80:PRO:HD2	2.33	0.42
1:B:284:PRO:HG2	1:B:287:VAL:HG23	2.02	0.42
1:A:29:ASP:HB3	1:A:30:TYR:H	1.69	0.42
1:A:336:GLN:HG2	1:A:395:GLU:OE1	2.19	0.42
1:B:112:ARG:HG2	1:B:160:GLU:HG3	2.01	0.42
1:A:312:ILE:HD13	1:A:382:LEU:HB2	2.01	0.42
1:B:130:PHE:HE1	1:B:132:VAL:CG2	2.31	0.42
1:B:151:ALA:HB2	1:B:423:PRO:HG3	2.00	0.41
1:B:312:ILE:HD13	1:B:382:LEU:HB2	2.01	0.41
1:A:284:PRO:HG2	1:A:287:VAL:HG23	2.02	0.41
2:C:75:LYS:O	2:C:79:CYS:SG	2.78	0.41
2:C:60:CYS:SG	2:C:70:CYS:CB	3.08	0.41
1:A:58:ASP:O	1:A:64:LEU:HG	2.20	0.41
1:B:99:THR:HA	1:B:173:THR:HA	2.02	0.41
1:B:198:MET:HE1	1:B:244:LEU:CD1	2.49	0.41
1:A:99:THR:HA	1:A:173:THR:HA	2.02	0.41
1:B:228:ARG:NH1	1:B:246:ARG:HD2	2.36	0.41
2:D:75:LYS:O	2:D:79:CYS:SG	2.79	0.41
1:A:79:GLN:HA	1:A:89:MET:HE1	2.02	0.41
1:B:207:THR:O	1:B:216:THR:N	2.54	0.41
1:A:207:THR:O	1:A:216:THR:N	2.54	0.41
1:A:228:ARG:NH1	1:A:246:ARG:HD2	2.36	0.41
1:B:102:PHE:N	1:B:170:LEU:CD1	2.80	0.41
1:B:59:VAL:HG13	1:B:60:LYS:HG2	2.03	0.41
1:B:58:ASP:O	1:B:64:LEU:HG	2.20	0.41
1:A:102:PHE:H	1:A:170:LEU:HD12	1.86	0.41
1:B:285:VAL:O	1:B:289:SER:OG	2.30	0.41
2:D:60:CYS:SG	2:D:70:CYS:CB	3.08	0.41
1:A:59:VAL:HG13	1:A:60:LYS:HG2	2.03	0.40
1:A:58:ASP:O	1:A:64:LEU:CD1	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:42:THR:O	2:C:91:ASP:HB2	2.21	0.40
2:D:42:THR:O	2:D:91:ASP:HB2	2.21	0.40
1:B:83:VAL:HA	1:B:84:PRO:HD2	1.93	0.40
2:C:102:LEU:HD13	2:D:99:TYR:CE1	2.56	0.40
1:A:219:ASN:O	1:A:220:SER:C	2.60	0.40
1:A:320:VAL:HG22	1:A:406:ILE:HG12	2.03	0.40
1:A:355:ILE:O	1:A:359:SER:N	2.33	0.40
1:B:58:ASP:O	1:B:64:LEU:CD1	2.70	0.40
1:A:51:ASP:OD1	1:A:239:SER:OG	2.37	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	363/396 (92%)	348 (96%)	15 (4%)	0	100	100
1	B	363/396 (92%)	348 (96%)	15 (4%)	0	100	100
2	C	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	D	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
3	E	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
3	F	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
All	All	916/990 (92%)	874 (95%)	42 (5%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains [i](#)

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	329/344 (96%)	316 (96%)	13 (4%)	31	51
1	B	329/344 (96%)	316 (96%)	13 (4%)	31	51
2	C	72/72 (100%)	71 (99%)	1 (1%)	67	79
2	D	72/72 (100%)	71 (99%)	1 (1%)	67	79
3	E	13/13 (100%)	12 (92%)	1 (8%)	13	22
3	F	13/13 (100%)	13 (100%)	0	100	100
All	All	828/858 (96%)	799 (96%)	29 (4%)	36	56

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

Mol	Chain	Res	Type
1	A	70	ASP
1	A	73	THR
1	A	75	PRO
1	A	77	LEU
1	A	78	THR
1	A	79	GLN
1	A	84	PRO
1	A	129	LEU
1	A	170	LEU
1	A	201	SER
1	A	205	THR
1	A	208	MET
1	A	399	SER
2	C	87	ASP
3	E	4	ARG
2	D	87	ASP
1	B	70	ASP
1	B	73	THR
1	B	75	PRO
1	B	77	LEU
1	B	78	THR
1	B	79	GLN
1	B	84	PRO
1	B	129	LEU
1	B	170	LEU
1	B	201	SER
1	B	205	THR

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Mol	Chain	Res	Type
1	B	208	MET
1	B	399	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
1	A	305	ASN
1	A	387	HIS
1	A	410	ASN
1	B	188	ASN
1	B	305	ASN
1	B	387	HIS
1	B	410	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

