



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:46 PM UTC

PDB ID : 1YY9 / pdb_00001yy9
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

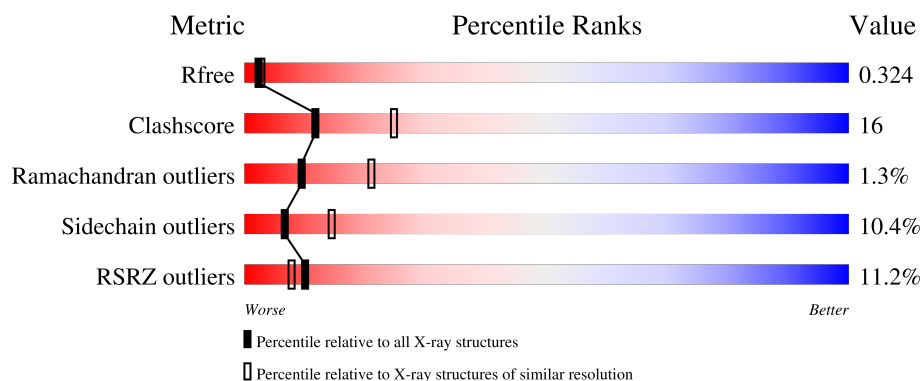
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	624	8% 67% 27% • •
2	C	213	9% 59% 34% 6% •
3	D	221	21% 66% 25% 8%
4	B	9	67% 33%
5	E	2	100%

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Mol	Chain	Length	Quality of chain
5	F	2	 100%
5	G	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	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

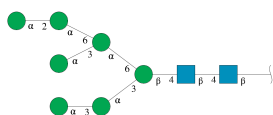
- Molecule 2 is a protein called Cetuximab Fab Light chain.

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.



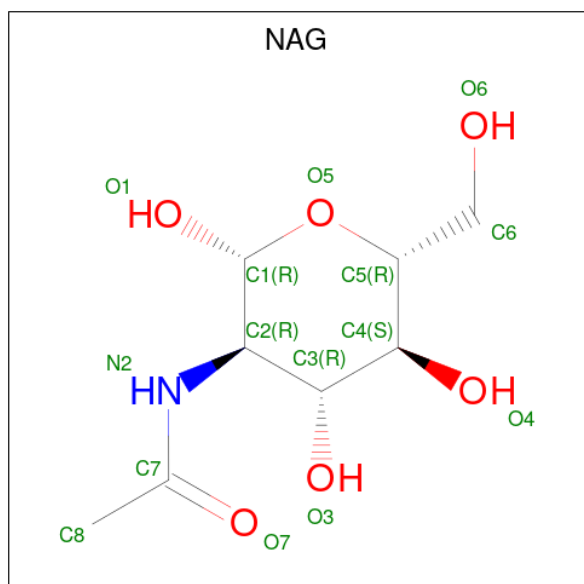
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	9	Total	C	N	O	0	0	0
			105	58	2	45			

- 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 (CCD ID: 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		

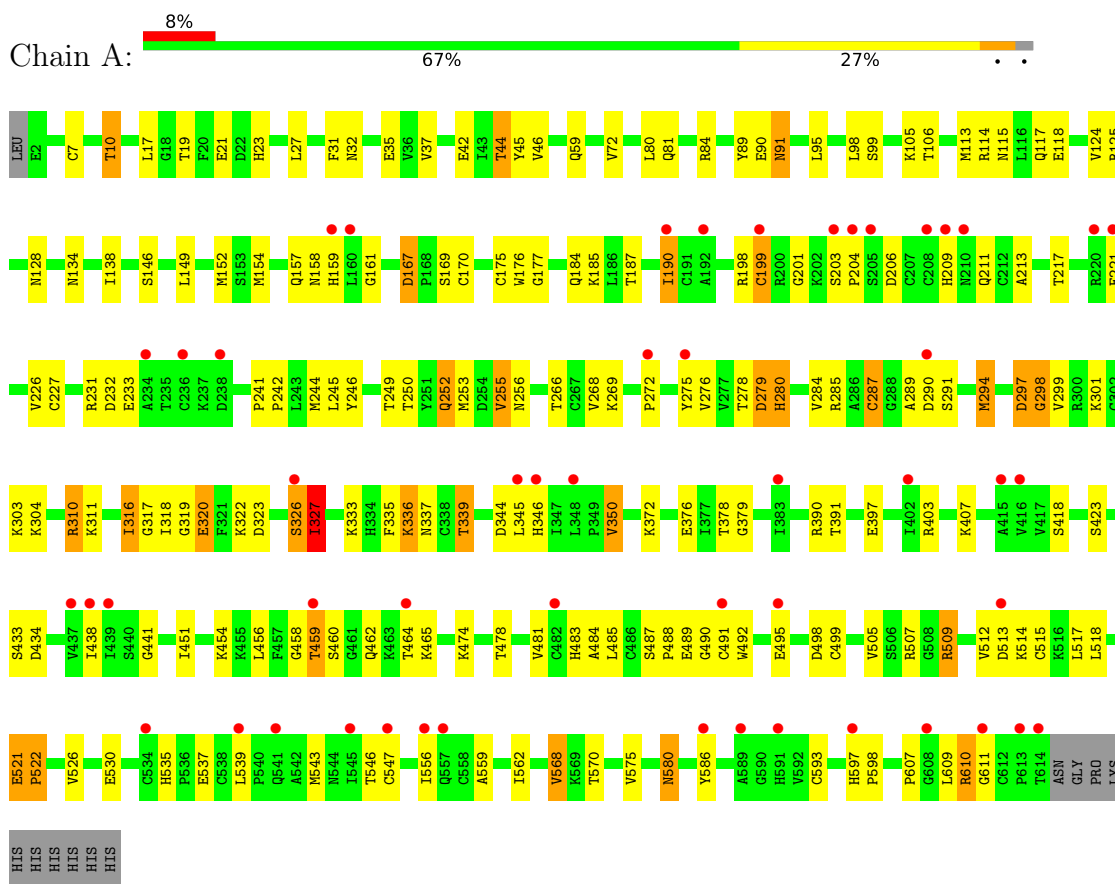
- Molecule 7 is water.

