WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 11:04 PM BST

PDB ID	:	1WWL
Title	:	Crystal structure of CD14
Authors	:	Kim, J.-I.; Lee, C.J.; Jin, M.S.; Lee, C.-H.; Paik, S.-G.; Lee, H.; Lee, J.-O.
Deposited on	:	2005-01-06
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

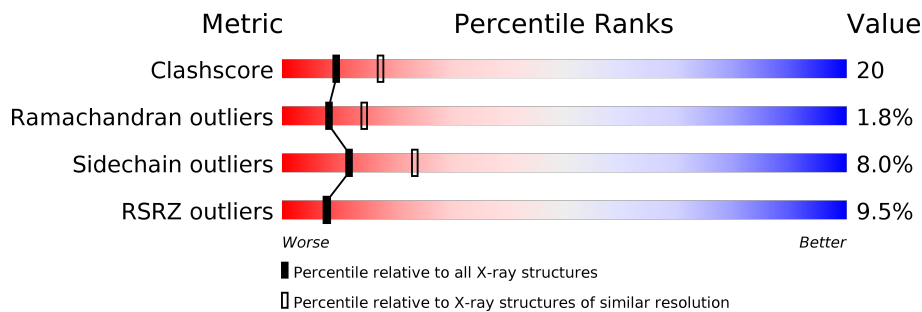|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.50 Å.

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

Metric	Percentile Ranks	Value
Clashscore		20
Ramachandran outliers		1.8%
Sidechain outliers		8.0%
RSRZ outliers		9.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 <=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	312	10% · 61% · 32% · 5%
1	B	312	9% · 67% · 28% · 5%
2	C	2	50% · 50%
2	D	2	50% · 50%
2	E	2	100%
2	F	2	50% · 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5235 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 Monocyte differentiation antigen CD14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total 2335	C 1472	N 404	O 450	S 9	0	0	0
1	B	312	Total 2364	C 1489	N 408	O 458	S 9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	-	cloning artifact	UNP P10810
A	4	ASP	-	cloning artifact	UNP P10810
B	3	ALA	-	cloning artifact	UNP P10810
B	4	ASP	-	cloning artifact	UNP P10810

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

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

• Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	185	Total	O	0	0
			185	185		
4	B	211	Total	O	0	0
			211	211		

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: Monocyte differentiation antigen CD14
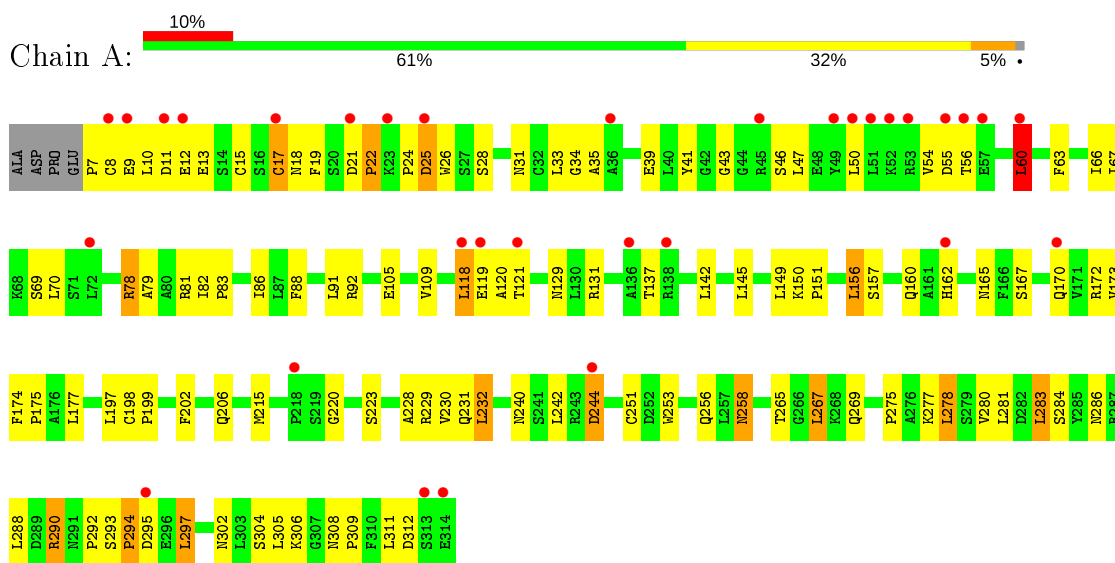
- Molecule 1: Monocyte differentiation antigen CD14
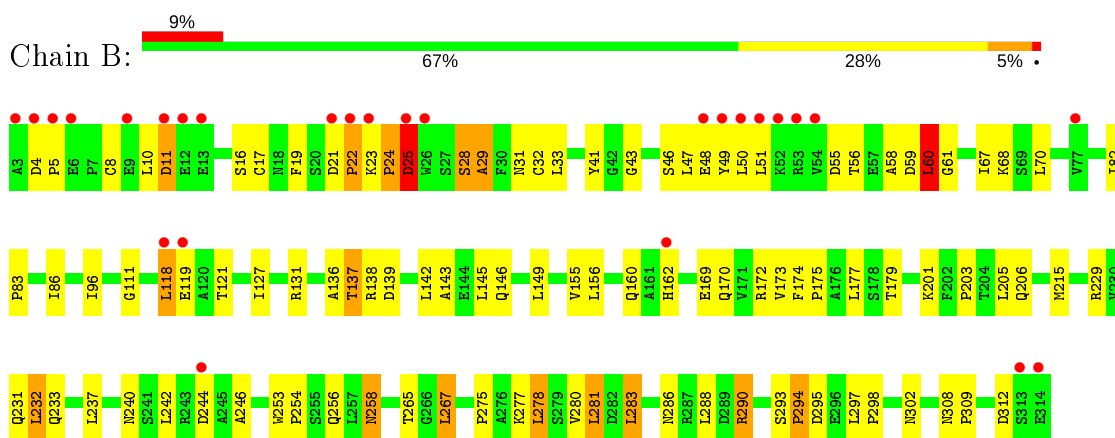
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

NAG1
NAG2

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

Chain D: 50% 50%

NAG1
NAG2

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

Chain E: 100%

NAG1
NAG2

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

Chain F: 50% 50%

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.52Å 117.70Å 102.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.79 – 2.50 29.73 – 2.48	Depositor EDS
% Data completeness (in resolution range)	96.1 (19.79-2.50) 94.9 (29.73-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	6.64 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.278 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	37.5	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 72.6	EDS
L-test for twinning[2]	$<|L|> = 0.46$, $<L^2> = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5235	wwPDB-VP
Average B, all atoms (Å^2)	51.0	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 45.04 % 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 1.3996e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: 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	0.50	0/2380	0.76	2/3240 (0.1%)
1	B	0.53	0/2410	0.82	2/3283 (0.1%)
All	All	0.52	0/4790	0.79	4/6523 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	ASP	N-CA-C	5.99	127.16	111.00
1	B	278	LEU	CA-CB-CG	5.86	128.79	115.30
1	A	167	SER	N-CA-C	-5.40	96.41	111.00
1	A	278	LEU	CA-CB-CG	5.35	127.60	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2335	0	2343	106	0
1	B	2364	0	2364	87	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	28	0	25	0	0
3	A	14	0	13	1	0
3	B	14	0	13	0	0
4	A	185	0	0	12	0
4	B	211	0	0	10	0
All	All	5235	0	4833	189	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 20.