8 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	G	1	4	14,14,15	0.35	0	17,19,21	0.60	0
4	NAG	G	2	4	14,14,15	0.49	0	17,19,21	1.18	1 (5%)
4	NAG	H	1	1,4	14,14,15	0.84	0	17,19,21	2.62	5 (29%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	H	2	4	14,14,15	1.00	0	17,19,21	1.96	5 (29%)
4	NAG	I	1	1,4	14,14,15	0.84	0	17,19,21	2.62	5 (29%)
4	NAG	I	2	4	14,14,15	1.00	0	17,19,21	1.95	5 (29%)
4	NAG	J	1	4	14,14,15	0.34	0	17,19,21	0.60	0
4	NAG	J	2	4	14,14,15	0.49	0	17,19,21	1.18	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
4	NAG	G	1	4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	3/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	3/6/23/26	0/1/1/1
4	NAG	J	1	4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	C4-C3-C2	-5.59	102.82	111.02
4	H	1	NAG	C4-C3-C2	-5.58	102.84	111.02
4	H	1	NAG	C1-O5-C5	5.46	119.59	112.19
4	I	1	NAG	C1-O5-C5	5.45	119.57	112.19
4	H	1	NAG	O4-C4-C5	5.00	121.72	109.30
4	I	1	NAG	O4-C4-C5	5.00	121.71	109.30
4	G	2	NAG	C1-O5-C5	3.92	117.50	112.19
4	J	2	NAG	C1-O5-C5	3.91	117.49	112.19
4	H	2	NAG	O5-C1-C2	-3.49	105.78	111.29
4	H	2	NAG	C4-C3-C2	-3.49	105.91	111.02
4	I	2	NAG	C4-C3-C2	-3.48	105.91	111.02
4	I	2	NAG	O5-C1-C2	-3.48	105.79	111.29
4	H	1	NAG	C3-C4-C5	-3.41	104.15	110.24
4	I	1	NAG	C3-C4-C5	-3.41	104.16	110.24
4	I	1	NAG	O4-C4-C3	3.25	117.87	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	O4-C4-C3	3.24	117.85	110.35
4	H	2	NAG	C3-C4-C5	-3.03	104.83	110.24
4	I	2	NAG	C3-C4-C5	-3.02	104.85	110.24
4	I	2	NAG	O6-C6-C5	-2.96	101.14	111.29
4	H	2	NAG	O6-C6-C5	-2.96	101.14	111.29
4	H	2	NAG	O4-C4-C3	-2.86	103.74	110.35
4	I	2	NAG	O4-C4-C3	-2.85	103.75	110.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

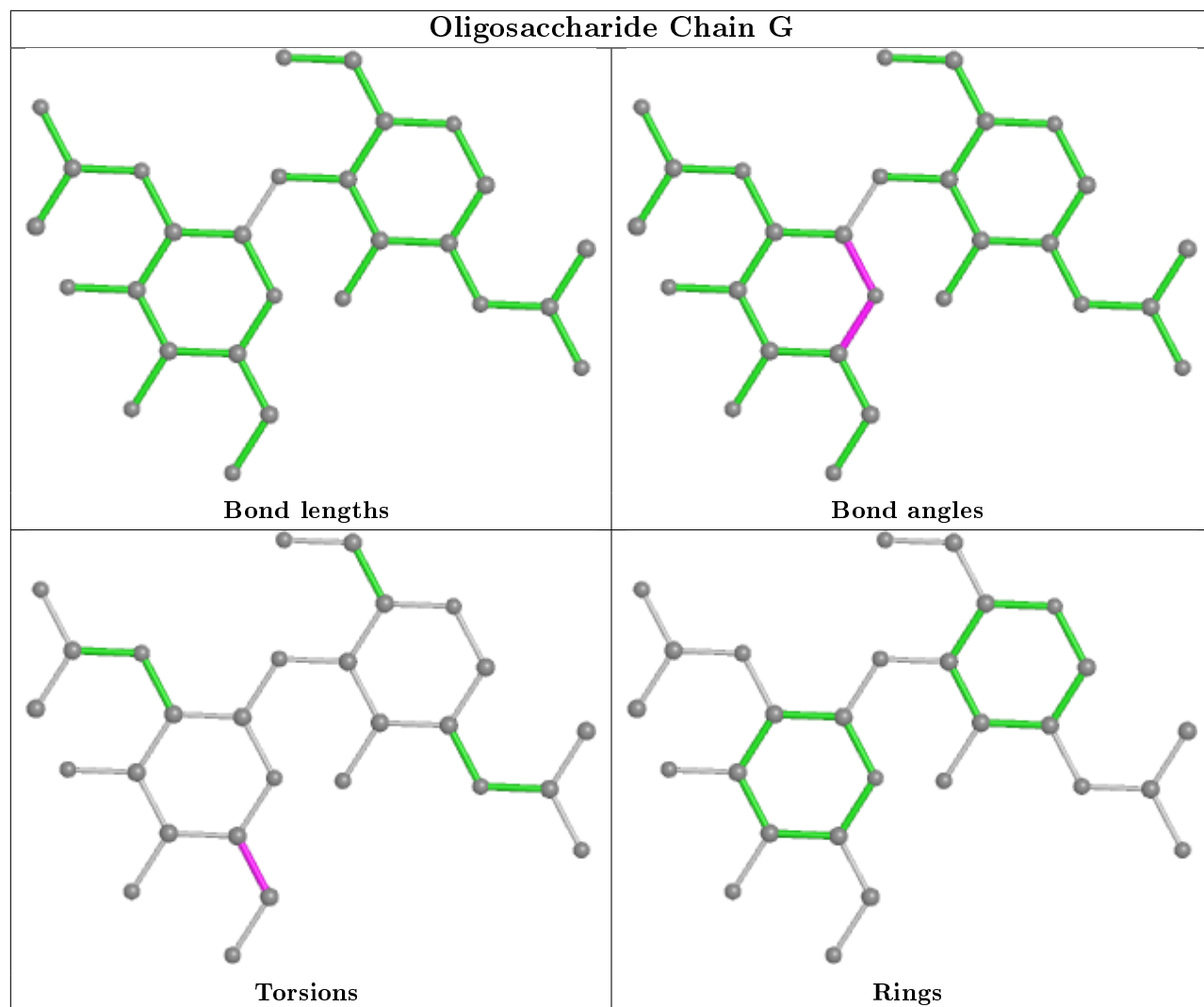
Mol	Chain	Res	Type	Atoms
4	J	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C3-C2-N2-C7
4	H	2	NAG	C3-C2-N2-C7