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		

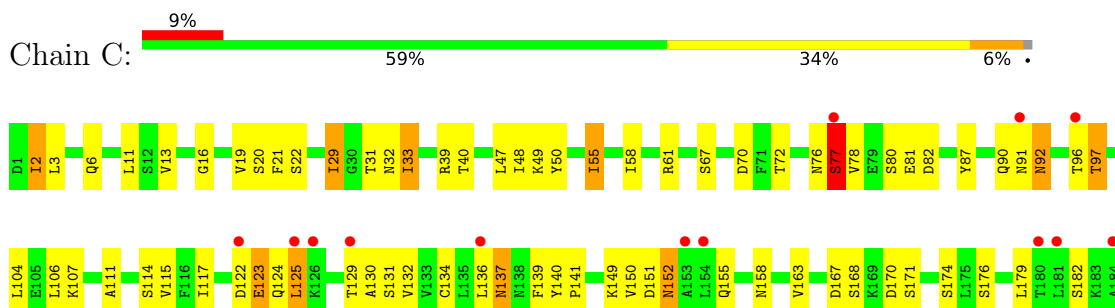
3 Residue-property plots

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: Epidermal Growth Factor Receptor

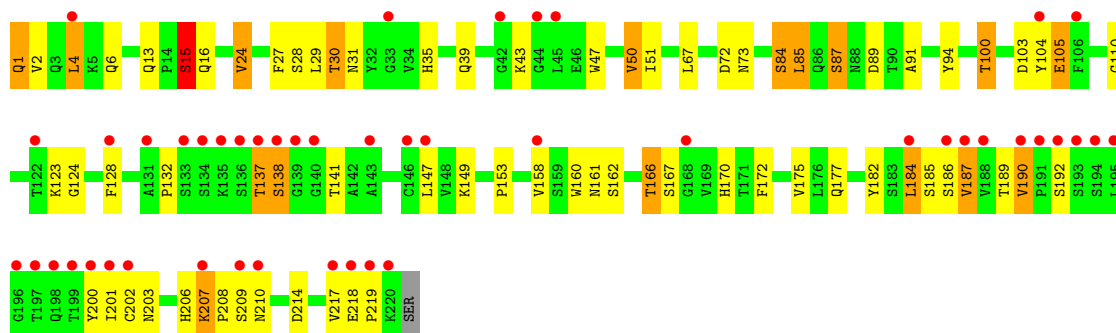


• Molecule 2: Cetuximab Fab Light chain





- Molecule 3: Cetuximab Fab Heavy chain



- 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



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



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



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



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 40.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.00-2.60) 98.2 (40.00-2.60)	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 , 0.324	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)	0.34 , 34.9	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

5.1 Standard geometry

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

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	0.81	1/4745 (0.0%)	1.03	7/6426 (0.1%)
2	C	0.79	2/1643 (0.1%)	1.06	2/2237 (0.1%)
3	D	0.83	1/1692 (0.1%)	1.01	3/2316 (0.1%)
All	All	0.81	4/8080 (0.0%)	1.03	12/10979 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	182	TYR	C-N	-5.59	1.26	1.33
2	C	70	ASP	C-O	5.32	1.30	1.24
1	A	95	LEU	N-CA	5.09	1.52	1.46
2	C	33	ILE	CA-CB	5.03	1.61	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	SER	N-CA-C	6.32	118.56	109.14
3	D	187	VAL	N-CA-C	6.24	118.38	108.89
2	C	92	ASN	N-CA-C	5.77	118.44	111.40
1	A	490	GLY	N-CA-C	5.58	119.98	112.17
1	A	287	CYS	N-CA-C	5.52	118.45	110.28
1	A	327	ILE	N-CA-C	-5.49	102.11	109.30
1	A	522	PRO	CB-CA-C	5.34	120.37	111.56
2	C	185	ASP	N-CA-C	-5.28	104.96	111.40
1	A	118	GLU	N-CA-C	5.21	117.90	109.40
3	D	190	VAL	N-CA-C	5.17	113.43	109.19
3	D	217	VAL	N-CA-C	5.07	114.78	106.72
1	A	327	ILE	CB-CA-C	-5.02	103.78	111.71

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	4653	0	4451	129	0
2	C	1609	0	1535	61	0
3	D	1648	0	1584	68	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
7	C	6	0	0	0	0
7	D	15	0	0	0	0
All	All	8225	0	7798	253	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 16.