All (189) 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:293:SER:HB3	1:B:294:PRO:HD2	1.34	1.03
1:B:231:GLN:HE22	1:B:256:GLN:H	1.15	0.93
1:A:69:SER:HA	4:A:1423:HOH:O	1.70	0.91
1:A:206:GLN:HG3	4:A:1577:HOH:O	1.70	0.91
1:A:293:SER:HB3	1:A:294:PRO:HD2	1.52	0.88
1:B:121:THR:HG22	4:B:1468:HOH:O	1.75	0.86
1:A:290:ARG:HE	1:A:290:ARG:HA	1.45	0.82
1:A:288:LEU:H	1:A:308:ASN:HD22	1.27	0.82
1:A:8:CYS:O	1:A:9:GLU:HG3	1.82	0.79
1:A:231:GLN:HE21	1:A:232:LEU:H	1.30	0.79
1:B:118:LEU:HD21	1:B:121:THR:HB	1.65	0.78
1:B:286:ASN:HB2	1:B:308:ASN:HD21	1.51	0.76
1:B:281:LEU:HD13	1:B:283:LEU:HD22	1.69	0.73
1:B:293:SER:HB3	1:B:294:PRO:CD	2.17	0.73
1:A:311:LEU:O	1:B:277:LYS:HE3	1.88	0.73
1:B:33:LEU:HD12	1:B:70:LEU:HD23	1.70	0.71
1:B:231:GLN:NE2	1:B:256:GLN:HB2	2.06	0.71
1:B:131:ARG:HH11	1:B:160:GLN:NE2	1.89	0.70
1:A:309:PRO:HA	1:A:312:ASP:OD2	1.94	0.68
1:B:281:LEU:CD1	1:B:283:LEU:HD22	2.23	0.68
1:A:251:CYS:HB3	4:A:1522:HOH:O	1.93	0.68
1:B:231:GLN:NE2	1:B:256:GLN:H	1.90	0.67
1:A:294:PRO:HD3	1:B:294:PRO:HB3	1.77	0.66
1:A:197:LEU:HD13	1:A:230:VAL:HG21	1.78	0.66
1:A:231:GLN:HE21	1:A:232:LEU:N	1.93	0.66
1:A:7:PRO:HG2	1:A:25:ASP:HB2	1.77	0.65
1:A:33:LEU:HD12	1:A:34:GLY:H	1.62	0.65
1:A:33:LEU:HD13	1:A:70:LEU:HD23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ASP:HB3	1:B:58:ALA:HB2	1.80	0.63
1:A:118:LEU:HD22	1:A:119:GLU:N	2.15	0.62
1:A:118:LEU:HD21	1:A:121:THR:HB	1.82	0.62
1:A:22:PRO:O	1:A:24:PRO:HD3	2.00	0.62
1:B:145:LEU:O	1:B:149:LEU:HD13	1.99	0.61
1:B:28:SER:O	1:B:29:ALA:HB2	2.01	0.61
1:A:31:ASN:C	1:A:33:LEU:H	2.02	0.61
1:A:60:LEU:HD12	1:A:60:LEU:O	2.00	0.61
1:B:23:LYS:N	1:B:24:PRO:HD3	2.15	0.61
1:A:288:LEU:H	1:A:308:ASN:ND2	1.98	0.61
1:A:118:LEU:C	1:A:118:LEU:HD13	2.22	0.60
1:B:229:ARG:NE	4:B:1560:HOH:O	2.34	0.60
1:B:47:LEU:HD12	1:B:82:ILE:HG12	1.84	0.60
1:B:293:SER:CB	1:B:294:PRO:HD2	2.21	0.59
1:A:228:ALA:HB3	1:A:230:VAL:HG23	1.85	0.58
1:B:309:PRO:HA	1:B:312:ASP:OD2	2.03	0.58
1:A:286:ASN:HB2	1:A:308:ASN:HD21	1.68	0.58
1:B:232:LEU:C	1:B:232:LEU:HD23	2.24	0.58
1:A:231:GLN:NE2	1:A:256:GLN:HB2	2.19	0.57
1:A:47:LEU:O	1:A:50:LEU:HD13	2.04	0.57
1:B:5:PRO:HD2	4:B:1576:HOH:O	2.04	0.57
1:A:294:PRO:HB3	1:B:294:PRO:HD3	1.85	0.57
1:A:258:ASN:HD22	1:A:258:ASN:C	2.09	0.56
1:A:256:GLN:HG2	4:A:1465:HOH:O	2.05	0.56
1:A:82:ILE:O	1:A:109:VAL:HA	2.06	0.56
1:B:4:ASP:N	1:B:5:PRO:HD3	2.21	0.56
1:B:137:THR:OG1	1:B:138:ARG:N	2.39	0.55
1:B:83:PRO:HG2	1:B:86:ILE:CG1	2.36	0.55
1:A:215:MET:H	1:A:240:ASN:ND2	2.05	0.55
1:B:139:ASP:HB2	4:B:1472:HOH:O	2.06	0.55
1:B:258:ASN:C	1:B:258:ASN:HD22	2.11	0.54
1:A:172:ARG:HG3	1:A:173:VAL:H	1.73	0.54
1:B:169:GLU:HB2	1:B:170:GLN:NE2	2.23	0.54
1:B:83:PRO:HG2	1:B:86:ILE:HG12	1.89	0.54
1:A:118:LEU:HD12	1:A:118:LEU:H	1.73	0.53
1:B:246:ALA:HB1	4:B:1452:HOH:O	2.07	0.53
1:A:12:GLU:HA	4:A:1441:HOH:O	2.08	0.53
1:A:131:ARG:HH11	1:A:160:GLN:HE21	1.54	0.53
1:A:240:ASN:O	1:A:265:THR:HA	2.09	0.53
1:A:54:VAL:HG12	1:A:55:ASP:N	2.24	0.53
1:B:232:LEU:O	1:B:232:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ALA:N	4:A:1422:HOH:O	2.40	0.53
1:A:165:ASN:HD22	3:A:1415:NAG:C7	2.21	0.53
1:A:19:PHE:HB3	1:A:24:PRO:HG2	1.90	0.53
1:A:13:GLU:HG2	4:A:1532:HOH:O	2.09	0.52
1:B:215:MET:H	1:B:240:ASN:ND2	2.07	0.52
1:A:129:ASN:OD1	1:A:157:SER:HB3	2.10	0.52
1:A:244:ASP:OD2	1:A:269:GLN:HG2	2.09	0.52
1:A:41:TYR:CZ	1:A:43:GLY:HA2	2.44	0.52
1:B:162:HIS:HB2	4:B:1495:HOH:O	2.09	0.52
1:A:18:ASN:OD1	1:A:18:ASN:C	2.48	0.51
1:B:10:LEU:HD12	1:B:11:ASP:H	1.75	0.51
1:A:145:LEU:O	1:A:149:LEU:HD13	2.11	0.51
1:B:68:LYS:HG3	1:B:96:ILE:HD12	1.93	0.51
1:A:56:THR:O	1:A:56:THR:HG22	2.12	0.50
1:A:232:LEU:HD23	1:A:232:LEU:O	2.11	0.50
1:A:242:LEU:HB2	1:A:267:LEU:HD13	1.92	0.50
1:B:22:PRO:C	1:B:24:PRO:HD3	2.32	0.50
1:B:111:GLY:O	1:B:136:ALA:HB2	2.12	0.50
1:B:46:SER:OG	1:B:48:GLU:HG3	2.12	0.50
1:A:121:THR:O	1:A:121:THR:HG23	2.12	0.49
1:A:253:TRP:CD1	1:A:275:PRO:HG3	2.47	0.49
1:A:215:MET:H	1:A:240:ASN:HD22	1.58	0.49
1:B:51:LEU:HD23	1:B:86:ILE:HD11	1.93	0.49
1:B:155:VAL:HG22	1:B:179:THR:HB	1.93	0.49
1:A:290:ARG:NE	1:A:290:ARG:HA	2.21	0.49
1:B:121:THR:HG23	1:B:121:THR:O	2.12	0.49
1:A:31:ASN:C	1:A:33:LEU:N	2.66	0.49