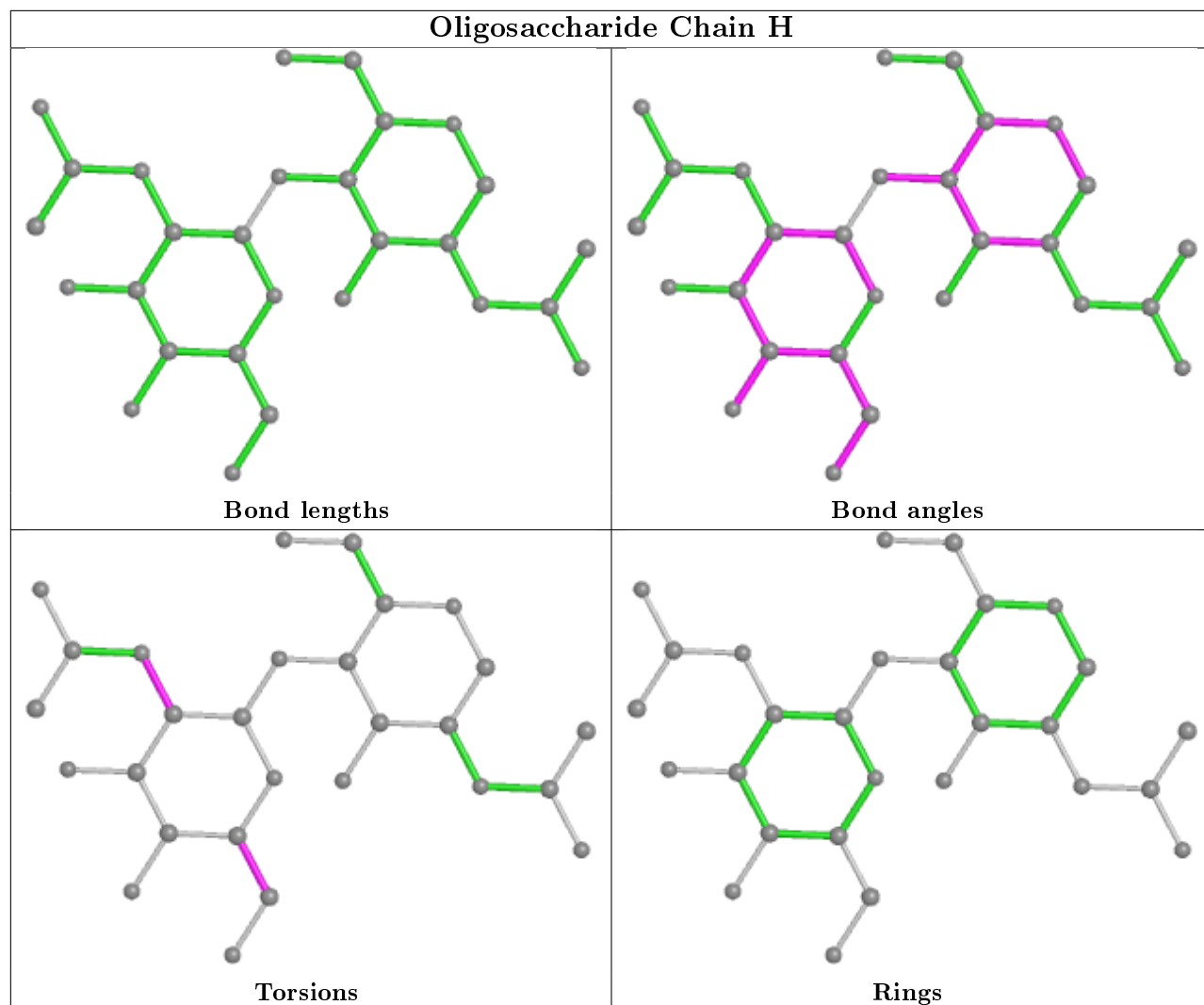
There are no ring outliers.