All (253) 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
1:A:149:LEU:HA	1:A:152:MET:HE2	1.61	0.82
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE21	3:D:1:GLN:H1	1.31	0.78
1:A:458:GLY:H	1:A:462:GLN:HE22	1.32	0.78
1:A:244:MET:HE2	1:A:255:VAL:HA	1.66	0.77
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: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
3:D:162:SER:H	3:D:203:ASN:ND2	1.88	0.70
3:D:1:GLN:HE21	3:D:1:GLN:N	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:246:TYR:HD1	1:A:253:MET:HE1	1.57	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:OE1	1:A:320:GLU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:543:MET:HE2	1:A:543:MET:HA	1.82	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
1:A:253:MET:HE1	1:A:575:VAL:HG11	1.83	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:89:TYR:CD2	1:A:90:GLU:HB2	2.37	0.60
1:A:114:ARG:HA	1:A:176:TRP:CD1	2.37	0.60
2:C:136:LEU:CD2	2:C:196:VAL:HG21	2.28	0.60
1:A:535:HIS:CD2	1:A:537:GLU:HB2	2.37	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
3:D:184:LEU:HG	3:D:185:SER:N	2.19	0.58
1:A:90:GLU:O	1:A:91:ASN:C	2.45	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:OE1	3:D:16:GLN:HA	2.04	0.57
1:A:244:MET:CE	1:A:255:VAL:HA	2.32	0.57
1:A:294:MET:HE3	1:A:294:MET:C	2.30	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
1:A:80:LEU:HD23	1:A:113:MET:HE1	1.87	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:597:HIS:ND1	1:A:598:PRO:HD2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:31:PHE:O	1:A:32:ASN:C	2.51	0.54
7:A:5797:HOH:O	3:D:100:THR:CG2	2.55	0.54
1:A:46:VAL:HG12	1:A:72:VAL:HB	1.89	0.54
1:A:154:MET:HE2	1:A:154:MET:HA	1.89	0.54
6:A:3891:NAG:H83	6:A:3891:NAG:H3	1.90	0.53
2:C:50:TYR:OH	3:D:103:ASP:OD2	2.27	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
1:A:407:LYS:NZ	1:A:434:ASP:CG	2.67	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
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
1:A:149:LEU:HA	1:A:152:MET:CE	2.36	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:76:ASN:O	2:C:77:SER:C	2.51	0.52
2:C:31:THR:O	2:C:50:TYR:HA	2.10	0.52
2:C:151:ASP:O	2:C:152:ASN:HB2	2.09	0.52
3:D:29:LEU:HB2	3:D:73:ASN:OD1	2.10	0.51
1:A:407:LYS:HZ1	1:A:434:ASP:CG	2.17	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:483:HIS:CD2	1:A:484:ALA:N	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:209:PHE:HD1	2:C:210:ASN:CB	2.24	0.50
1:A:190:ILE:HG23	1:A:190:ILE:O	2.12	0.50
1:A:246:TYR:HD1	1:A:253:MET:CE	2.23	0.50
3:D:30:THR:HG22	3:D:31:ASN:OD1	2.11	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:203:SER:HB2	1:A:204:PRO:HD2	1.94	0.49
1:A:124:VAL:O	1:A:154:MET:HE3	2.12	0.49
2:C:129:THR:HG22	2:C:130:ALA:N	2.28	0.49
1:A:322:LYS:O	1:A:323:ASP:HB2	2.12	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:85:LEU:HD13	3:D:89:ASP:HB3	1.94	0.49
3:D:202:CYS:O	3:D:214:ASP:HA	2.12	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:294:MET:HE2	1:A:301:LYS:HB2	1.95	0.48
1:A:403:ARG:O	1:A:433:SER:HB2	2.13	0.48
2:C:39:ARG:O	2:C:40:THR:C	2.56	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
1:A:609:LEU:C	1:A:611:GLY:H	2.22	0.47
2:C:16:GLY:C	2:C:77:SER:HA	2.39	0.47
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: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:124:GLN:HG3	3:D:128:PHE:CZ	2.50	0.47
2:C:125:LEU:HD21	2:C:186:TYR:HD2	1.80	0.47
1:A:465:LYS:HZ2	3:D:100:THR:HG21	1.77	0.47
3:D:72:ASP:OD1	3:D:72:ASP:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:123:GLU:HG2	2:C:124:GLN:N	2.30	0.46
1:A:487:SER:C	1:A:489:GLU:H	2.24	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:6:GLN:HE22	3:D:94:TYR:HA	1.80	0.45
3:D:206:HIS:HD2	3:D:209:SER:OG	2.00	0.45
4:B:6:MAN:O6	4:B:6:MAN:C5	2.64	0.45
1:A:318:ILE:HG22	1:A:319:GLY:N	2.31	0.45
1:A:252:GLN:HE21	1:A:252:GLN:C	2.24	0.45
1:A:311:LYS:H	1:A:339:THR:HB	1.81	0.44
2:C:132:VAL:HB	2:C:179:LEU:HB3	1.98	0.44
2:C:47:LEU:C	2:C:48:ILE:HG12	2.42	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:96:THR:HG21	3:D:104:TYR:CG	2.53	0.43
2:C:192:TYR:HB2	2:C:209:PHE:CZ	2.53	0.43
3:D:105:GLU:O	3:D:105:GLU:HG2	2.19	0.43
2:C:209:PHE:C	2:C:209:PHE:CD1	2.96	0.43
3:D:172:PHE:HE1	3:D:187:VAL:HG22	1.83	0.43
1:A:465:LYS:HZ1	3:D:100:THR:HG21	1.81	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
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:284:VAL:CG1	1:A:285:ARG:N	2.82	0.43
1:A:586:TYR:O	1:A:593:CYS:HA	2.18	0.43
3:D:51:ILE:HG23	3:D:51:ILE:O	2.18	0.42
1:A:278:THR:C	1:A:280:HIS:H	2.27	0.42
1:A:35:GLU:OE1	1:A:59:GLN:NE2	2.50	0.42
1:A:333:LYS:C	1:A:335:PHE:H	2.26	0.42
3:D:210:ASN:O	3:D:210:ASN:CG	2.62	0.42
3:D:39:GLN:O	3:D:91:ALA:HB1	2.19	0.42
3:D:132:PRO:HG2	3:D:219:PRO:HD3	2.01	0.42
1:A:407:LYS:NZ	1:A:434:ASP:OD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASP:O	1:A:298:GLY:C	2.63	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:150:VAL:C	2:C:152:ASN:H	2.27	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:21:PHE:O	2:C:72:THR:HA	2.19	0.42
2:C:107:LYS:HA	2:C:140:TYR:OH	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:7:CYS:SG	1:A:37:VAL:HG22	2.60	0.41
1:A:513:ASP:OD1	1:A:513:ASP:N	2.48	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:HD12	3:D:67:LEU:HA	1.71	0.41
1:A:209:HIS:HD2	1:A:211:GLN:N	2.07	0.41
1:A:509:ARG:H	1:A:509:ARG:NE	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
3:D:87:SER:C	3:D:89:ASP:N	2.77	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
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
1:A:580:ASN:HD22	1:A:580:ASN:C	2.29	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%)	9	21
2	C	209/213 (98%)	189 (90%)	17 (8%)	3 (1%)	9	19
3	D	218/221 (99%)	200 (92%)	16 (7%)	2 (1%)	14	30
All	All	1038/1058 (98%)	932 (90%)	93 (9%)	13 (1%)	9	21

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 [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	520/545 (95%)	473 (91%)	47 (9%)	9	20
2	C	184/188 (98%)	160 (87%)	24 (13%)	4	8
3	D	186/191 (97%)	164 (88%)	22 (12%)	5	10
All	All	890/924 (96%)	797 (90%)	93 (10%)	7	14

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	27	LEU
1	A	44	THR
1	A	91	ASN
1	A	105	LYS
1	A	106	THR
1	A	167	ASP
1	A	190	ILE
1	A	199	CYS
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	269	LYS
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	336	LYS
1	A	339	THR
1	A	350	VAL
1	A	378	THR
1	A	390	ARG
1	A	391	THR
1	A	438	ILE
1	A	456	LEU
1	A	459	THR
1	A	460	SER

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Mol	Chain	Res	Type
1	A	464	THR
1	A	474	LYS
1	A	478	THR
1	A	481	VAL
1	A	499	CYS
1	A	505	VAL
1	A	509	ARG
1	A	514	LYS
1	A	556	ILE
1	A	562	ILE
1	A	568	VAL
1	A	570	THR
1	A	580	ASN
2	C	2	ILE
2	C	13	VAL
2	C	20	SER
2	C	22	SER
2	C	29	ILE
2	C	33	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	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	163	VAL
2	C	168	SER
2	C	176	SER
2	C	185	ASP
2	C	202	SER
3	D	1	GLN
3	D	4	LEU
3	D	15	SER
3	D	24	VAL
3	D	30	THR

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Mol	Chain	Res	Type
3	D	43	LYS
3	D	50	VAL
3	D	84	SER
3	D	85	LEU
3	D	87	SER
3	D	100	THR
3	D	105	GLU
3	D	137	THR
3	D	141	THR
3	D	166	THR
3	D	175	VAL
3	D	184	LEU
3	D	189	THR
3	D	190	VAL
3	D	192	SER
3	D	207	LYS
3	D	218	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	23	HIS
1	A	134	ASN
1	A	158	ASN
1	A	164	GLN
1	A	209	HIS
1	A	210	ASN
1	A	252	GLN
1	A	280	HIS
1	A	462	GLN
1	A	483	HIS
1	A	535	HIS
1	A	554	ASN
1	A	580	ASN
2	C	6	GLN
2	C	92	ASN
2	C	137	ASN
2	C	152	ASN
2	C	160	GLN
2	C	198	HIS
3	D	1	GLN