1:B:47:LEU:HB3	1:B:50:LEU:HD13	1.95	0.49
1:B:59:ASP:O	1:B:61:GLY:N	2.37	0.49
1:A:294:PRO:HG2	1:A:295:ASP:H	1.78	0.48
1:A:292:PRO:HB2	1:A:297:LEU:HD22	1.96	0.48
1:B:294:PRO:HG2	1:B:295:ASP:H	1.77	0.48
1:A:47:LEU:HB3	1:A:50:LEU:HD13	1.94	0.48
1:B:127:ILE:HG12	1:B:155:VAL:HB	1.96	0.48
1:B:23:LYS:HE2	1:B:49:TYR:CD2	2.48	0.48
1:B:232:LEU:CD2	1:B:254:PRO:HG2	2.44	0.48
1:A:83:PRO:HG2	1:A:86:ILE:HG12	1.96	0.47
1:B:290:ARG:HA	1:B:290:ARG:HE	1.78	0.47
1:B:10:LEU:HD22	1:B:31:ASN:O	2.14	0.47
1:B:33:LEU:CD1	1:B:70:LEU:HD23	2.40	0.47
1:B:118:LEU:H	1:B:118:LEU:CD1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PRO:HD2	1:A:26:TRP:CZ2	2.49	0.47
1:A:229:ARG:HB3	4:A:1449:HOH:O	2.15	0.47
1:A:231:GLN:HE22	1:A:256:GLN:H	1.63	0.47
1:A:173:VAL:O	1:A:175:PRO:HD3	2.14	0.47
1:B:232:LEU:HD22	1:B:254:PRO:HG2	1.96	0.47
1:B:288:LEU:O	1:B:309:PRO:HD2	2.15	0.47
1:A:177:LEU:HD23	1:A:202:PHE:HD2	1.80	0.47
1:A:60:LEU:HG	1:A:60:LEU:H	1.29	0.46
1:B:174:PHE:HB3	1:B:177:LEU:HB2	1.96	0.46
1:B:143:ALA:O	1:B:146:GLN:HB2	2.15	0.46
1:B:173:VAL:O	1:B:175:PRO:HD3	2.15	0.46
1:B:240:ASN:O	1:B:265:THR:HA	2.15	0.46
1:A:311:LEU:O	1:B:277:LYS:CE	2.62	0.46
1:A:231:GLN:NE2	1:A:232:LEU:H	2.07	0.46
1:A:253:TRP:CG	1:A:275:PRO:HG3	2.51	0.46
1:A:283:LEU:HB3	1:A:305:LEU:HD23	1.98	0.46
1:B:131:ARG:NH1	1:B:160:GLN:NE2	2.62	0.46
1:A:174:PHE:HB3	1:A:177:LEU:HB2	1.98	0.45
1:A:172:ARG:HG3	1:A:173:VAL:N	2.30	0.45
1:A:228:ALA:CB	1:A:230:VAL:HG23	2.46	0.45
1:A:88:PHE:HD2	1:A:91:LEU:HD12	1.81	0.45
1:B:47:LEU:O	1:B:50:LEU:HD13	2.16	0.45
1:A:46:SER:HA	1:A:81:ARG:HB3	1.97	0.45
1:A:119:GLU:HA	4:A:1447:HOH:O	2.17	0.45
1:B:275:PRO:O	1:B:298:PRO:HB3	2.17	0.45
1:B:8:CYS:HA	1:B:17:CYS:HA	1.98	0.45
1:A:118:LEU:N	1:A:118:LEU:CD1	2.80	0.44
1:A:50:LEU:N	1:A:50:LEU:HD12	2.33	0.44
1:A:10:LEU:HD13	1:A:35:ALA:HB2	2.00	0.44
1:B:265:THR:OG1	1:B:267:LEU:HD22	2.17	0.44
1:B:32:CYS:O	1:B:33:LEU:C	2.56	0.44
1:B:41:TYR:CZ	1:B:43:GLY:HA2	2.52	0.44
1:A:8:CYS:HA	1:A:17:CYS:HA	1.98	0.44
1:B:60:LEU:HD11	1:B:67:ILE:HG13	2.00	0.44
1:A:242:LEU:HG	1:A:265:THR:HB	2.00	0.43
1:B:118:LEU:HD22	1:B:119:GLU:N	2.33	0.43
1:B:8:CYS:HA	1:B:16:SER:O	2.17	0.43
1:A:119:GLU:O	1:A:120:ALA:HB3	2.18	0.43
1:A:33:LEU:C	1:A:35:ALA:H	2.21	0.43
1:B:28:SER:O	1:B:29:ALA:CB	2.65	0.43
1:A:230:VAL:HG12	1:A:231:GLN:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:HD23	1:A:232:LEU:C	2.39	0.43
1:A:39:GLU:HB2	4:A:1510:HOH:O	2.18	0.43
1:B:253:TRP:O	1:B:254:PRO:C	2.56	0.43
1:B:290:ARG:HA	1:B:290:ARG:NE	2.33	0.43
1:B:21:ASP:O	1:B:24:PRO:HD3	2.18	0.43
1:B:201:LYS:C	1:B:203:PRO:HD3	2.39	0.43
1:B:237:LEU:HD22	4:B:1455:HOH:O	2.19	0.43
1:A:150:LYS:HB3	1:A:151:PRO:HD2	2.01	0.43
1:A:293:SER:HB3	1:A:294:PRO:CD	2.37	0.43
1:B:242:LEU:HB2	1:B:267:LEU:HD13	2.00	0.43
1:A:92:ARG:HG3	1:A:121:THR:OG1	2.19	0.42
1:A:284:SER:HB2	1:A:306:LYS:O	2.18	0.42
1:A:28:SER:O	1:A:31:ASN:HB2	2.20	0.42
1:A:118:LEU:HD11	1:A:121:THR:HB	2.00	0.42
1:B:4:ASP:CG	4:B:1624:HOH:O	2.57	0.42
1:A:162:HIS:CG	1:A:162:HIS:O	2.73	0.41
1:A:78:ARG:HA	1:A:105:GLU:O	2.21	0.41
1:A:10:LEU:O	1:A:10:LEU:HG	2.21	0.41
1:A:156:LEU:HB2	1:A:177:LEU:HD11	2.03	0.41
1:A:9:GLU:O	1:A:15:CYS:HA	2.20	0.41
1:A:198:CYS:HA	1:A:199:PRO:HD3	1.90	0.41
1:A:56:THR:O	1:A:92:ARG:NH2	2.50	0.41
1:B:19:PHE:HA	4:B:1574:HOH:O	2.19	0.41
1:B:233:GLN:HG3	4:B:1519:HOH:O	2.20	0.41
1:A:63:PHE:HD2	1:A:66:ILE:HD12	1.85	0.41
1:B:205:LEU:HD12	1:B:205:LEU:HA	1.83	0.41
1:B:215:MET:H	1:B:240:ASN:HD22	1.68	0.41
1:A:293:SER:CB	1:A:294:PRO:HD2	2.33	0.41
1:A:220:GLY:O	1:A:223:SER:HB3	2.21	0.41
1:A:292:PRO:HB2	4:A:1477:HOH:O	2.20	0.41
1:A:11:ASP:O	1:A:12:GLU:HB2	2.21	0.40
1:A:170:GLN:NE2	4:A:1488:HOH:O	2.54	0.40
1:A:67:ILE:HA	1:A:70:LEU:HG	2.03	0.40
1:A:41:TYR:CE2	1:A:43:GLY:HA2	2.56	0.40
1:B:206:GLN:OE1	1:B:233:GLN:NE2	2.54	0.40
1:B:23:LYS:HG2	1:B:49:TYR:CE2	2.56	0.40
1:B:24:PRO:HB2	1:B:25:ASP:H	1.65	0.40
1:B:10:LEU:HD12	1:B:11:ASP:N	2.36	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	306/312 (98%)	271 (89%)	31 (10%)	4 (1%)	12	21
1	B	310/312 (99%)	281 (91%)	22 (7%)	7 (2%)	6	10
All	All	616/624 (99%)	552 (90%)	53 (9%)	11 (2%)	8	14

