



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 08:22 AM BST

PDB ID : 1YY9
Title : Structure of the extracellular domain of the epidermal growth factor receptor in complex with the Fab fragment of cetuximab/Erbitux/IMC-C225
Authors : Li, S.; Schmitz, K.R.; Jeffrey, P.D.; Wiltzius, J.J.W.; Kussie, P.; Ferguson, K.M.
Deposited on : 2005-02-24
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

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

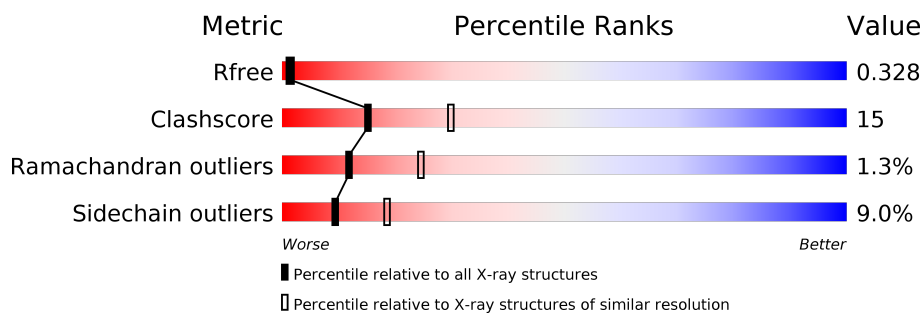
1 Overall quality at a glance

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)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	624	<div> <div>68%</div> <div>27%</div> <div>• •</div> </div>
2	C	213	<div> <div>62%</div> <div>31%</div> <div>5% •</div> </div>
3	D	221	<div> <div>68%</div> <div>26%</div> <div>5%</div> </div>
4	B	9	<div> <div>67%</div> <div>33%</div> </div>
5	E	2	<div> <div>100%</div> </div>
5	F	2	<div> <div>100%</div> </div>
5	G	2	<div> <div>100%</div> </div>

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	G	1	X	-	-	-
5	NAG	G	2	X	-	-	-
6	NAG	A	5041	X	-	-	-
6	NAG	A	625	X	-	-	-
6	NAG	D	881	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8225 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 Epidermal Growth Factor Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	613	4653	2879	828	886	60	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	LYS	SER	conflict	UNP P00533
A	610	ARG	GLU	conflict	UNP P00533
A	619	HIS	-	expression tag	UNP P00533
A	620	HIS	-	expression tag	UNP P00533
A	621	HIS	-	expression tag	UNP P00533
A	622	HIS	-	expression tag	UNP P00533
A	623	HIS	-	expression tag	UNP P00533
A	624	HIS	-	expression tag	UNP P00533

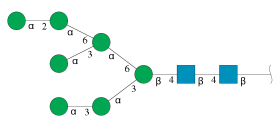
- Molecule 2 is a protein called Cetuximab Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	211	1609	1003	270	332	4	0	0	0

- Molecule 3 is a protein called Cetuximab Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	220	1648	1046	271	326	5	0	0	0

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



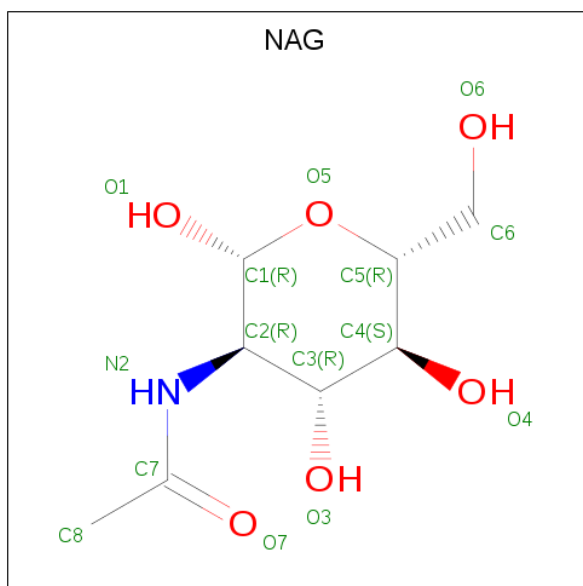
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	9	Total	C	N	O	0	0	0
			105	58	2	45			

- 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	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

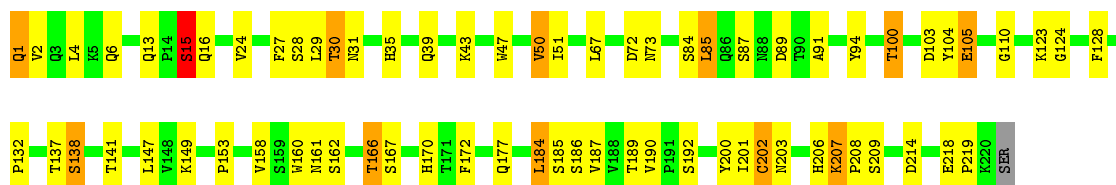
- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	35	Total	O	0	0
			35	35		
7	C	6	Total	O	0	0
			6	6		
7	D	15	Total	O	0	0
			15	15		



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

Chain B: 67% 33%



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

Chain E: 100%



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

Chain F: 100%



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

Chain G: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.82Å 70.86Å 147.12Å 90.00° 102.48° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 30.06 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.00-2.60) 98.3 (30.06-2.61)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.239 , 0.289 0.291 , 0.328	Depositor DCC
R_{free} test set	2352 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8225	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.66	0/4745	0.76	0/6426
2	C	0.65	0/1643	0.79	0/2237
3	D	0.68	0/1692	0.76	0/2316
All	All	0.66	0/8080	0.77	0/10979

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	4653	0	4451	120	0
2	C	1609	0	1535	58	0
3	D	1648	0	1584	65	0
4	B	105	0	88	5	0
5	E	28	0	25	0	0
5	F	28	0	25	0	0
5	G	28	0	25	0	0
6	A	56	0	52	1	0
6	D	14	0	13	0	0
7	A	35	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	6	0	0	0	0
7	D	15	0	0	0	0
All	All	8225	0	7798	239	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 15.