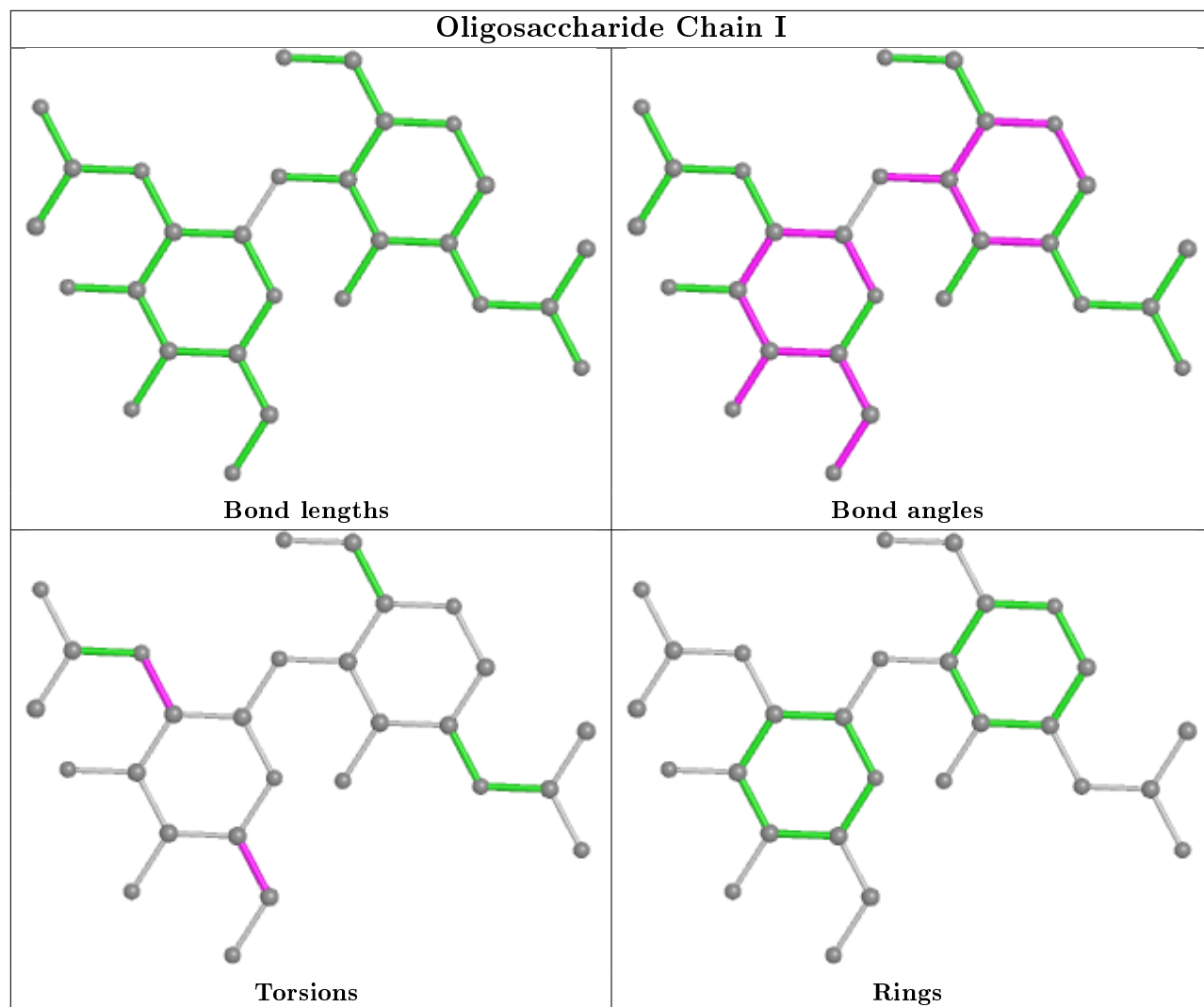
6 monomers are involved in 6 short contacts:

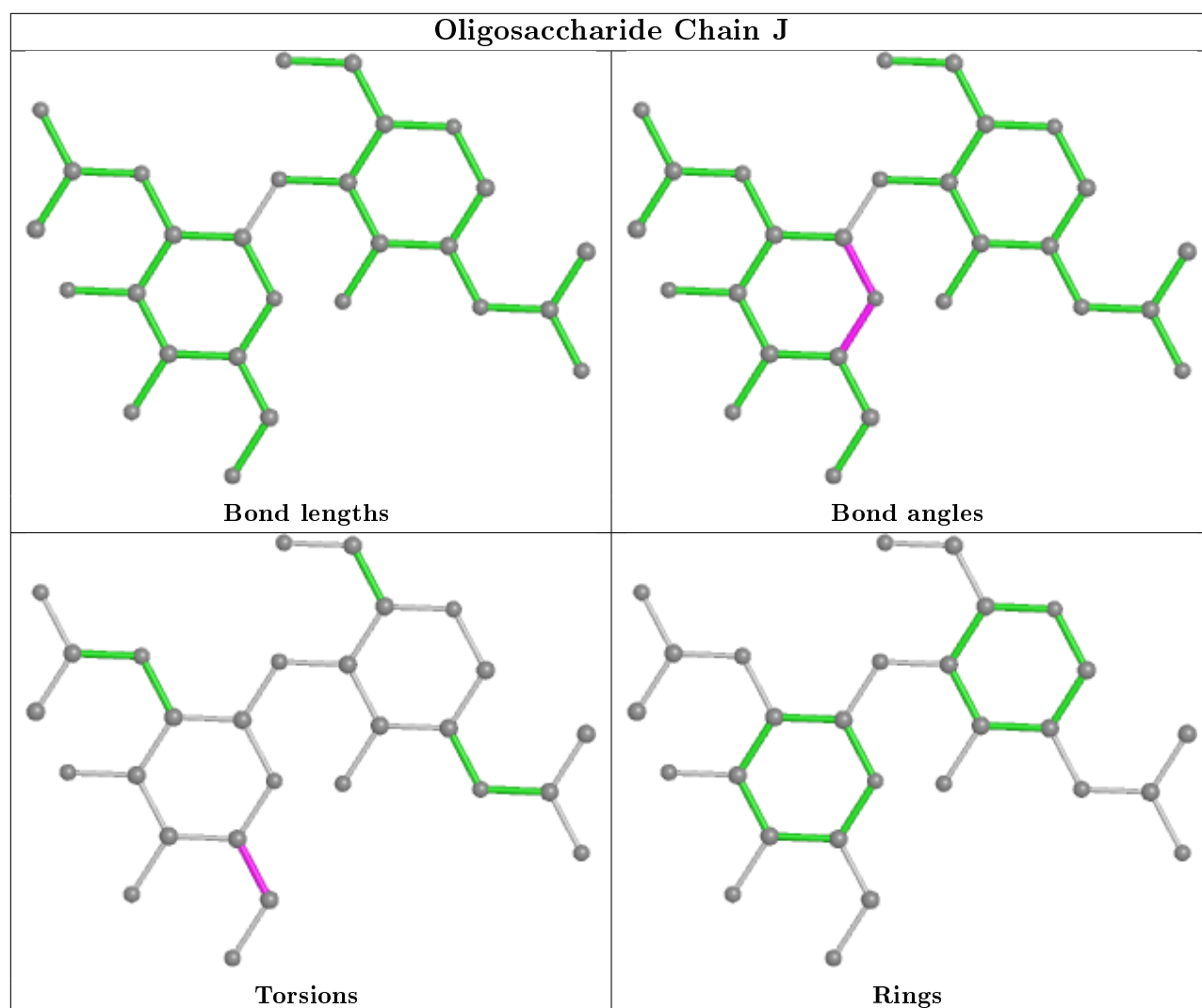
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	2	NAG	1	0
4	G	1	NAG	2	0
4	J	1	NAG	2	0
4	I	1	NAG	1	0
4	H	1	NAG	1	0
4	H	2	NAG	1	0

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](#)

4 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	$\# Z  > 2$
5	NAG	B	1004	1	14,14,15	0.40	0	17,19,21	1.17	2 (11%)
5	NAG	D	1001	2	14,14,15	0.50	0	17,19,21	0.63	1 (5%)
5	NAG	C	202	2	14,14,15	0.49	0	17,19,21	0.64	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	1004	1	14,14,15	0.41	0	17,19,21	1.17	2 (11%)