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	PRO
1	B	24	PRO
1	B	25	ASP
1	B	29	ALA
1	B	60	LEU
1	A	60	LEU
1	A	79	ALA
1	B	294	PRO
1	B	56	THR
1	A	294	PRO
1	B	22	PRO

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	260/264 (98%)	238 (92%)	22 (8%)	10	21
1	B	263/264 (100%)	243 (92%)	20 (8%)	13	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	523/528 (99%)	481 (92%)	42 (8%)	12	23

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	CYS
1	A	21	ASP
1	A	25	ASP
1	A	60	LEU
1	A	78	ARG
1	A	118	LEU
1	A	137	THR
1	A	142	LEU
1	A	156	LEU
1	A	232	LEU
1	A	244	ASP
1	A	258	ASN
1	A	267	LEU
1	A	277	LYS
1	A	278	LEU
1	A	280	VAL
1	A	281	LEU
1	A	283	LEU
1	A	290	ARG
1	A	297	LEU
1	A	302	ASN
1	A	304	SER
1	B	11	ASP
1	B	25	ASP
1	B	28	SER
1	B	60	LEU
1	B	118	LEU
1	B	137	THR
1	B	142	LEU
1	B	156	LEU
1	B	172	ARG
1	B	232	LEU
1	B	244	ASP
1	B	258	ASN
1	B	267	LEU
1	B	278	LEU
1	B	280	VAL

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Mol	Chain	Res	Type
1	B	281	LEU
1	B	283	LEU
1	B	290	ARG
1	B	297	LEU
1	B	302	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	160	GLN
1	A	162	HIS
1	A	212	ASN
1	A	231	GLN
1	A	233	GLN
1	A	240	ASN
1	A	258	ASN
1	A	299	GLN
1	A	302	ASN
1	A	308	ASN
1	B	31	ASN
1	B	160	GLN
1	B	170	GLN
1	B	212	ASN
1	B	231	GLN
1	B	233	GLN
1	B	240	ASN
1	B	258	ASN
1	B	291	ASN
1	B	302	ASN
1	B	308	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
2	NAG	C	1	1,2	14,14,15	0.52	0	17,19,21	0.85	1 (5%)
2	NAG	C	2	2	14,14,15	0.56	0	17,19,21	0.69	0
2	NAG	D	1	1,2	14,14,15	0.48	0	17,19,21	0.89	1 (5%)
2	NAG	D	2	2	14,14,15	0.61	0	17,19,21	0.67	0
2	NAG	E	1	1,2	14,14,15	0.63	0	17,19,21	0.88	0
2	NAG	E	2	2	14,14,15	0.81	0	17,19,21	1.00	0
2	NAG	F	1	1,2	14,14,15	0.67	0	17,19,21	0.95	1 (5%)
2	NAG	F	2	2	14,14,15	0.64	0	17,19,21	0.70	0

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C2-N2-C7	-2.72	119.03	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C2-N2-C7	-2.34	119.57	122.90
2	C	1	NAG	C2-N2-C7	-2.09	119.92	122.90

There are no chirality outliers.