All (239) 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)
4:B:6:MAN:C6	4:B:6:MAN:O6	1.92	1.18
1:A:10:THR:HG22	1:A:42:GLU:OE1	1.56	1.05
1:A:157:GLN:HB3	1:A:159:HIS:NE2	1.80	0.96
2:C:136:LEU:HD21	2:C:196:VAL:HG21	1.48	0.95
1:A:44:THR:HG23	1:A:45:TYR:CD1	2.08	0.87
1:A:23:HIS:CE1	1:A:44:THR:HG22	2.13	0.84
2:C:80:SER:HA	2:C:106:LEU:HD11	1.63	0.80
2:C:115:VAL:HG22	2:C:136:LEU:HD22	1.61	0.80
1:A:209:HIS:HD2	1:A:211:GLN:H	1.30	0.79
1:A:17:LEU:H	1:A:23:HIS:HD2	1.31	0.79
1:A:227:CYS:SG	1:A:231:ARG:HB3	2.22	0.79
4:B:4:MAN:H61	4:B:5:MAN:H5	1.63	0.78
2:C:186:TYR:O	2:C:187:GLU:HB2	1.83	0.78
3:D:1:GLN:H1	3:D:1:GLN:HE21	1.31	0.78
1:A:458:GLY:H	1:A:462:GLN:HE22	1.32	0.78
1:A:232:ASP:O	1:A:233:GLU:HG2	1.85	0.76
1:A:515:CYS:SG	1:A:526:VAL:HG22	2.25	0.76
1:A:521:GLU:CB	1:A:522:PRO:CD	2.64	0.76
3:D:4:LEU:HD22	3:D:24:VAL:HG22	1.68	0.75
1:A:44:THR:CG2	1:A:45:TYR:HD1	1.99	0.75
2:C:32:ASN:HB3	2:C:91:ASN:HB3	1.69	0.74
1:A:244:MET:HE2	1:A:255:VAL:HA	1.70	0.73
1:A:465:LYS:NZ	3:D:100:THR:HG21	2.03	0.73
1:A:483:HIS:HD2	1:A:485:LEU:H	1.34	0.73
2:C:167:ASP:O	2:C:171:SER:HA	1.88	0.73
2:C:115:VAL:HG22	2:C:136:LEU:CD2	2.19	0.72
3:D:184:LEU:HG	3:D:185:SER:H	1.53	0.72
1:A:521:GLU:CB	1:A:522:PRO:HD3	2.19	0.72
3:D:13:GLN:HB2	3:D:16:GLN:CG	2.18	0.72
3:D:35:HIS:ND1	3:D:50:VAL:HG13	2.05	0.71
1:A:253:MET:HE1	1:A:575:VAL:HG11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:162:SER:H	3:D:203:ASN:ND2	1.88	0.70
3:D:1:GLN:N	3:D:1:GLN:HE21	1.89	0.70
1:A:99:SER:HA	1:A:128:ASN:O	1.92	0.70
3:D:13:GLN:HB2	3:D:16:GLN:HG2	1.74	0.69
1:A:376:GLU:OE1	1:A:403:ARG:NH1	2.27	0.68
2:C:82:ASP:O	2:C:104:LEU:HD23	1.94	0.68
1:A:44:THR:CG2	1:A:45:TYR:CD1	2.75	0.68
1:A:138:ILE:HD12	1:A:184:GLN:HG3	1.77	0.67
1:A:459:THR:H	1:A:462:GLN:HE21	1.41	0.67
1:A:327:ILE:HD11	1:A:345:LEU:HD22	1.76	0.66
1:A:291:SER:HB2	1:A:303:LYS:O	1.96	0.66
1:A:459:THR:H	1:A:462:GLN:NE2	1.93	0.66
1:A:17:LEU:H	1:A:23:HIS:CD2	2.14	0.66
1:A:297:ASP:O	1:A:299:VAL:N	2.29	0.66
1:A:289:ALA:O	1:A:290:ASP:HB2	1.95	0.65
1:A:289:ALA:O	1:A:290:ASP:CB	2.45	0.65
1:A:326:SER:HB2	1:A:346:HIS:O	1.97	0.65
1:A:320:GLU:N	1:A:320:GLU:OE1	2.25	0.64
2:C:115:VAL:HG13	2:C:136:LEU:CD2	2.28	0.64
1:A:509:ARG:CD	1:A:509:ARG:H	2.10	0.63
3:D:35:HIS:CE1	3:D:50:VAL:CG1	2.80	0.63
3:D:137:THR:HG22	3:D:138:SER:H	1.63	0.63
1:A:607:PRO:O	1:A:610:ARG:HG2	1.98	0.63
1:A:157:GLN:HB3	1:A:159:HIS:CE1	2.34	0.62
1:A:336:LYS:O	1:A:337:ASN:HB2	2.00	0.61
1:A:535:HIS:CD2	1:A:537:GLU:H	2.17	0.61
3:D:28:SER:OG	3:D:30:THR:HB	2.01	0.61
2:C:90:GLN:HE21	2:C:97:THR:HB	1.66	0.60
2:C:137:ASN:HD21	3:D:170:HIS:HD2	1.49	0.60
3:D:162:SER:H	3:D:203:ASN:HD21	1.48	0.60
4:B:4:MAN:H61	4:B:5:MAN:C5	2.30	0.60
1:A:114:ARG:HA	1:A:176:TRP:CD1	2.37	0.60
1:A:89:TYR:CD2	1:A:90:GLU:HB2	2.37	0.60
1:A:80:LEU:HD23	1:A:113:MET:HE2	1.84	0.60
2:C:136:LEU:CD2	2:C:196:VAL:HG21	2.28	0.60
1:A:149:LEU:HA	1:A:152:MET:HE1	1.84	0.59
1:A:535:HIS:CD2	1:A:537:GLU:HB2	2.37	0.59
1:A:465:LYS:HZ1	3:D:100:THR:HG21	1.67	0.59
1:A:272:PRO:HG2	1:A:275:TYR:CD1	2.37	0.59
1:A:198:ARG:HG3	1:A:213:ALA:O	2.03	0.59
1:A:17:LEU:N	1:A:23:HIS:HD2	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:184:LEU:HG	3:D:185:SER:N	2.19	0.58
1:A:244:MET:CE	1:A:255:VAL:HA	2.32	0.58
2:C:6:GLN:HE22	2:C:87:TYR:HA	1.69	0.58
2:C:136:LEU:HD21	2:C:196:VAL:CG2	2.29	0.58
1:A:201:GLY:HA3	1:A:206:ASP:OD1	2.04	0.57
3:D:35:HIS:CE1	3:D:50:VAL:HG11	2.39	0.57
1:A:134:ASN:ND2	1:A:177:GLY:HA2	2.19	0.57
1:A:19:THR:HG22	1:A:21:GLU:H	1.68	0.57
1:A:316:ILE:HD11	1:A:327:ILE:HG12	1.85	0.57
3:D:16:GLN:HA	3:D:16:GLN:OE1	2.04	0.57
3:D:147:LEU:HD12	3:D:184:LEU:O	2.05	0.57
3:D:13:GLN:HB2	3:D:16:GLN:HG3	1.86	0.57
1:A:217:THR:O	1:A:217:THR:HG22	2.04	0.56
3:D:1:GLN:H1	3:D:1:GLN:NE2	2.00	0.56
1:A:546:THR:O	1:A:546:THR:HG22	2.06	0.56
1:A:245:LEU:HG	1:A:256:ASN:HB2	1.87	0.56
1:A:317:GLY:O	1:A:322:LYS:HA	2.06	0.56
2:C:155:GLN:HB3	2:C:158:ASN:HD21	1.71	0.56
1:A:149:LEU:HA	1:A:152:MET:CE	2.36	0.56
1:A:597:HIS:ND1	1:A:598:PRO:HD2	2.21	0.55
3:D:172:PHE:O	3:D:184:LEU:HD11	2.06	0.55
1:A:483:HIS:CD2	1:A:485:LEU:H	2.20	0.55
1:A:451:ILE:HD11	1:A:491:CYS:O	2.07	0.55
2:C:117:ILE:HD12	2:C:194:CYS:HB2	1.89	0.55
1:A:209:HIS:CD2	1:A:211:GLN:H	2.19	0.55
2:C:115:VAL:HG13	2:C:136:LEU:HD21	1.88	0.55
3:D:47:TRP:HZ2	3:D:50:VAL:HG22	1.71	0.55
1:A:246:TYR:HD1	1:A:253:MET:HE1	1.72	0.54
7:A:5797:HOH:O	3:D:100:THR:CG2	2.55	0.54
1:A:407:LYS:HZ1	1:A:434:ASP:CG	2.10	0.54
1:A:46:VAL:HG12	1:A:72:VAL:HB	1.89	0.54
1:A:90:GLU:O	1:A:91:ASN:C	2.45	0.53
6:A:3891:NAG:H3	6:A:3891:NAG:H83	1.90	0.53
1:A:158:ASN:HD21	1:A:161:GLY:H	1.57	0.53
1:A:310:ARG:HA	1:A:339:THR:HG21	1.90	0.53
1:A:284:VAL:HG12	1:A:285:ARG:N	2.24	0.53
1:A:213:ALA:HB3	1:A:226:VAL:HG13	1.90	0.53
1:A:23:HIS:HE1	1:A:44:THR:HG22	1.65	0.53
1:A:80:LEU:HD23	1:A:113:MET:CE	2.39	0.53
3:D:161:ASN:HD21	3:D:200:TYR:HA	1.74	0.53
2:C:209:PHE:HD1	2:C:210:ASN:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:137:ASN:HD21	3:D:170:HIS:CD2	2.27	0.52
3:D:206:HIS:CE1	3:D:208:PRO:HG2	2.45	0.52
1:A:81:GLN:HA	1:A:115:ASN:O	2.08	0.52
2:C:2:ILE:HD13	2:C:29:ILE:HD11	1.91	0.52
3:D:1:GLN:N	3:D:1:GLN:NE2	2.57	0.52
2:C:151:ASP:O	2:C:152:ASN:HB2	2.09	0.52
2:C:31:THR:O	2:C:50:TYR:HA	2.10	0.52
3:D:29:LEU:HB2	3:D:73:ASN:OD1	2.10	0.51