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Mol	Chain	Res	Type
3	D	6	GLN
3	D	13	GLN
3	D	83	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	0.55	0	17,19,21	1.65	4 (23%)
4	NAG	B	2	4	14,14,15	0.64	0	17,19,21	1.52	1 (5%)
4	BMA	B	3	4	11,11,12	0.73	0	15,15,17	1.26	3 (20%)
4	MAN	B	4	4	11,11,12	0.88	0	15,15,17	1.54	4 (26%)
4	MAN	B	5	4	11,11,12	0.97	1 (9%)	15,15,17	2.31	3 (20%)
4	MAN	B	6	4	11,11,12	3.74	2 (18%)	15,15,17	2.06	3 (20%)
4	MAN	B	7	4	11,11,12	0.61	0	15,15,17	1.02	1 (6%)
4	MAN	B	8	4	11,11,12	1.46	2 (18%)	15,15,17	2.18	6 (40%)
4	MAN	B	9	4	11,11,12	1.51	2 (18%)	15,15,17	1.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	1	5,1	14,14,15	0.52	0	17,19,21	1.65	4 (23%)
5	NAG	E	2	5	14,14,15	0.57	0	17,19,21	1.23	2 (11%)
5	NAG	F	1	5,1	14,14,15	0.71	0	17,19,21	1.33	1 (5%)
5	NAG	F	2	5	14,14,15	0.53	0	17,19,21	1.42	1 (5%)
5	NAG	G	1	5,1	14,14,15	0.86	1 (7%)	17,19,21	1.21	2 (11%)
5	NAG	G	2	5	14,14,15	0.49	0	17,19,21	1.42	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	-	1/6/23/26	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	5,1	-	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	5,1	-	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	5,1	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	11.86	1.92	1.42
4	B	8	MAN	O5-C1	3.02	1.48	1.43
4	B	6	MAN	C6-C5	2.98	1.61	1.51
4	B	5	MAN	O6-C6	2.81	1.54	1.42
4	B	9	MAN	O5-C5	2.78	1.48	1.43
4	B	9	MAN	C2-C3	2.50	1.56	1.52
5	G	1	NAG	C1-C2	2.50	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8	MAN	C6-C5	2.14	1.59	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	6	MAN	C1-O5-C5	6.01	120.24	112.19
4	B	5	MAN	C1-O5-C5	5.93	120.13	112.19
4	B	8	MAN	O3-C3-C4	5.39	123.08	110.38
4	B	5	MAN	O2-C2-C1	4.50	119.52	109.22
4	B	6	MAN	O6-C6-C5	-4.43	96.23	111.33
5	E	1	NAG	C1-O5-C5	4.37	118.04	112.19
4	B	2	NAG	C1-O5-C5	4.30	117.94	112.19
5	F	2	NAG	C1-O5-C5	3.61	117.02	112.19
4	B	5	MAN	O2-C2-C3	-3.60	102.69	110.15
4	B	1	NAG	O5-C1-C2	-3.54	105.81	111.29
4	B	1	NAG	O7-C7-C8	-3.36	116.08	122.05
4	B	8	MAN	O3-C3-C2	-3.20	103.51	110.05
5	G	2	NAG	C1-O5-C5	3.15	116.41	112.19
5	E	1	NAG	C4-C3-C2	2.99	115.39	111.02
5	G	1	NAG	C1-O5-C5	2.93	116.11	112.19
5	F	1	NAG	O5-C1-C2	-2.93	106.76	111.29
5	E	1	NAG	O5-C1-C2	-2.76	107.02	111.29
4	B	4	MAN	C1-O5-C5	2.73	115.84	112.19
4	B	8	MAN	O5-C1-C2	-2.72	104.30	110.79
4	B	1	NAG	C1-O5-C5	2.64	115.73	112.19
5	G	2	NAG	O5-C1-C2	-2.63	107.22	111.29
5	G	2	NAG	C3-C4-C5	2.62	114.97	110.23
4	B	4	MAN	C2-C3-C4	-2.59	106.31	110.86
4	B	4	MAN	O3-C3-C4	2.57	116.43	110.38
4	B	3	BMA	O5-C5-C6	2.48	112.49	107.66
4	B	8	MAN	O6-C6-C5	2.48	119.77	111.33
4	B	8	MAN	C3-C4-C5	2.44	114.66	110.23
4	B	6	MAN	O5-C5-C6	2.41	112.36	107.66
4	B	7	MAN	O5-C5-C6	2.41	112.35	107.66
4	B	4	MAN	O2-C2-C1	2.23	114.32	109.22
4	B	3	BMA	O5-C1-C2	-2.19	105.57	110.79
4	B	8	MAN	C2-C3-C4	-2.16	107.07	110.86
5	E	2	NAG	C8-C7-N2	2.14	119.66	116.12
5	G	1	NAG	O4-C4-C3	2.12	115.36	110.38
4	B	1	NAG	O7-C7-N2	2.10	125.70	121.98
5	E	1	NAG	O4-C4-C3	-2.04	105.56	110.38
4	B	3	BMA	C1-C2-C3	2.03	112.61	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2	NAG	O5-C1-C2	-2.02	108.17	111.29

All (2) chirality outliers are listed below:

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

All (25) 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	6	MAN	O5-C5-C6-O6
4	B	5	MAN	C4-C5-C6-O6
4	B	4	MAN	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
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	1	NAG	C8-C7-N2-C2
5	G	1	NAG	C4-C5-C6-O6
5	E	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
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	2	NAG	C1-C2-N2-C7
4	B	8	MAN	O5-C5-C6-O6