All (16) torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings
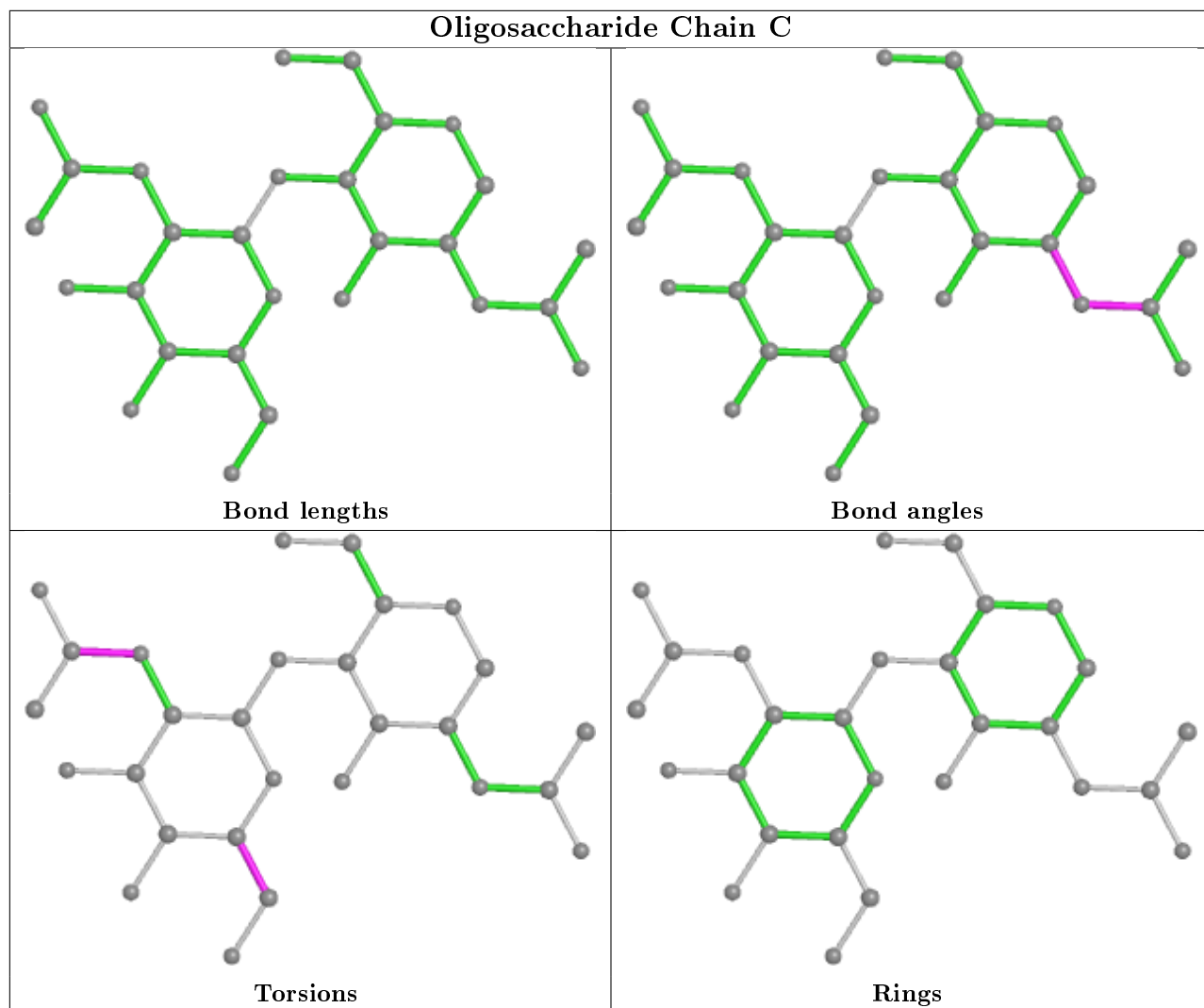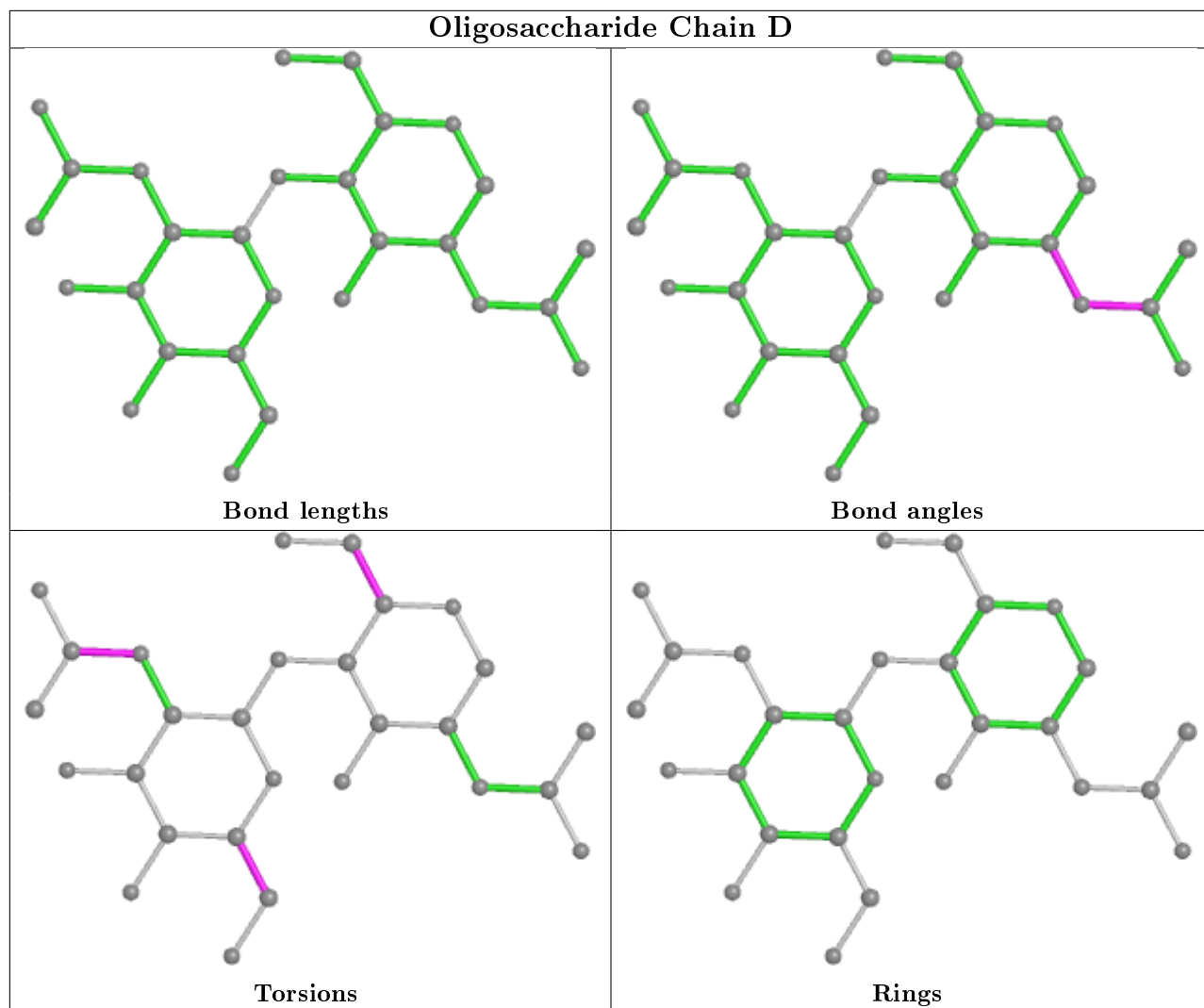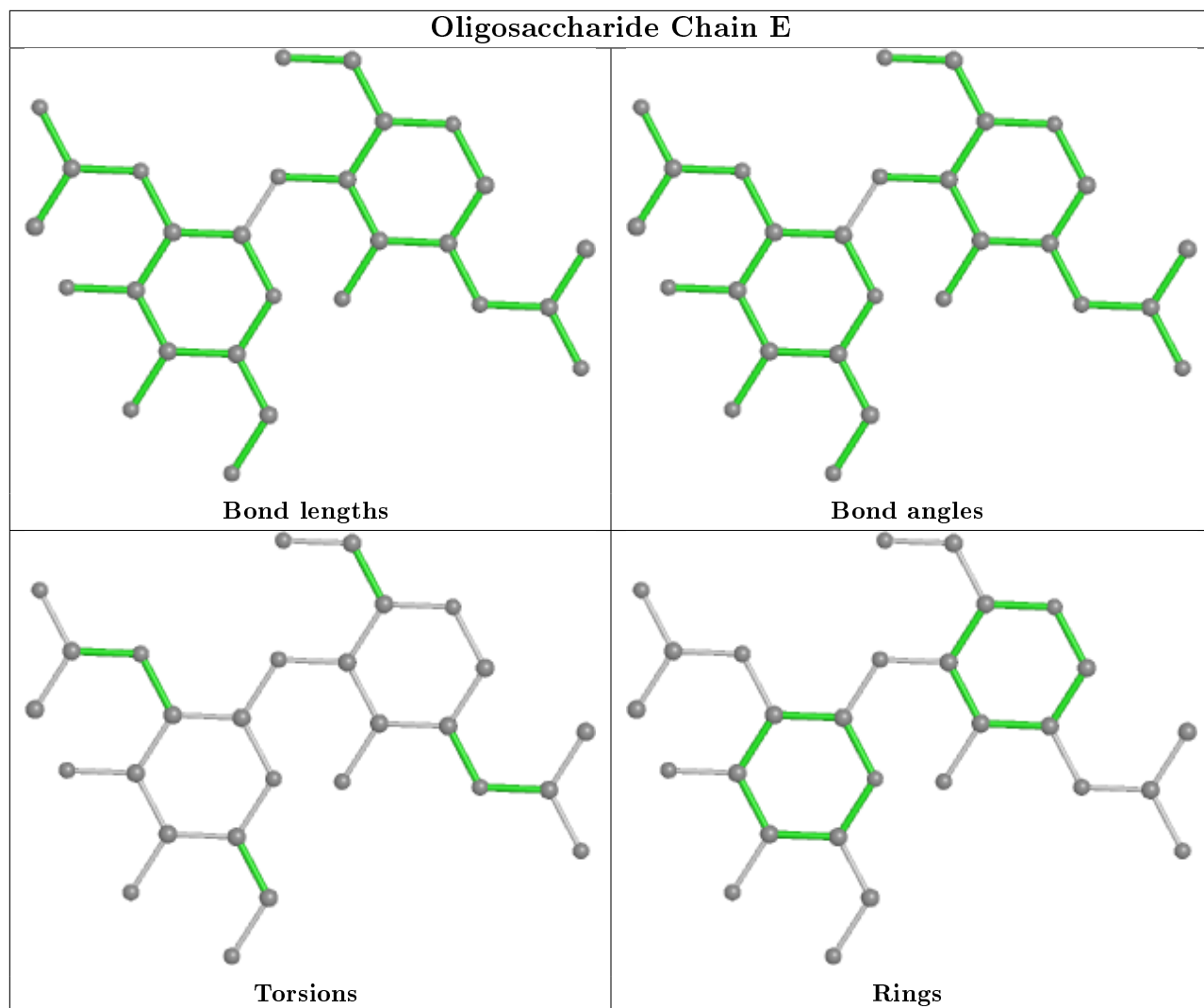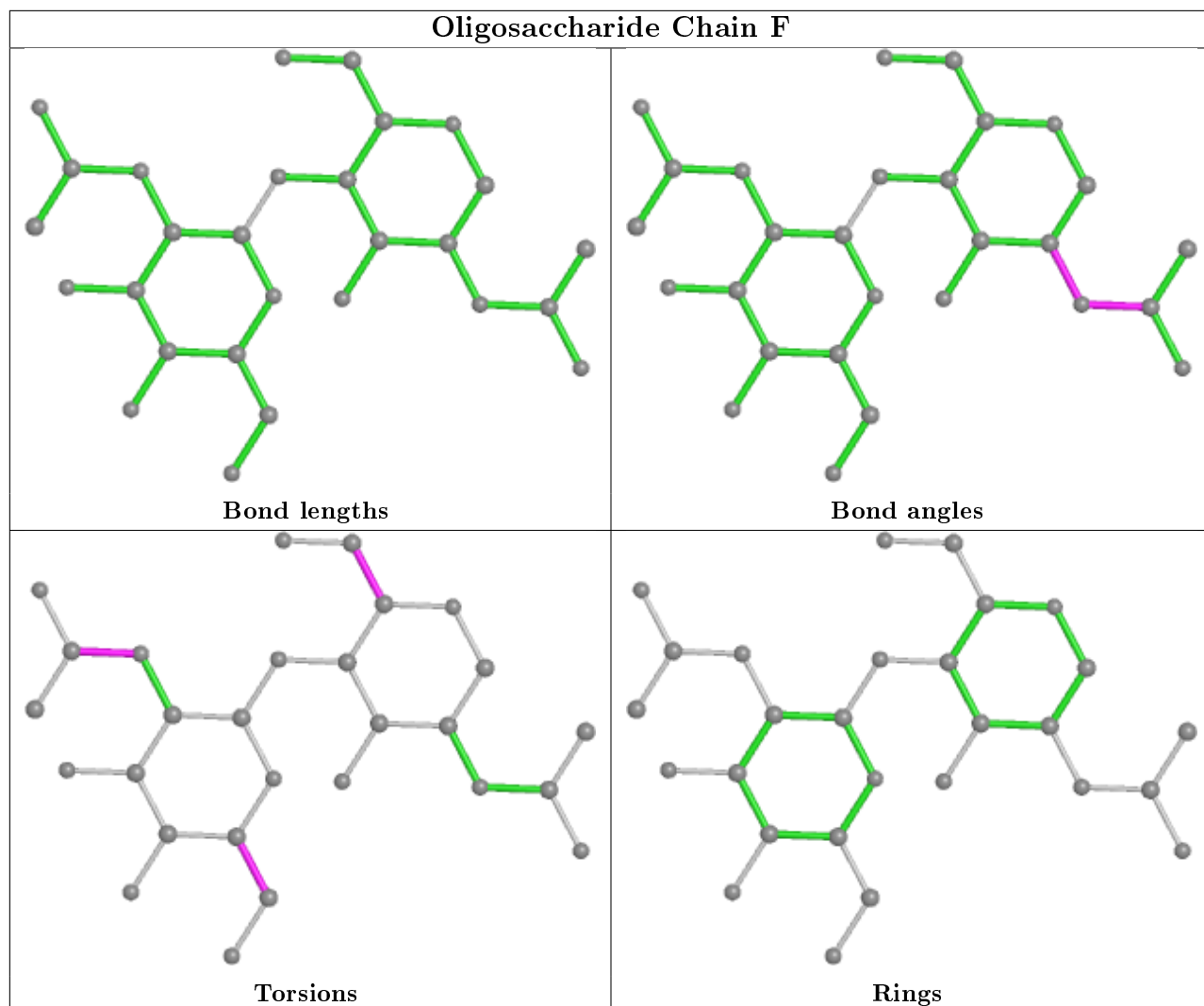
5.6 Ligand geometry (i)