2:C:29:ILE:O	2:C:29:ILE:HG23	2.09	0.51
2:C:198:HIS:CD2	2:C:200:GLY:H	2.28	0.51
1:A:276:VAL:HG11	1:A:287:CYS:SG	2.51	0.51
3:D:149:LYS:HE2	3:D:177:GLN:HE22	1.75	0.51
1:A:316:ILE:CD1	1:A:327:ILE:HG12	2.41	0.51
1:A:539:LEU:HG	1:A:559:ALA:HA	1.92	0.51
1:A:372:LYS:HE2	1:A:397:GLU:OE2	2.11	0.51
1:A:246:TYR:HD1	1:A:253:MET:CE	2.23	0.50
1:A:483:HIS:CD2	1:A:484:ALA:N	2.79	0.50
2:C:209:PHE:HD1	2:C:210:ASN:CB	2.24	0.50
1:A:190:ILE:O	1:A:190:ILE:HG23	2.12	0.50
3:D:30:THR:HG22	3:D:31:ASN:OD1	2.11	0.50
1:A:322:LYS:O	1:A:323:ASP:HB2	2.12	0.50
2:C:124:GLN:HE22	2:C:131:SER:HB2	1.77	0.50
3:D:35:HIS:ND1	3:D:50:VAL:CG1	2.74	0.50
1:A:31:PHE:O	1:A:32:ASN:C	2.51	0.49
1:A:203:SER:HB2	1:A:204:PRO:HD2	1.94	0.49
2:C:129:THR:HG22	2:C:130:ALA:N	2.28	0.49
2:C:115:VAL:HG13	2:C:136:LEU:HD23	1.94	0.49
3:D:158:VAL:HG11	3:D:186:SER:CB	2.43	0.49
3:D:161:ASN:ND2	3:D:201:ILE:H	2.08	0.49
3:D:170:HIS:O	3:D:187:VAL:HG22	2.12	0.49
3:D:202:CYS:O	3:D:214:ASP:HA	2.12	0.49
3:D:85:LEU:HD13	3:D:89:ASP:HB3	1.94	0.49
3:D:6:GLN:HE21	3:D:110:GLY:HA3	1.78	0.48
1:A:117:GLN:NE2	1:A:185:LYS:HB2	2.29	0.48
1:A:403:ARG:O	1:A:433:SER:HB2	2.13	0.48
1:A:407:LYS:NZ	1:A:434:ASP:CG	2.67	0.48
3:D:123:LYS:HE2	3:D:124:GLY:O	2.13	0.48
1:A:418:SER:HA	1:A:441:GLY:O	2.14	0.48
2:C:141:PRO:O	2:C:198:HIS:HE1	1.96	0.47
2:C:129:THR:HA	2:C:182:SER:HA	1.96	0.47
2:C:50:TYR:OH	3:D:103:ASP:OD2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:55:ILE:HG22	2:C:58:ILE:HD13	1.97	0.47
3:D:153:PRO:O	3:D:206:HIS:HE1	1.97	0.47
2:C:32:ASN:HD22	2:C:92:ASN:HD22	1.62	0.47
3:D:207:LYS:N	3:D:208:PRO:HD2	2.28	0.47
1:A:84:ARG:NH2	1:A:227:CYS:O	2.48	0.47
2:C:76:ASN:O	2:C:77:SER:C	2.51	0.47
2:C:167:ASP:HB3	2:C:170:ASP:OD1	2.15	0.47
2:C:174:SER:O	3:D:172:PHE:HE2	1.97	0.47
2:C:125:LEU:HD21	2:C:186:TYR:HD2	1.80	0.47
2:C:124:GLN:HG3	3:D:128:PHE:CZ	2.50	0.47
1:A:458:GLY:H	1:A:462:GLN:NE2	2.07	0.46
3:D:15:SER:HA	3:D:84:SER:HA	1.97	0.46
3:D:35:HIS:CE1	3:D:50:VAL:HG13	2.50	0.46
2:C:123:GLU:HG2	2:C:124:GLN:N	2.30	0.46
3:D:170:HIS:HB2	3:D:187:VAL:HG23	1.98	0.45
1:A:546:THR:O	1:A:547:CYS:HB3	2.17	0.45
3:D:206:HIS:HD2	3:D:209:SER:OG	2.00	0.45
3:D:6:GLN:HE22	3:D:94:TYR:HA	1.80	0.45
4:B:6:MAN:C5	4:B:6:MAN:O6	2.64	0.45
1:A:318:ILE:HG22	1:A:319:GLY:N	2.31	0.45
1:A:311:LYS:H	1:A:339:THR:HB	1.81	0.44
1:A:154:MET:HA	1:A:154:MET:HE2	1.98	0.44
2:C:132:VAL:HB	2:C:179:LEU:HB3	1.98	0.44
1:A:126:PHE:H	1:A:154:MET:HE2	1.82	0.44
1:A:170:CYS:SG	1:A:175:CYS:HB3	2.58	0.44
3:D:166:THR:HG22	3:D:167:SER:N	2.33	0.44
1:A:495:GLU:O	1:A:498:ASP:HB2	2.18	0.44
3:D:149:LYS:HE2	3:D:177:GLN:NE2	2.32	0.44
2:C:2:ILE:HD11	2:C:29:ILE:HD12	1.99	0.44
1:A:146:SER:HA	1:A:149:LEU:HG	1.99	0.44
3:D:47:TRP:CZ2	3:D:50:VAL:HG22	2.51	0.44
1:A:485:LEU:HD13	1:A:512:VAL:HA	2.00	0.43
2:C:192:TYR:HB2	2:C:209:PHE:CZ	2.53	0.43
2:C:96:THR:HG21	3:D:104:TYR:CG	2.53	0.43
3:D:105:GLU:O	3:D:105:GLU:HG2	2.19	0.43
1:A:284:VAL:CG1	1:A:285:ARG:N	2.82	0.43
2:C:39:ARG:O	2:C:40:THR:C	2.56	0.43
3:D:172:PHE:HE1	3:D:187:VAL:HG22	1.83	0.43
1:A:546:THR:O	1:A:546:THR:CG2	2.66	0.43
3:D:2:VAL:HG13	3:D:27:PHE:CD2	2.53	0.43
2:C:124:GLN:HG3	3:D:128:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PRO:HA	1:A:242:PRO:HD3	1.77	0.43
1:A:167:ASP:OD1	1:A:169:SER:HB2	2.17	0.43
1:A:586:TYR:O	1:A:593:CYS:HA	2.18	0.43
1:A:609:LEU:C	1:A:611:GLY:H	2.22	0.42
2:C:16:GLY:C	2:C:77:SER:HA	2.39	0.42
3:D:51:ILE:HG23	3:D:51:ILE:O	2.18	0.42
3:D:72:ASP:OD1	3:D:72:ASP:C	2.57	0.42
1:A:35:GLU:OE1	1:A:59:GLN:NE2	2.50	0.42
3:D:132:PRO:HG2	3:D:219:PRO:HD3	2.01	0.42
3:D:39:GLN:O	3:D:91:ALA:HB1	2.19	0.42
2:C:11:LEU:HD21	2:C:19:VAL:CG1	2.49	0.42
1:A:252:GLN:HE21	1:A:252:GLN:CA	2.33	0.42
1:A:350:VAL:HG22	7:A:5798:HOH:O	2.19	0.42
1:A:526:VAL:HA	1:A:530:GLU:O	2.19	0.42
2:C:186:TYR:O	2:C:187:GLU:CB	2.59	0.42
2:C:16:GLY:O	2:C:77:SER:HA	2.20	0.42
2:C:80:SER:HA	2:C:106:LEU:CD1	2.43	0.42
1:A:98:LEU:HD21	1:A:125:ARG:HG2	2.01	0.42
2:C:107:LYS:HA	2:C:140:TYR:OH	2.19	0.42
2:C:21:PHE:O	2:C:72:THR:HA	2.19	0.42
3:D:160:TRP:HZ2	3:D:186:SER:O	2.03	0.42
1:A:344:ASP:OD1	1:A:379:GLY:HA3	2.20	0.41
2:C:174:SER:O	3:D:172:PHE:CE2	2.73	0.41
1:A:513:ASP:OD1	1:A:513:ASP:N	2.48	0.41
1:A:7:CYS:SG	1:A:37:VAL:HG22	2.60	0.41
2:C:3:LEU:HD23	2:C:3:LEU:HA	1.86	0.41
2:C:47:LEU:HA	2:C:58:ILE:HG12	2.01	0.41
3:D:172:PHE:HE1	3:D:187:VAL:CG2	2.33	0.41
3:D:67:LEU:HA	3:D:67:LEU:HD12	1.71	0.41
1:A:209:HIS:HD2	1:A:211:GLN:N	2.07	0.41
1:A:509:ARG:NE	1:A:509:ARG:H	2.19	0.41
1:A:517:LEU:O	1:A:518:LEU:HB2	2.19	0.41
1:A:138:ILE:CD1	1:A:184:GLN:HG3	2.49	0.41
4:B:4:MAN:C6	4:B:5:MAN:H5	2.44	0.41
1:A:187:THR:O	1:A:199:CYS:SG	2.79	0.41
1:A:568:VAL:HG11	7:A:5818:HOH:O	2.21	0.41
2:C:122:ASP:O	2:C:123:GLU:HB3	2.21	0.41
1:A:454:LYS:HD2	1:A:454:LYS:N	2.36	0.41
2:C:111:ALA:O	2:C:139:PHE:HA	2.21	0.41
1:A:252:GLN:HE21	1:A:252:GLN:C	2.24	0.40
1:A:487:SER:C	1:A:489:GLU:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:LYS:HB3	2:C:152:ASN:HA	2.01	0.40
1:A:517:LEU:O	1:A:518:LEU:CB	2.69	0.40
1:A:423:SER:HB2	1:A:492:TRP: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	611/624 (98%)	543 (89%)	60 (10%)	8 (1%)	12	24
2	C	209/213 (98%)	189 (90%)	17 (8%)	3 (1%)	11	22
3	D	218/221 (99%)	200 (92%)	16 (7%)	2 (1%)	17	35
All	All	1038/1058 (98%)	932 (90%)	93 (9%)	13 (1%)	12	24