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	B	1004	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1001	2	-	2/6/23/26	0/1/1/1
5	NAG	C	202	2	-	2/6/23/26	0/1/1/1
5	NAG	A	1004	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1004	NAG	C8-C7-N2	2.34	120.06	116.10
5	A	1004	NAG	C8-C7-N2	2.32	120.03	116.10
5	C	202	NAG	C1-O5-C5	2.09	115.02	112.19
5	D	1001	NAG	C1-O5-C5	2.08	115.02	112.19
5	A	1004	NAG	C2-N2-C7	-2.03	120.01	122.90
5	B	1004	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1001	NAG	O5-C5-C6-O6
5	C	202	NAG	O5-C5-C6-O6
5	D	1001	NAG	C4-C5-C6-O6
5	C	202	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1004	NAG	3	0
5	A	1004	NAG	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	375/396 (94%)	0.44	31 (8%) 11 13	31, 69, 122, 147	0
1	B	375/396 (94%)	0.66	46 (12%) 4 4	31, 69, 122, 147	0
2	C	84/84 (100%)	0.04	0 100 100	30, 52, 92, 97	0
2	D	84/84 (100%)	0.05	0 100 100	30, 52, 92, 97	0
3	E	15/15 (100%)	0.14	0 100 100	44, 61, 100, 115	0
3	F	15/15 (100%)	0.00	0 100 100	44, 61, 100, 115	0
All	All	948/990 (95%)	0.44	77 (8%) 12 14	30, 64, 117, 147	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	SER	6.2
1	B	59	VAL	6.0
1	A	76	ALA	5.9
1	B	104	VAL	5.8
1	B	72	LYS	5.6
1	B	204	GLY	5.3
1	B	64	LEU	4.6
1	B	60	LYS	4.6
1	B	205	THR	4.4
1	B	50	THR	4.4
1	A	122	GLY	4.4
1	A	77	LEU	4.3
1	A	95	ARG	4.3
1	B	180	PRO	4.2
1	B	85	GLU	4.2
1	B	56	ILE	4.2
1	B	95	ARG	4.2
1	A	78	THR	4.1
1	A	127	ASN	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	423	PRO	3.9
1	B	122	GLY	3.6
1	B	179	ALA	3.6
1	A	104	VAL	3.6
1	B	75	PRO	3.5
1	B	61	SER	3.4
1	B	78	THR	3.4
1	A	116	TYR	3.4
1	A	423	PRO	3.4
1	A	56	ILE	3.3
1	B	102	PHE	3.3
1	A	64	LEU	3.3
1	A	150	GLU	3.2
1	B	81	PRO	3.2
1	A	79	GLN	3.1
1	B	79	GLN	3.1
1	A	124	ASN	3.0
1	A	71	SER	3.0
1	B	80	ASP	3.0
1	B	150	GLU	3.0
1	B	58	ASP	2.9
1	A	126	THR	2.9
1	A	59	VAL	2.9
1	B	36	ILE	2.8
1	A	169	THR	2.8
1	B	76	ALA	2.8
1	B	239	SER	2.8
1	B	57	SER	2.7
1	B	123	LEU	2.7
1	A	72	LYS	2.7
1	A	93	VAL	2.6
1	B	413	ASP	2.6
1	A	123	LEU	2.6
1	B	73	THR	2.6
1	A	179	ALA	2.5
1	A	60	LYS	2.5
1	B	77	LEU	2.5
1	A	80	ASP	2.5
1	B	74	SER	2.4
1	A	75	PRO	2.4
1	B	219	ASN	2.4
1	A	74	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	85	GLU	2.4
1	B	84	PRO	2.4
1	A	205	THR	2.3
1	B	240	ALA	2.3
1	B	203	ASP	2.3
1	B	65	SER	2.2
1	B	106	SER	2.2
1	A	239	SER	2.2
1	A	157	ILE	2.2
1	B	124	ASN	2.2
1	B	55	TRP	2.1
1	A	419	THR	2.1
1	B	132	VAL	2.1
1	B	166	GLU	2.1
1	B	115	PHE	2.1
1	B	62	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

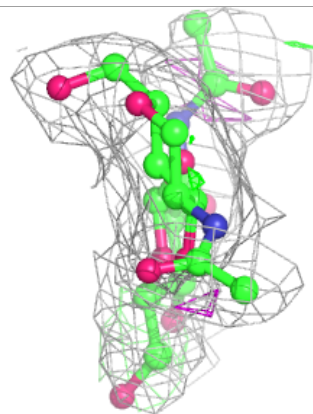
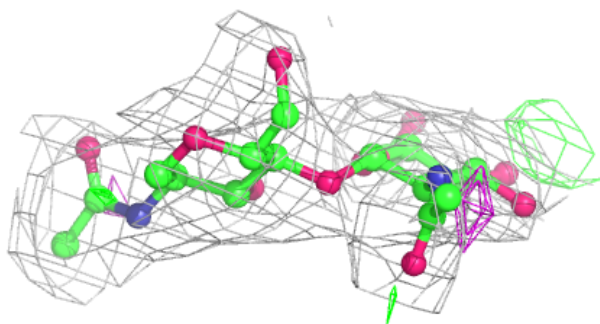
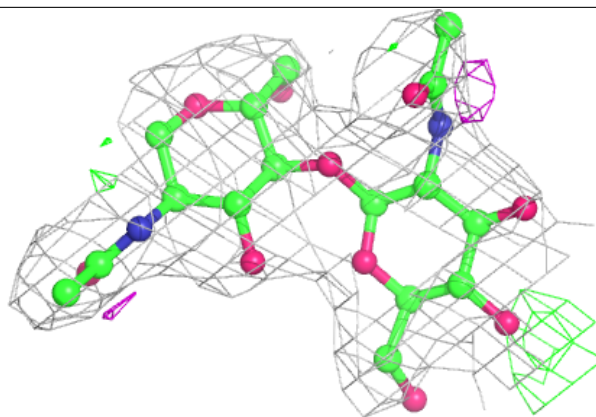
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	I	2	14/15	0.73	0.27	41,96,111,121	0
4	NAG	H	2	14/15	0.75	0.32	41,96,111,121	0
4	NAG	G	2	14/15	0.77	0.23	41,63,113,116	0
4	NAG	J	2	14/15	0.83	0.19	41,63,113,116	0
4	NAG	I	1	14/15	0.87	0.17	48,67,107,112	0
4	NAG	H	1	14/15	0.89	0.13	48,67,107,112	0
4	NAG	G	1	14/15	0.90	0.17	19,44,66,69	0
4	NAG	J	1	14/15	0.94	0.16	19,44,66,69	0