2 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	$\#|Z| > 2$
3	NAG	B	1415	1	14,14,15	0.98	1 (7%)	17,19,21	0.84	0
3	NAG	A	1415	1	14,14,15	0.66	0	17,19,21	0.66	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
3	NAG	B	1415	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1415	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1415	NAG	C1-C2	3.06	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1415	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	308/312 (98%)	0.39	32 (10%)	6	6	20, 47, 109, 130	0
1	B	312/312 (100%)	0.30	27 (8%)	10	10	16, 41, 97, 111	0
All	All	620/624 (99%)	0.34	59 (9%)	8	8	16, 44, 104, 130	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	ASP	9.7
1	B	50	LEU	8.9
1	B	12	GLU	6.4
1	A	45	ARG	6.0
1	A	314	GLU	5.6
1	B	51	LEU	4.9
1	A	52	LYS	4.9
1	A	55	ASP	4.9
1	B	54	VAL	4.5
1	A	49	TYR	4.3
1	B	314	GLU	4.3
1	B	313	SER	4.0
1	B	49	TYR	3.9
1	B	53	ARG	3.8
1	A	53	ARG	3.8
1	B	48	GLU	3.8
1	B	52	LYS	3.7
1	B	13	GLU	3.7
1	A	51	LEU	3.6
1	A	23	LYS	3.6
1	A	136	ALA	3.6
1	A	138	ARG	3.4
1	A	25	ASP	3.4
1	A	17	CYS	3.4