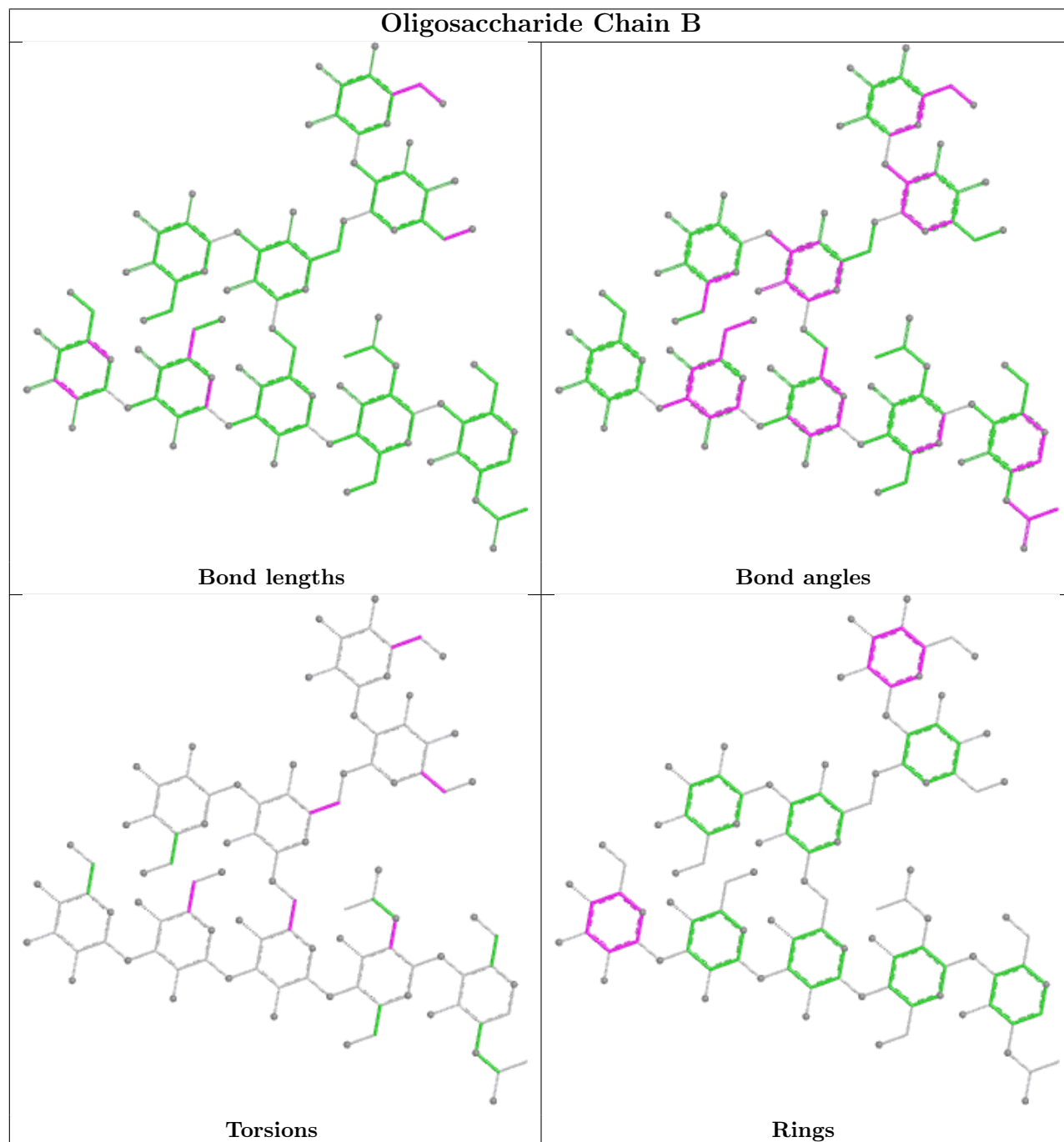
All (2) ring outliers are listed below:

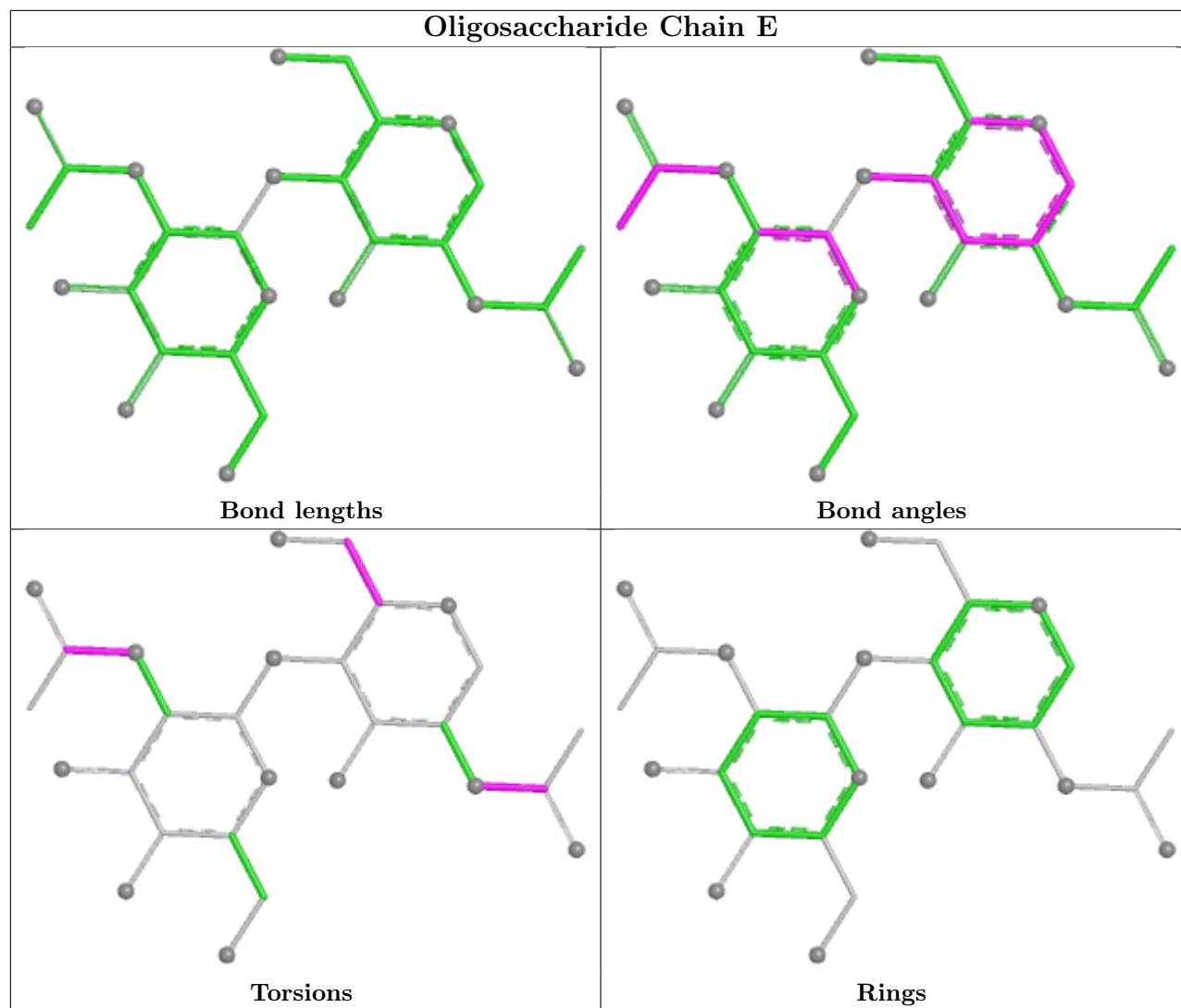
Mol	Chain	Res	Type	Atoms
4	B	9	MAN	C1-C2-C3-C4-C5-O5
4	B	6	MAN	C1-C2-C3-C4-C5-O5