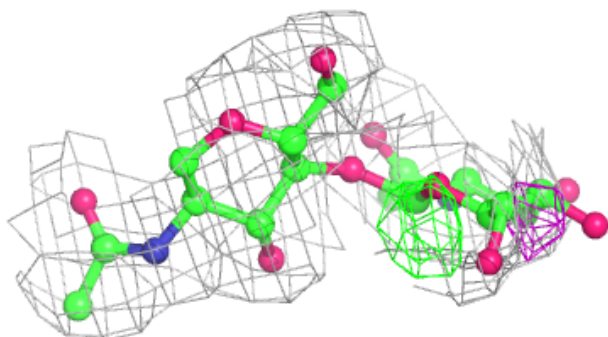
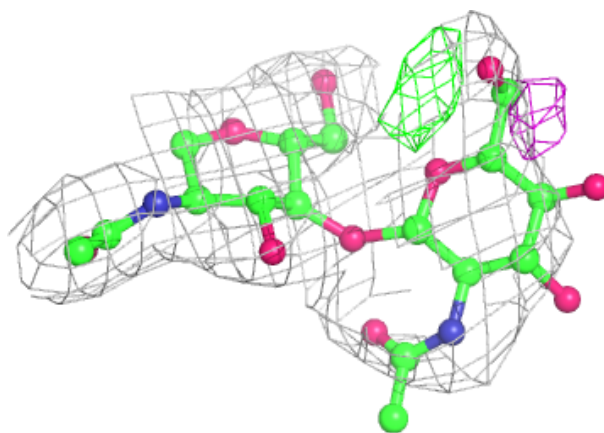
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