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	GLY
2	C	187	GLU
3	D	138	SER
1	A	507	ARG
2	C	77	SER
2	C	152	ASN
1	A	221	GLU
1	A	297	ASP
1	A	610	ARG
1	A	279	ASP
1	A	521	GLU
3	D	15	SER
1	A	488	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	520/545 (95%)	479 (92%)	41 (8%)	12	24
2	C	184/188 (98%)	163 (89%)	21 (11%)	5	10
3	D	186/191 (97%)	168 (90%)	18 (10%)	8	15
All	All	890/924 (96%)	810 (91%)	80 (9%)	9	18

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	74	ARG
1	A	105	LYS
1	A	106	THR
1	A	158	ASN
1	A	167	ASP
1	A	199	CYS
1	A	231	ARG
1	A	249	THR
1	A	250	THR
1	A	252	GLN
1	A	255	VAL
1	A	266	THR
1	A	268	VAL
1	A	279	ASP
1	A	280	HIS
1	A	294	MET
1	A	304	LYS
1	A	310	ARG
1	A	316	ILE
1	A	320	GLU
1	A	327	ILE
1	A	339	THR
1	A	350	VAL
1	A	378	THR
1	A	390	ARG

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Mol	Chain	Res	Type
1	A	391	THR
1	A	460	SER
1	A	464	THR
1	A	474	LYS
1	A	478	THR
1	A	505	VAL
1	A	507	ARG
1	A	509	ARG
1	A	514	LYS
1	A	553	ASP
1	A	556	ILE
1	A	562	ILE
1	A	570	THR
1	A	580	ASN
1	A	610	ARG
2	C	2	ILE
2	C	20	SER
2	C	22	SER
2	C	29	ILE
2	C	49	LYS
2	C	55	ILE
2	C	61	ARG
2	C	67	SER
2	C	77	SER
2	C	78	VAL
2	C	80	SER
2	C	81	GLU
2	C	97	THR
2	C	114	SER
2	C	123	GLU
2	C	125	LEU
2	C	134	CYS
2	C	137	ASN
2	C	168	SER
2	C	176	SER
2	C	202	SER
3	D	1	GLN
3	D	15	SER
3	D	30	THR
3	D	43	LYS
3	D	50	VAL
3	D	85	LEU

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Mol	Chain	Res	Type
3	D	87	SER
3	D	100	THR
3	D	105	GLU
3	D	141	THR
3	D	166	THR
3	D	184	LEU
3	D	189	THR
3	D	190	VAL
3	D	192	SER
3	D	202	CYS
3	D	207	LYS
3	D	218	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	134	ASN
1	A	158	ASN
1	A	209	HIS
1	A	252	GLN
1	A	280	HIS
1	A	462	GLN
1	A	483	HIS
1	A	535	HIS
1	A	541	GLN
1	A	580	ASN
2	C	6	GLN
2	C	92	ASN
2	C	137	ASN
2	C	160	GLN
2	C	198	HIS
3	D	1	GLN
3	D	6	GLN
3	D	70	ASN
3	D	161	ASN
3	D	177	GLN
3	D	203	ASN
3	D	206	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