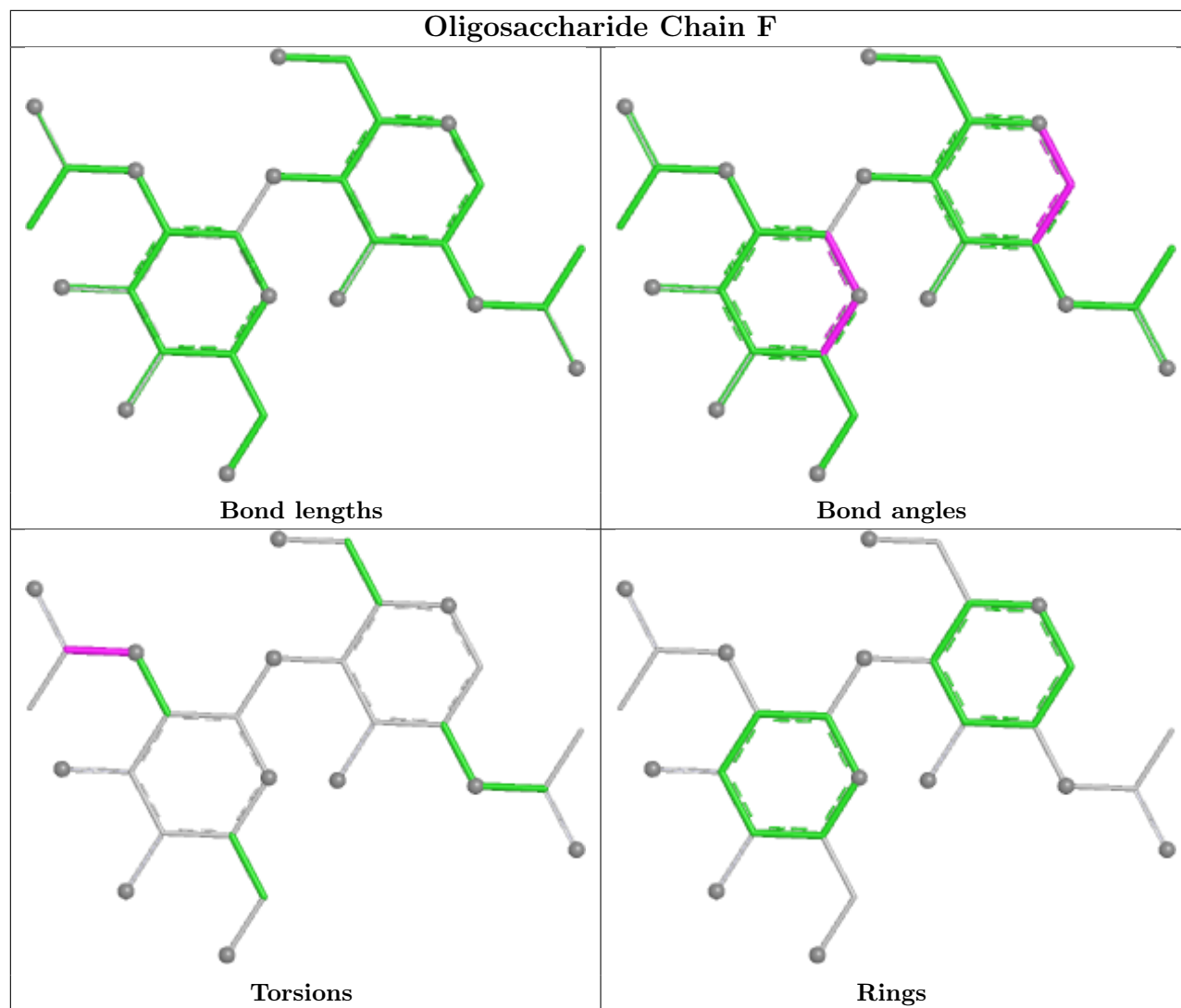
3 monomers are involved in 5 short contacts:

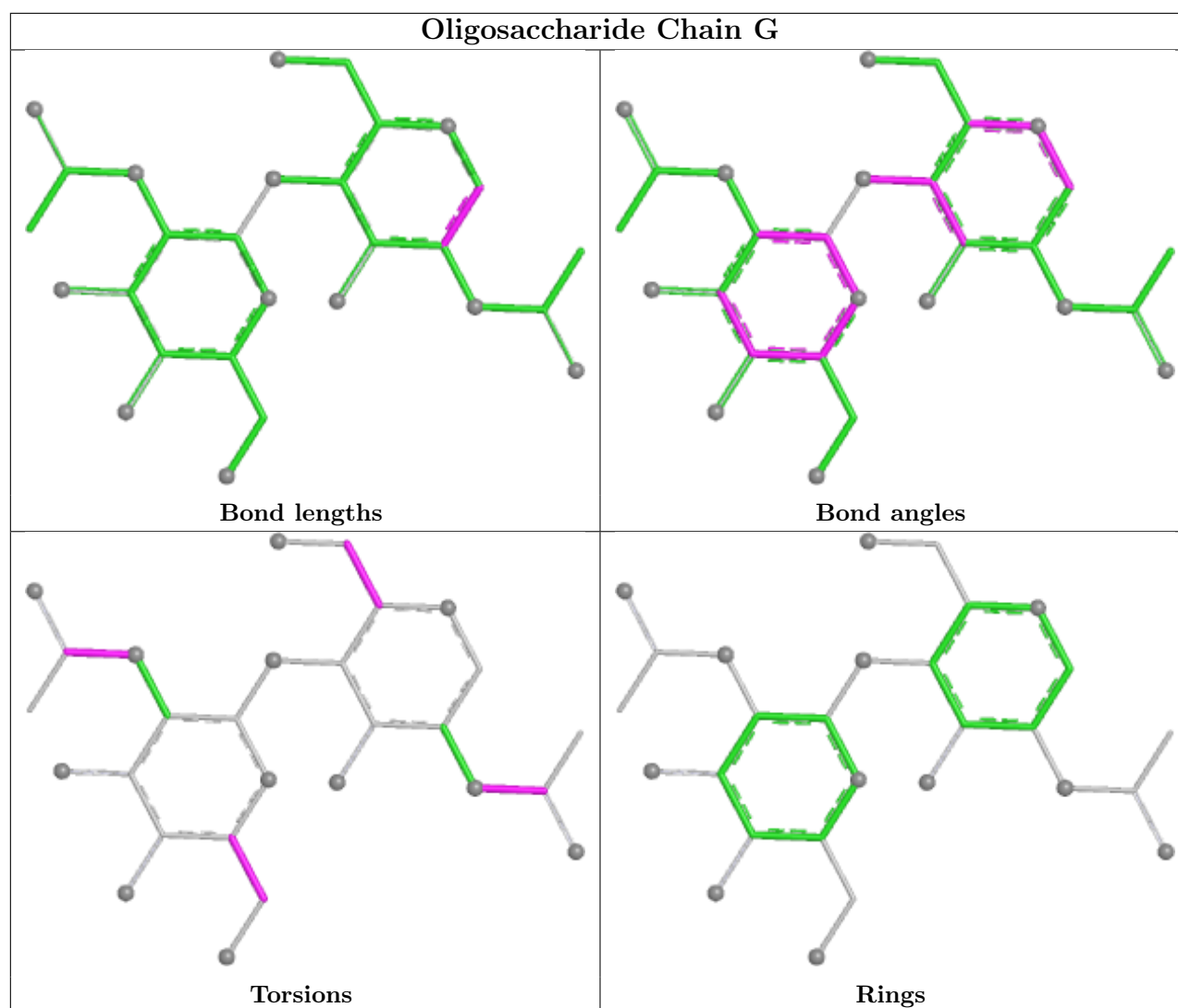
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	6	MAN	2	0
4	B	5	MAN	3	0
4	B	4	MAN	3	0