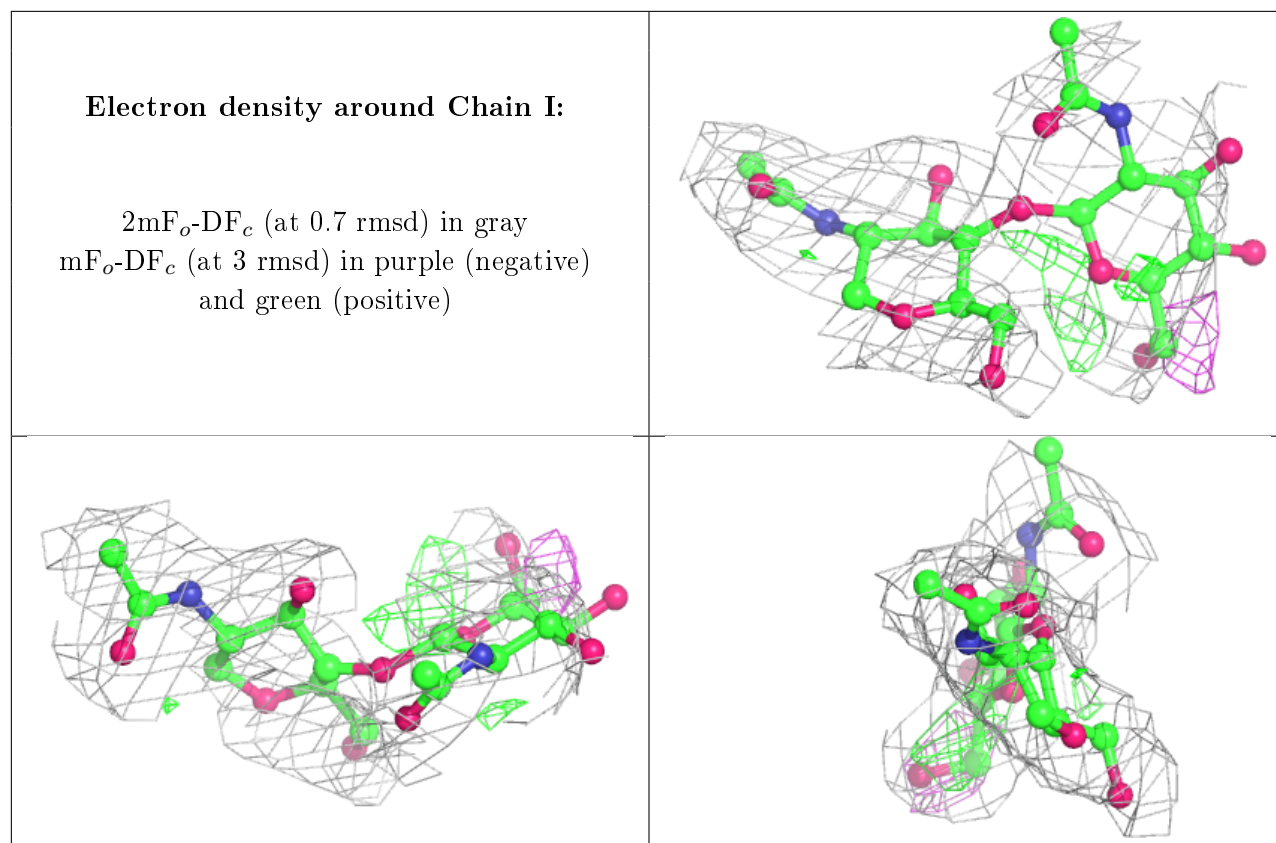
**Electron density around Chain G:**

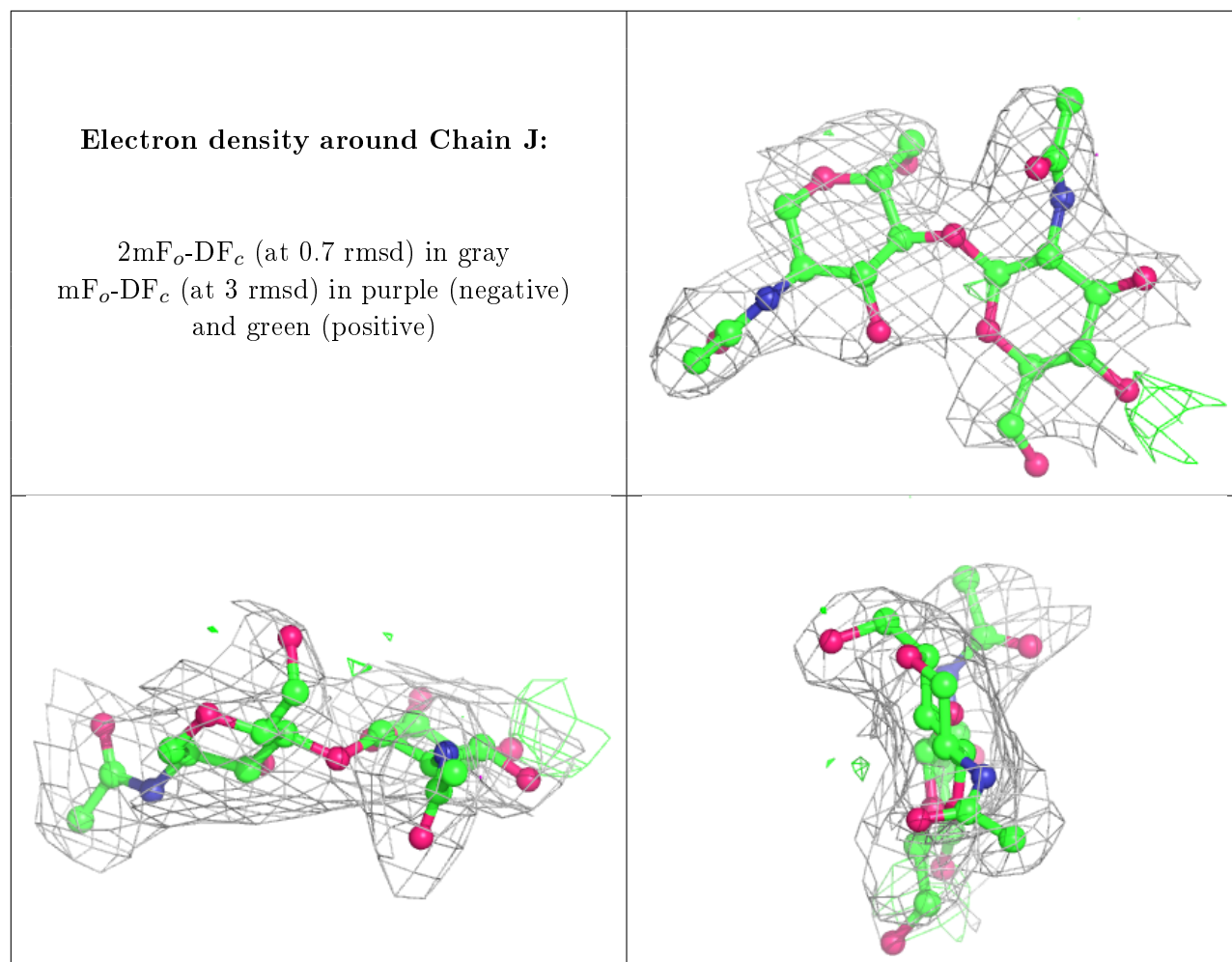
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain H:**

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







## 6.4 Ligands [\(i\)](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	B	1004	14/15	0.65	0.54	20,20,20,20	0
5	NAG	A	1004	14/15	0.66	0.42	20,20,20,20	0
5	NAG	D	1001	14/15	0.85	0.18	67,107,148,151	0
5	NAG	C	202	14/15	0.86	0.17	67,107,148,151	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.