15 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	B	1	1,4	14,14,15	0.56	0	17,19,21	1.63	4 (23%)
4	NAG	B	2	4	14,14,15	0.65	0	17,19,21	1.51	1 (5%)
4	BMA	B	3	4	11,11,12	0.75	0	15,15,17	1.58	3 (20%)
4	MAN	B	4	4	11,11,12	0.91	0	15,15,17	1.66	5 (33%)
4	MAN	B	5	4	11,11,12	0.97	1 (9%)	15,15,17	2.46	4 (26%)
4	MAN	B	6	4	11,11,12	3.72	2 (18%)	15,15,17	2.13	3 (20%)
4	MAN	B	7	4	11,11,12	0.63	0	15,15,17	1.21	1 (6%)
4	MAN	B	8	4	11,11,12	1.50	2 (18%)	15,15,17	2.39	6 (40%)
4	MAN	B	9	4	11,11,12	1.53	2 (18%)	15,15,17	1.34	1 (6%)
5	NAG	E	1	1,5	14,14,15	0.50	0	17,19,21	1.64	4 (23%)
5	NAG	E	2	5	14,14,15	0.57	0	17,19,21	1.21	1 (5%)
5	NAG	F	1	1,5	14,14,15	0.73	0	17,19,21	1.36	1 (5%)
5	NAG	F	2	5	14,14,15	0.52	0	17,19,21	1.44	1 (5%)
5	NAG	G	1	1,5	14,14,15	0.82	1 (7%)	17,19,21	1.19	2 (11%)
5	NAG	G	2	5	14,14,15	0.49	0	17,19,21	1.44	3 (17%)

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	B	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	BMA	B	3	4	-	2/2/19/22	0/1/1/1
4	MAN	B	4	4	-	2/2/19/22	0/1/1/1
4	MAN	B	5	4	-	2/2/19/22	0/1/1/1
4	MAN	B	6	4	-	2/2/19/22	1/1/1/1
4	MAN	B	7	4	-	0/2/19/22	0/1/1/1
4	MAN	B	8	4	-	1/2/19/22	0/1/1/1
4	MAN	B	9	4	-	0/2/19/22	1/1/1/1
5	NAG	E	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	NAG	G	1	1,5	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	G	2	5	1/1/5/7	4/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	6	MAN	O6-C6	11.80	1.92	1.42
4	B	8	MAN	O5-C1	3.16	1.48	1.43
4	B	6	MAN	C6-C5	2.97	1.61	1.51
4	B	5	MAN	O6-C6	2.80	1.54	1.42
4	B	9	MAN	O5-C5	2.67	1.48	1.43
4	B	9	MAN	C2-C3	2.58	1.56	1.52
5	G	1	NAG	C1-C2	2.28	1.55	1.52
4	B	8	MAN	C6-C5	2.13	1.59	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	6	MAN	C1-O5-C5	5.94	120.24	112.19
4	B	5	MAN	C1-O5-C5	5.86	120.13	112.19
4	B	8	MAN	O3-C3-C4	5.50	123.08	110.35
4	B	5	MAN	O2-C2-C1	5.07	119.52	109.15
4	B	6	MAN	O6-C6-C5	-4.39	96.23	111.29
5	E	1	NAG	C1-O5-C5	4.32	118.04	112.19
4	B	2	NAG	C1-O5-C5	4.25	117.94	112.19
4	B	8	MAN	O5-C1-C2	-4.19	104.30	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5	MAN	O2-C2-C3	-3.72	102.69	110.14
5	F	2	NAG	C1-O5-C5	3.56	117.02	112.19
4	B	1	NAG	O5-C1-C2	-3.47	105.81	111.29
4	B	8	MAN	O3-C3-C2	-3.38	103.51	109.99
4	B	3	BMA	O5-C5-C6	3.37	112.49	107.20
4	B	3	BMA	O5-C1-C2	-3.37	105.57	110.77
4	B	6	MAN	O5-C5-C6	3.29	112.36	107.20
4	B	7	MAN	O5-C5-C6	3.29	112.35	107.20
4	B	1	NAG	O7-C7-C8	-3.22	116.08	122.06
5	G	2	NAG	C1-O5-C5	3.11	116.41	112.19
5	E	1	NAG	C4-C3-C2	2.99	115.39	111.02
5	G	1	NAG	C1-O5-C5	2.89	116.11	112.19
5	F	1	NAG	O5-C1-C2	-2.87	106.76	111.29
5	E	1	NAG	O5-C1-C2	-2.70	107.02	111.29
4	B	4	MAN	C1-O5-C5	2.69	115.84	112.19
5	G	2	NAG	C3-C4-C5	2.65	114.97	110.24
4	B	4	MAN	C2-C3-C4	-2.65	106.31	110.89
4	B	4	MAN	O3-C3-C4	2.63	116.43	110.35
4	B	1	NAG	C1-O5-C5	2.61	115.73	112.19
5	G	2	NAG	O5-C1-C2	-2.58	107.22	111.29
4	B	9	MAN	O5-C1-C2	2.57	114.74	110.77
4	B	4	MAN	O2-C2-C1	2.53	114.32	109.15
4	B	8	MAN	C3-C4-C5	2.48	114.66	110.24
4	B	8	MAN	O6-C6-C5	2.47	119.77	111.29
4	B	3	BMA	C1-C2-C3	2.39	112.61	109.67
4	B	5	MAN	O5-C5-C6	2.32	110.85	107.20
4	B	4	MAN	O5-C5-C6	2.27	110.76	107.20
4	B	8	MAN	C2-C3-C4	-2.21	107.07	110.89
5	G	1	NAG	O4-C4-C3	2.17	115.36	110.35
5	E	2	NAG	C8-C7-N2	2.10	119.66	116.10
5	E	1	NAG	O4-C4-C3	-2.07	105.56	110.35
4	B	1	NAG	O7-C7-N2	2.04	125.70	121.95

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	1	NAG	C1
5	G	2	NAG	C1

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	2	NAG	C8-C7-N2-C2
5	F	2	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
4	B	5	MAN	O5-C5-C6-O6
4	B	5	MAN	C4-C5-C6-O6
4	B	6	MAN	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
4	B	4	MAN	O5-C5-C6-O6
5	E	1	NAG	C8-C7-N2-C2
5	G	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
4	B	4	MAN	C4-C5-C6-O6
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	G	1	NAG	C4-C5-C6-O6
4	B	6	MAN	C4-C5-C6-O6
4	B	3	BMA	C4-C5-C6-O6
5	G	1	NAG	C8-C7-N2-C2
4	B	3	BMA	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	G	1	NAG	O7-C7-N2-C2
4	B	8	MAN	O5-C5-C6-O6