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 [i](#)

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	0.62	0	17,19,21	1.67	3 (17%)
6	NAG	A	5041	1	14,14,15	0.92	1 (7%)	17,19,21	1.43	2 (11%)
6	NAG	A	5441	1	14,14,15	0.74	1 (7%)	17,19,21	1.56	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	625	1	14,14,15	1.04	1 (7%)	17,19,21	1.69	4 (23%)
6	NAG	A	3891	1	14,14,15	0.76	0	17,19,21	1.52	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	4/6/23/26	0/1/1/1
6	NAG	A	5041	1	1/1/5/7	5/6/23/26	0/1/1/1
6	NAG	A	5441	1	-	2/6/23/26	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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	625	NAG	C1-C2	3.06	1.56	1.52
6	A	5041	NAG	C1-C2	2.46	1.55	1.52
6	A	5441	NAG	C1-C2	2.02	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	4.76	118.56	112.19
6	A	3891	NAG	C2-N2-C7	4.35	128.74	122.90
6	A	5441	NAG	C1-O5-C5	4.18	117.79	112.19
6	A	625	NAG	O5-C1-C2	-3.74	105.51	111.29
6	D	881	NAG	C2-N2-C7	3.65	127.79	122.90
6	A	5041	NAG	O3-C3-C2	3.02	115.67	109.40
6	A	625	NAG	C1-O5-C5	-2.85	108.37	112.19
6	A	3891	NAG	C8-C7-N2	2.56	120.36	116.12
6	A	5441	NAG	O5-C1-C2	2.46	115.10	111.29
6	A	5041	NAG	O5-C1-C2	-2.37	107.62	111.29
6	A	3891	NAG	O7-C7-C8	-2.30	117.95	122.05
6	A	625	NAG	O5-C5-C6	2.11	111.76	107.66
6	A	5441	NAG	C4-C3-C2	2.05	114.02	111.02
6	A	5441	NAG	C2-N2-C7	2.04	125.63	122.90
6	D	881	NAG	O5-C5-C6	2.04	111.63	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	625	NAG	C3-C4-C5	-2.03	106.55	110.23

All (3) chirality outliers are listed below:

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

All (18) torsion outliers are listed below:

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	613/624 (98%)	0.82	51 (8%) 17 13	15, 32, 42, 50	0
2	C	211/213 (99%)	0.94	19 (9%) 15 11	25, 37, 43, 52	0
3	D	220/221 (99%)	1.39	47 (21%) 2 2	28, 38, 45, 54	0
All	All	1044/1058 (98%)	0.97	117 (11%) 10 8	15, 34, 43, 54	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	137	THR	6.6
3	D	196	GLY	5.9
3	D	135	LYS	5.7
3	D	200	TYR	5.1
3	D	199	THR	4.9
3	D	140	GLY	4.8
3	D	136	SER	4.4
1	A	160	LEU	4.1
3	D	201	ILE	4.0
3	D	186	SER	4.0
3	D	220	LYS	3.9
1	A	221	GLU	3.8
1	A	589	ALA	3.7
3	D	219	PRO	3.6
3	D	187	VAL	3.6
3	D	143	ALA	3.5
3	D	202	CYS	3.4
1	A	205	SER	3.4
1	A	491	CYS	3.3
3	D	192	SER	3.3
3	D	195	LEU	3.2
1	A	591	HIS	3.2
2	C	184	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	345	LEU	3.1
3	D	193	SER	3.1
3	D	218	GLU	3.1
1	A	416	VAL	3.0
1	A	236	CYS	3.0
2	C	153	ALA	3.0
3	D	139	GLY	3.0
1	A	611	GLY	3.0
1	A	586	TYR	2.9
3	D	197	THR	2.9
3	D	198	GLN	2.8
1	A	326	SER	2.8
2	C	96	THR	2.8
3	D	138	SER	2.8
1	A	539	LEU	2.8
2	C	136	LEU	2.7
1	A	597	HIS	2.7
2	C	122	ASP	2.7
1	A	208	CYS	2.7
3	D	168	GLY	2.7
2	C	91	ASN	2.7
3	D	45	LEU	2.7
1	A	459	THR	2.7
1	A	272	PRO	2.7
3	D	184	LEU	2.6
3	D	122	THR	2.6
1	A	534	CYS	2.6
1	A	547	CYS	2.6
3	D	188	VAL	2.6
1	A	203	SER	2.5
1	A	346	HIS	2.5
1	A	275	TYR	2.5
2	C	187	GLU	2.5
1	A	557	GLN	2.5
3	D	146	CYS	2.5
1	A	348	LEU	2.5
3	D	209	SER	2.5
2	C	185	ASP	2.5
3	D	190	VAL	2.5
2	C	181	LEU	2.4
3	D	147	LEU	2.4
1	A	209	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	133	SER	2.4
1	A	199	CYS	2.4
1	A	495	GLU	2.4
1	A	415	ALA	2.4
2	C	193	ALA	2.4
3	D	134	SER	2.4
1	A	220	ARG	2.4
3	D	106	PHE	2.4
1	A	210	ASN	2.4
3	D	217	VAL	2.4
1	A	190	ILE	2.3
3	D	194	SER	2.3
3	D	44	GLY	2.3
3	D	131	ALA	2.3
1	A	159	HIS	2.3
1	A	482	CYS	2.3
1	A	234	ALA	2.3
2	C	129	THR	2.3
1	A	613	PRO	2.3
3	D	4	LEU	2.3
1	A	204	PRO	2.2
3	D	191	PRO	2.2
2	C	154	LEU	2.2
2	C	180	THR	2.2
3	D	104	TYR	2.2
3	D	210	ASN	2.2
1	A	513	ASP	2.2
1	A	438	ILE	2.2
3	D	33	GLY	2.2
2	C	77	SER	2.2
3	D	158	VAL	2.2
1	A	383	ILE	2.2
1	A	464	THR	2.2
3	D	128	PHE	2.2
1	A	541	GLN	2.1
3	D	207	LYS	2.1
2	C	125	LEU	2.1
1	A	608	GLY	2.1
1	A	290	ASP	2.1
1	A	556	ILE	2.1
3	D	42	GLY	2.1
1	A	238	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	614	THR	2.1
1	A	545	ILE	2.1
2	C	211	ARG	2.1
1	A	192	ALA	2.0
1	A	402	ILE	2.0
1	A	439	ILE	2.0
2	C	186	TYR	2.0
2	C	126	LYS	2.0
1	A	437	VAL	2.0
2	C	192	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