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	RSRZ
1	B	22	PRO	3.2
1	A	244	ASP	3.2
1	A	313	SER	3.2
1	A	118	LEU	3.1
1	B	5	PRO	3.1
1	A	11	ASP	3.1
1	A	119	GLU	3.1
1	A	21	ASP	3.1
1	A	72	LEU	3.0
1	B	118	LEU	2.9
1	B	119	GLU	2.8
1	A	9	GLU	2.7
1	A	295	ASP	2.7
1	B	23	LYS	2.7
1	B	26	TRP	2.7
1	A	170	GLN	2.6
1	B	6	GLU	2.6
1	B	25	ASP	2.5
1	A	60	LEU	2.5
1	B	244	ASP	2.5
1	A	50	LEU	2.5
1	B	3	ALA	2.4
1	B	9	GLU	2.4
1	B	21	ASP	2.4
1	A	218	PRO	2.3
1	B	162	HIS	2.3
1	A	162	HIS	2.2
1	A	57	GLU	2.1
1	A	56	THR	2.1
1	A	121	THR	2.1
1	A	36	ALA	2.1
1	B	77	VAL	2.1
1	A	12	GLU	2.0
1	A	8	CYS	2.0
1	B	11	ASP	2.0

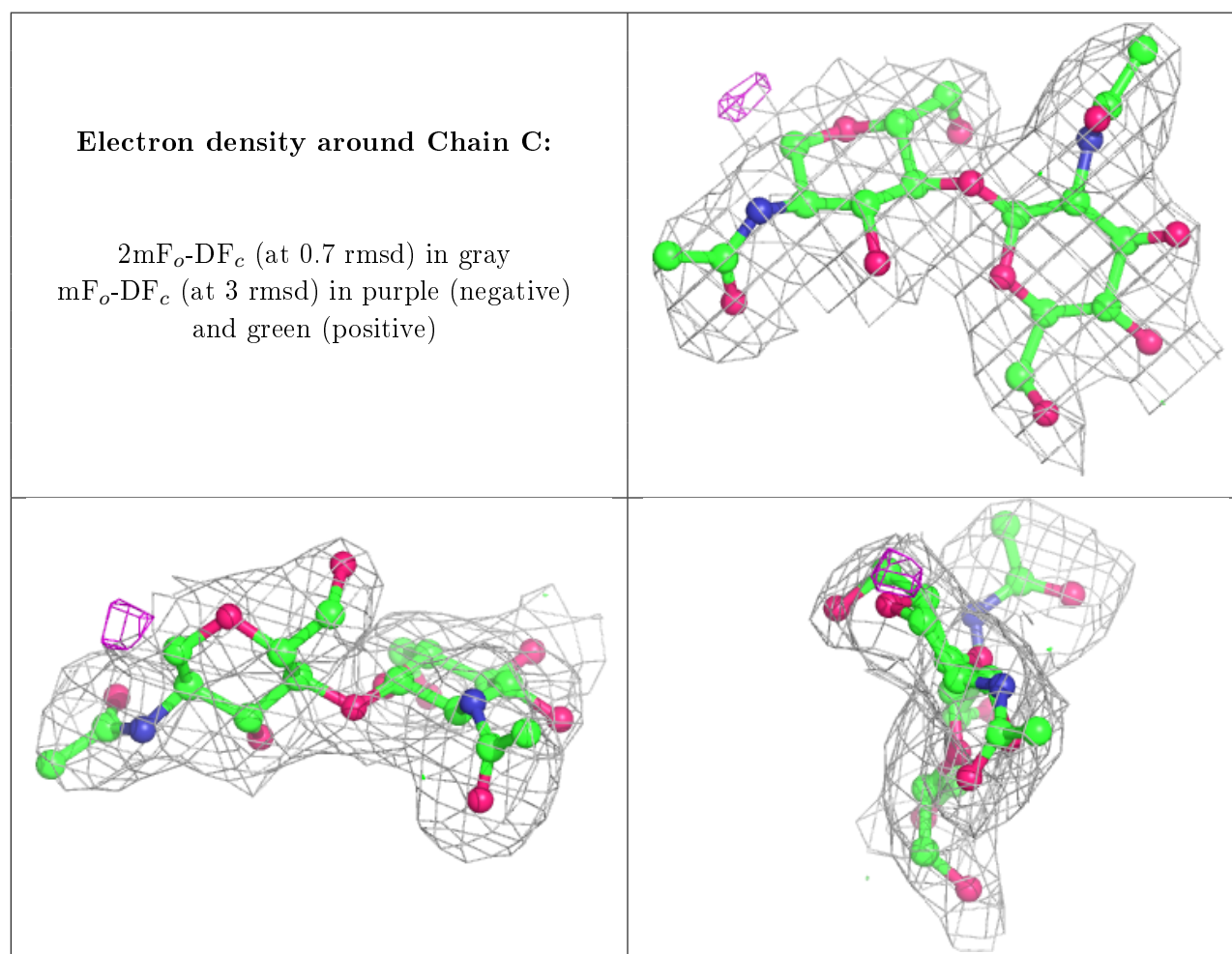## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
2	NAG	D	2	14/15	0.68	0.36	92,95,97,97	0
2	NAG	F	2	14/15	0.79	0.24	82,84,88,89	0
2	NAG	F	1	14/15	0.80	0.20	48,68,75,80	0
2	NAG	C	2	14/15	0.85	0.17	47,50,53,56	0
2	NAG	D	1	14/15	0.86	0.21	63,75,83,89	0
2	NAG	E	2	14/15	0.90	0.23	48,52,56,57	0
2	NAG	C	1	14/15	0.97	0.12	28,35,40,43	0
2	NAG	E	1	14/15	0.97	0.12	30,33,35,39	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 C:

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

Electron density around Chain D:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
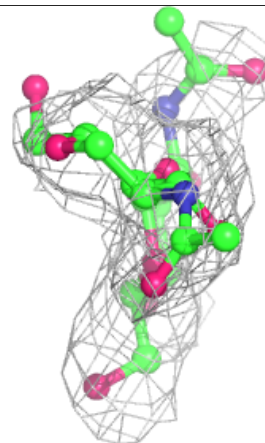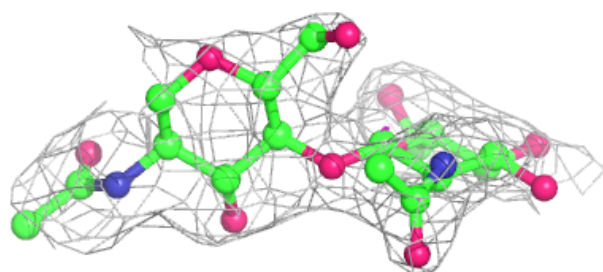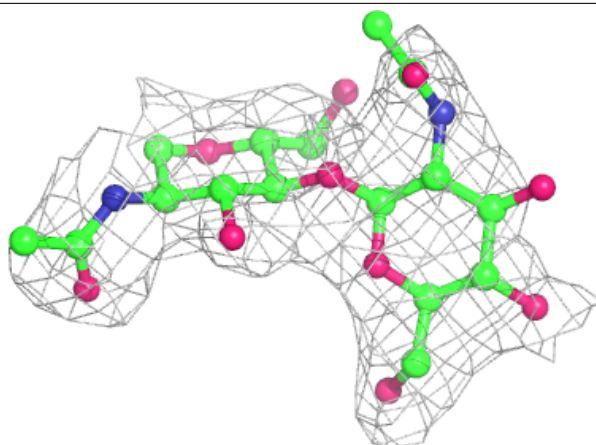
Electron density around Chain E:

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

Electron density around Chain F:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
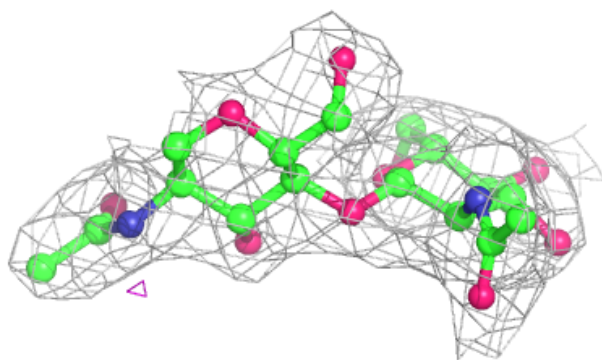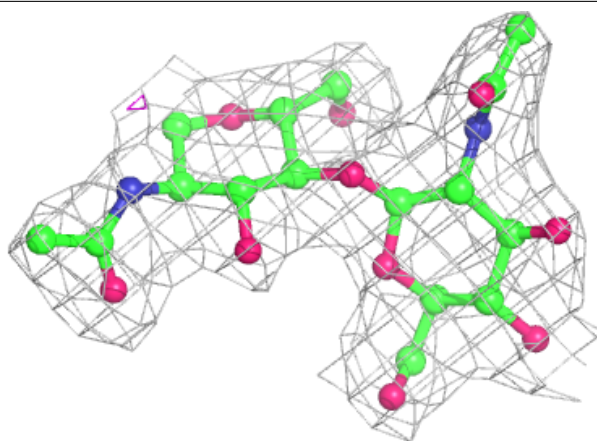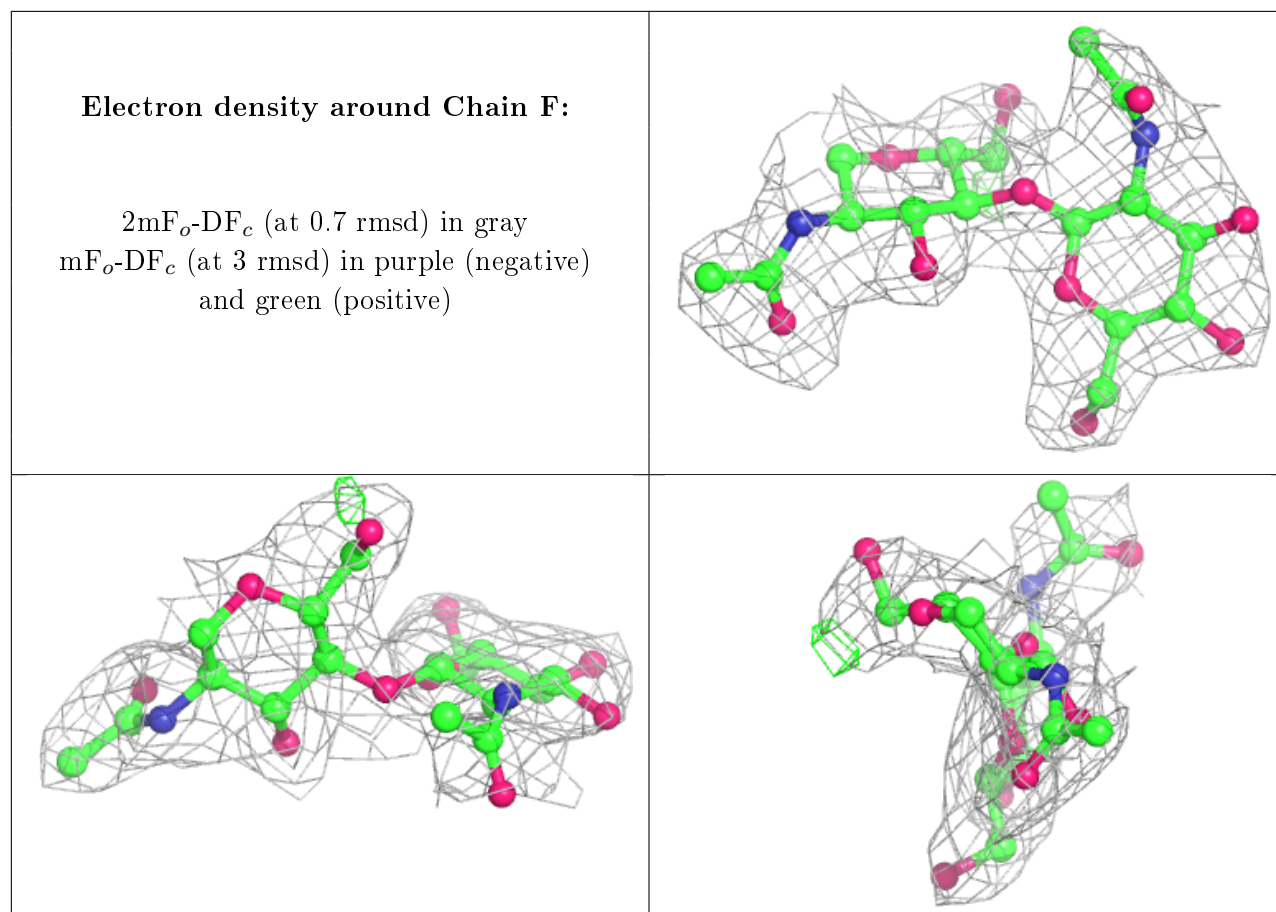
6.4 Ligands (i)

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
3	NAG	A	1415	14/15	0.62	0.39	88,95,99,99	0
3	NAG	B	1415	14/15	0.70	0.36	84,93,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.