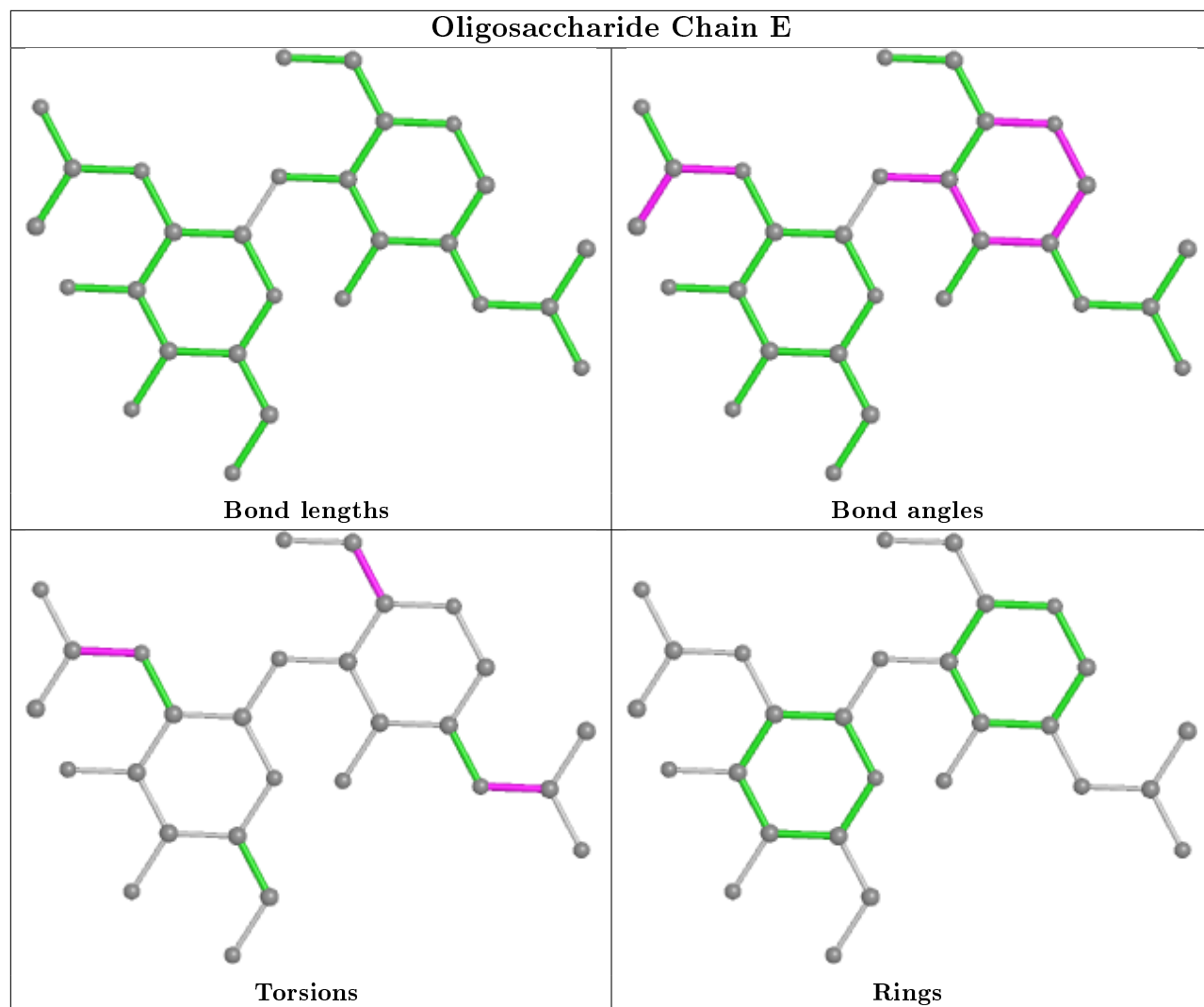
All (2) ring outliers are listed below:

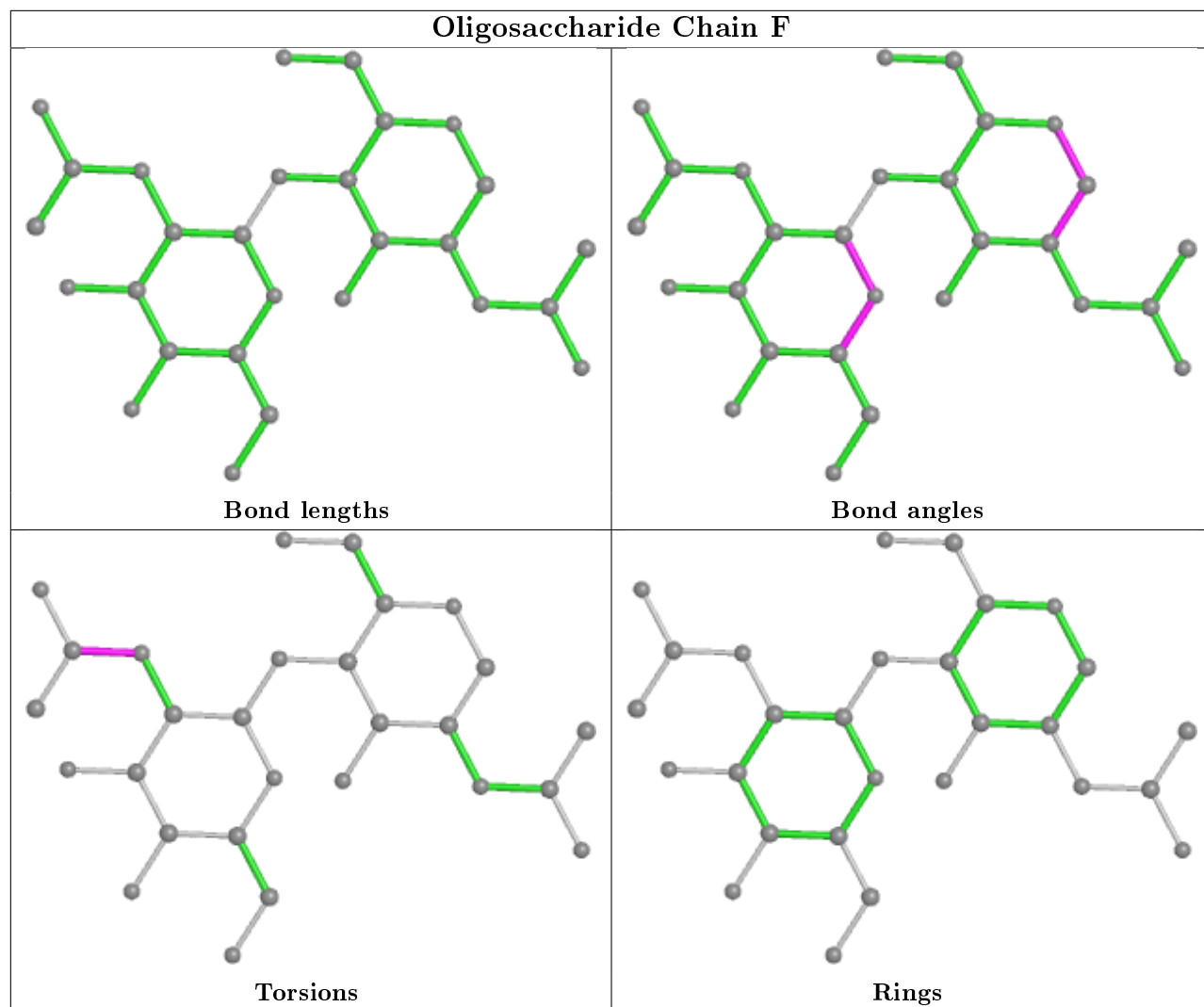
Mol	Chain	Res	Type	Atoms
4	B	9	MAN	C1-C2-C3-C4-C5-O5
4	B	6	MAN	C1-C2-C3-C4-C5-O5

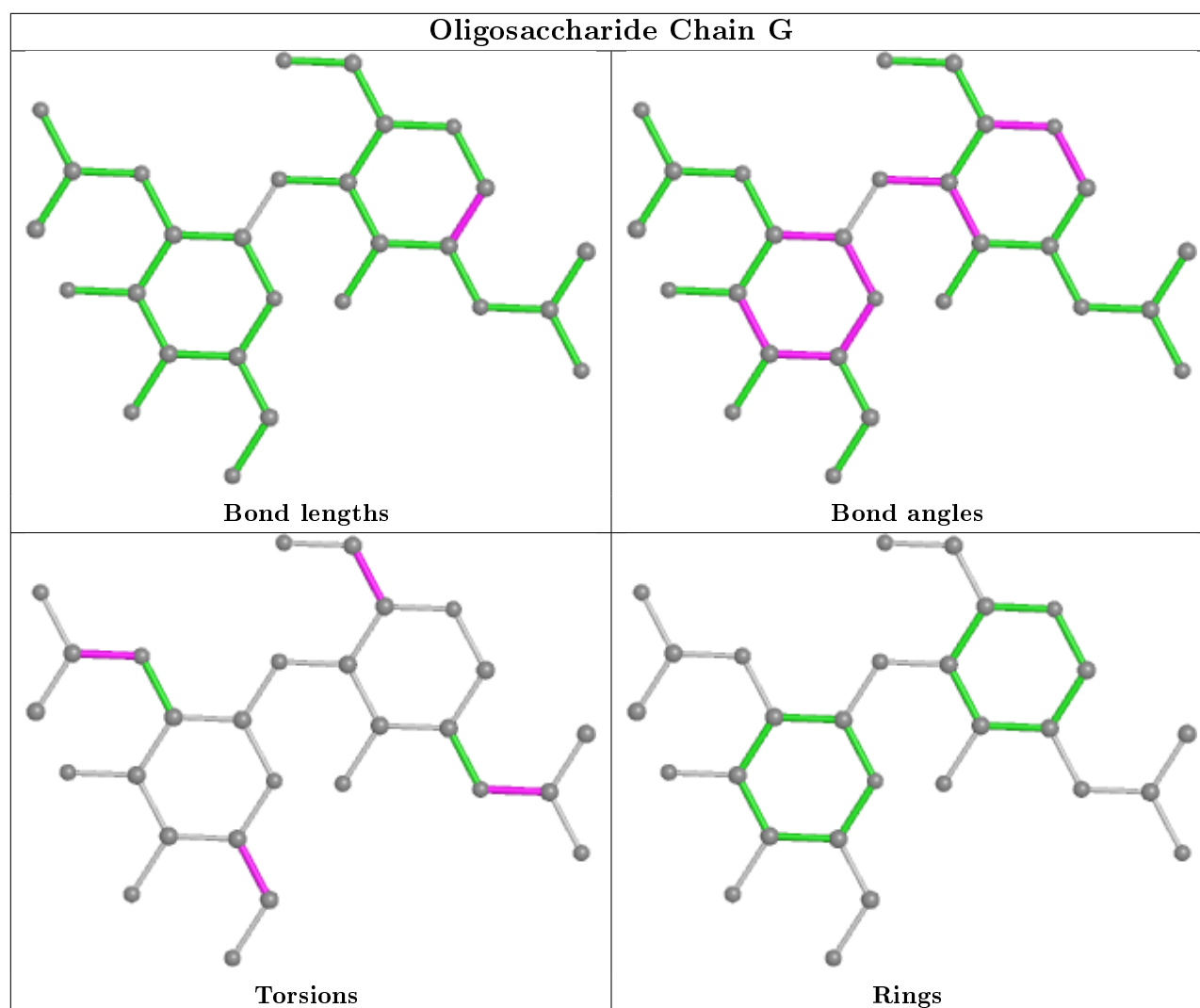
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4	MAN	3	0
4	B	6	MAN	2	0
4	B	5	MAN	3	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 ⓘ

5 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	$\# Z > 2$
6	NAG	D	881	3	14,14,15	0.61	0	17,19,21	1.70	3 (17%)
6	NAG	A	5041	1	14,14,15	0.87	1 (7%)	17,19,21	1.43	2 (11%)
6	NAG	A	625	1	14,14,15	0.98	1 (7%)	17,19,21	1.75	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	3891	1	14,14,15	0.74	0	17,19,21	1.51	4 (23%)
6	NAG	A	5441	1	14,14,15	0.70	0	17,19,21	1.54	3 (17%)

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
6	NAG	D	881	3	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	A	5041	1	1/1/5/7	6/6/23/26	0/1/1/1
6	NAG	A	625	1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	A	3891	1	-	3/6/23/26	0/1/1/1
6	NAG	A	5441	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	625	NAG	C1-C2	2.80	1.56	1.52
6	A	5041	NAG	C1-C2	2.25	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	881	NAG	C1-O5-C5	4.70	118.56	112.19
6	A	5441	NAG	C1-O5-C5	4.13	117.79	112.19
6	A	3891	NAG	C2-N2-C7	4.10	128.74	122.90
6	A	625	NAG	O5-C1-C2	-3.66	105.51	111.29
6	D	881	NAG	C2-N2-C7	3.43	127.79	122.90
6	A	5041	NAG	O3-C3-C2	3.00	115.67	109.47
6	A	625	NAG	O5-C5-C6	2.91	111.76	107.20
6	A	625	NAG	C1-O5-C5	-2.82	108.37	112.19
6	D	881	NAG	O5-C5-C6	2.82	111.63	107.20
6	A	3891	NAG	C8-C7-N2	2.52	120.36	116.10
6	A	5441	NAG	O5-C1-C2	2.42	115.10	111.29
6	A	5041	NAG	O5-C1-C2	-2.32	107.62	111.29
6	A	3891	NAG	O7-C7-C8	-2.21	117.95	122.06
6	A	625	NAG	C3-C4-C5	-2.07	106.55	110.24
6	A	3891	NAG	O5-C5-C6	2.06	110.44	107.20
6	A	5441	NAG	C4-C3-C2	2.05	114.02	111.02

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	D	881	NAG	C1
6	A	5041	NAG	C1
6	A	625	NAG	C1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	881	NAG	C3-C2-N2-C7
6	D	881	NAG	C8-C7-N2-C2
6	D	881	NAG	O7-C7-N2-C2
6	A	5041	NAG	C8-C7-N2-C2
6	A	5041	NAG	O7-C7-N2-C2
6	A	3891	NAG	C3-C2-N2-C7
6	A	3891	NAG	C8-C7-N2-C2
6	A	3891	NAG	O7-C7-N2-C2
6	A	625	NAG	C8-C7-N2-C2
6	A	625	NAG	O7-C7-N2-C2
6	A	625	NAG	O5-C5-C6-O6
6	A	5441	NAG	O5-C5-C6-O6
6	A	5441	NAG	C4-C5-C6-O6
6	A	5041	NAG	O5-C5-C6-O6
6	A	625	NAG	C4-C5-C6-O6
6	A	5041	NAG	C4-C5-C6-O6
6	A	5041	NAG	C3-C2-N2-C7
6	A	5041	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	3891	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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

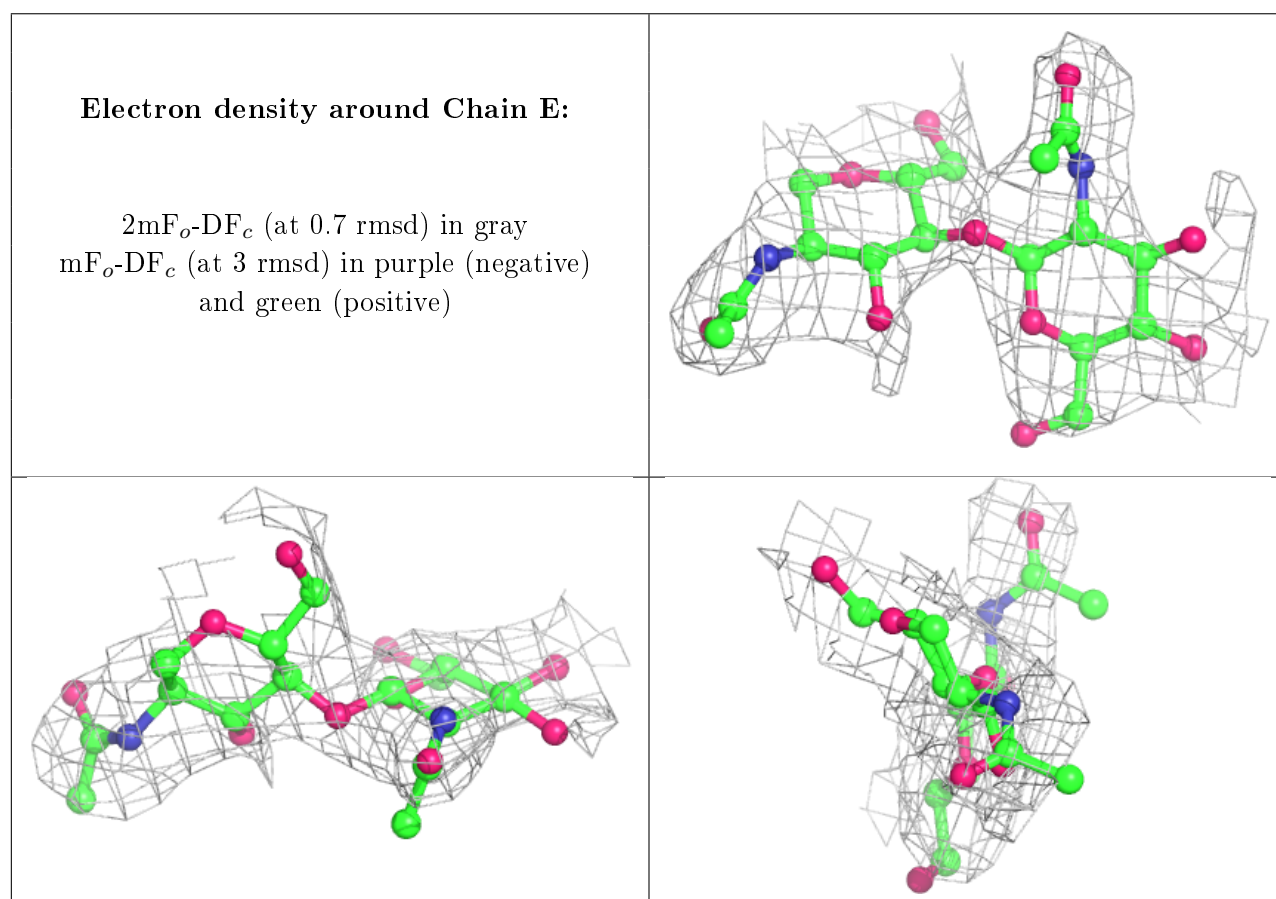
6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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6.3 Carbohydrates [i](#)

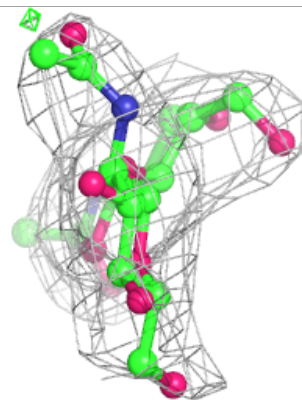
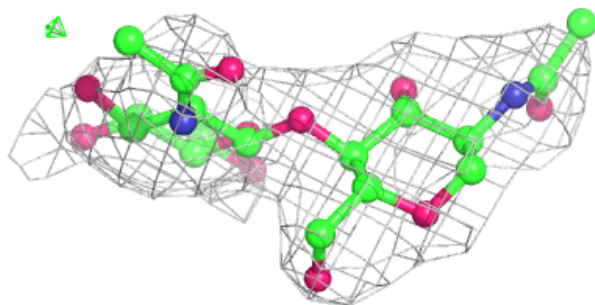
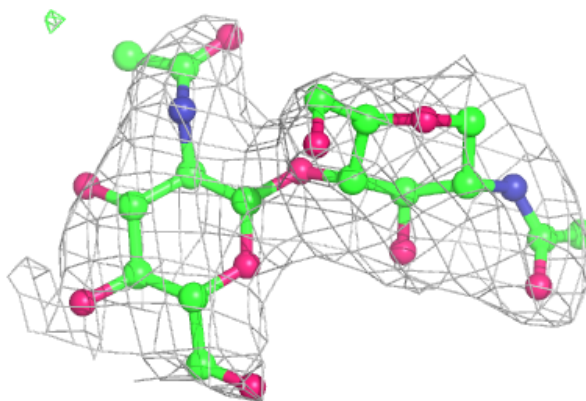
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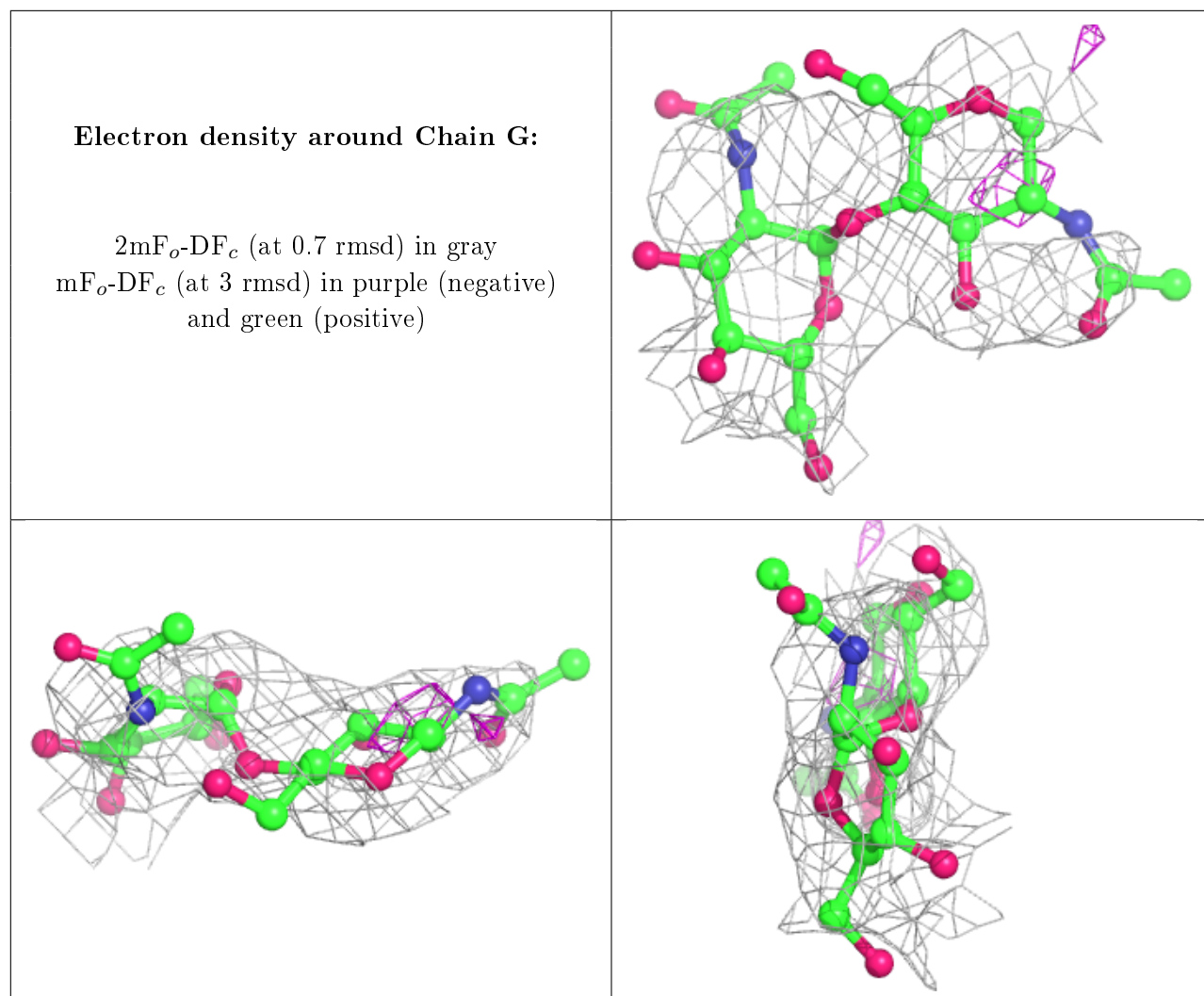
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain F:

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





6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.