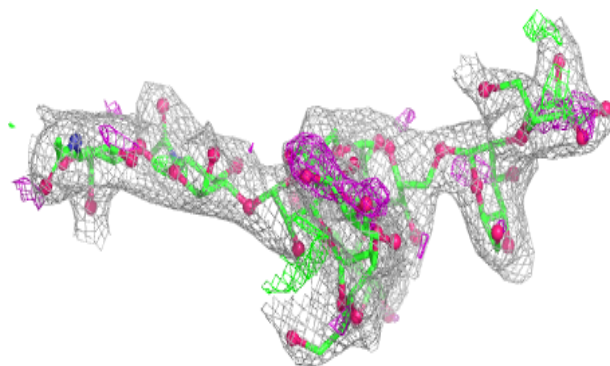
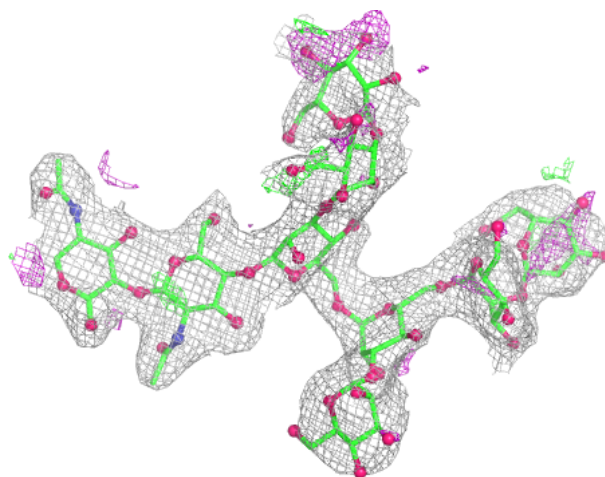
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	1	14/15	-	-	24,31,33,34	0
4	NAG	B	2	14/15	-	-	32,34,38,41	0
4	BMA	B	3	11/12	-	-	37,38,39,41	0
4	MAN	B	4	11/12	-	-	28,32,33,33	0
4	MAN	B	5	11/12	-	-	23,26,26,27	0
4	MAN	B	6	11/12	-	-	15,19,20,21	0
4	MAN	B	7	11/12	-	-	47,48,49,50	0
4	MAN	B	8	11/12	-	-	23,31,33,35	0
4	MAN	B	9	11/12	-	-	26,33,34,36	0
5	NAG	G	2	14/15	0.38	0.15	75,76,76,77	0
5	NAG	G	1	14/15	0.62	0.15	66,70,71,74	0
5	NAG	E	1	14/15	0.71	0.15	52,56,57,59	0
5	NAG	E	2	14/15	0.72	0.13	59,60,61,61	0
5	NAG	F	2	14/15	0.75	0.13	44,47,49,49	0
5	NAG	F	1	14/15	0.90	0.11	28,32,36,39	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.

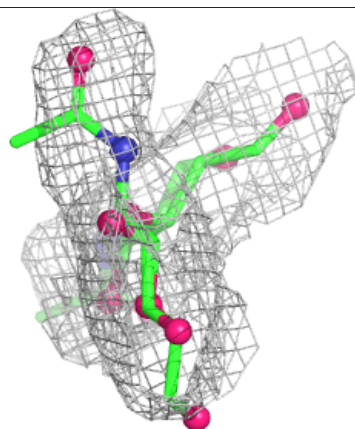
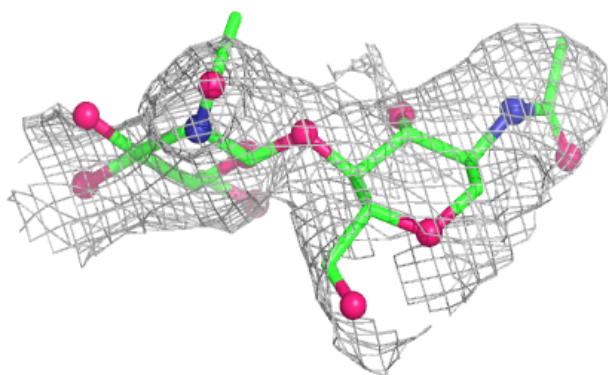
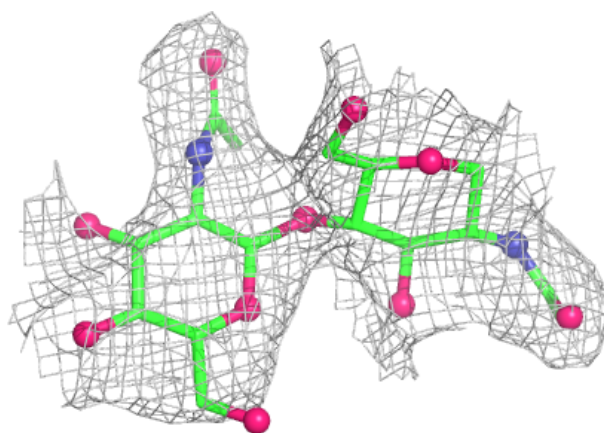
Electron density around Chain B:

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

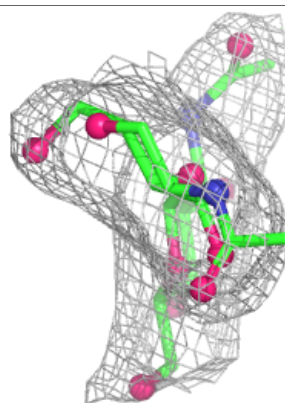
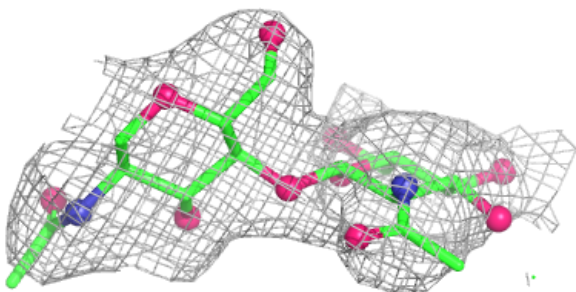
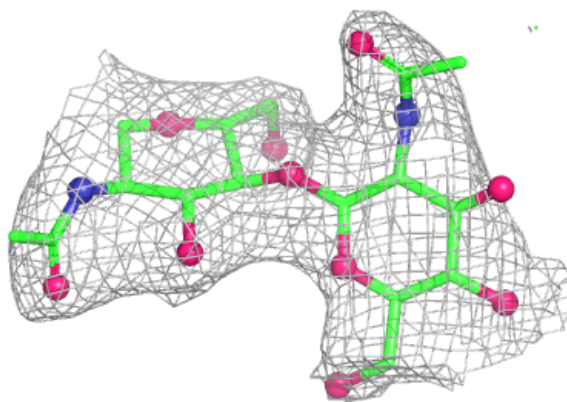


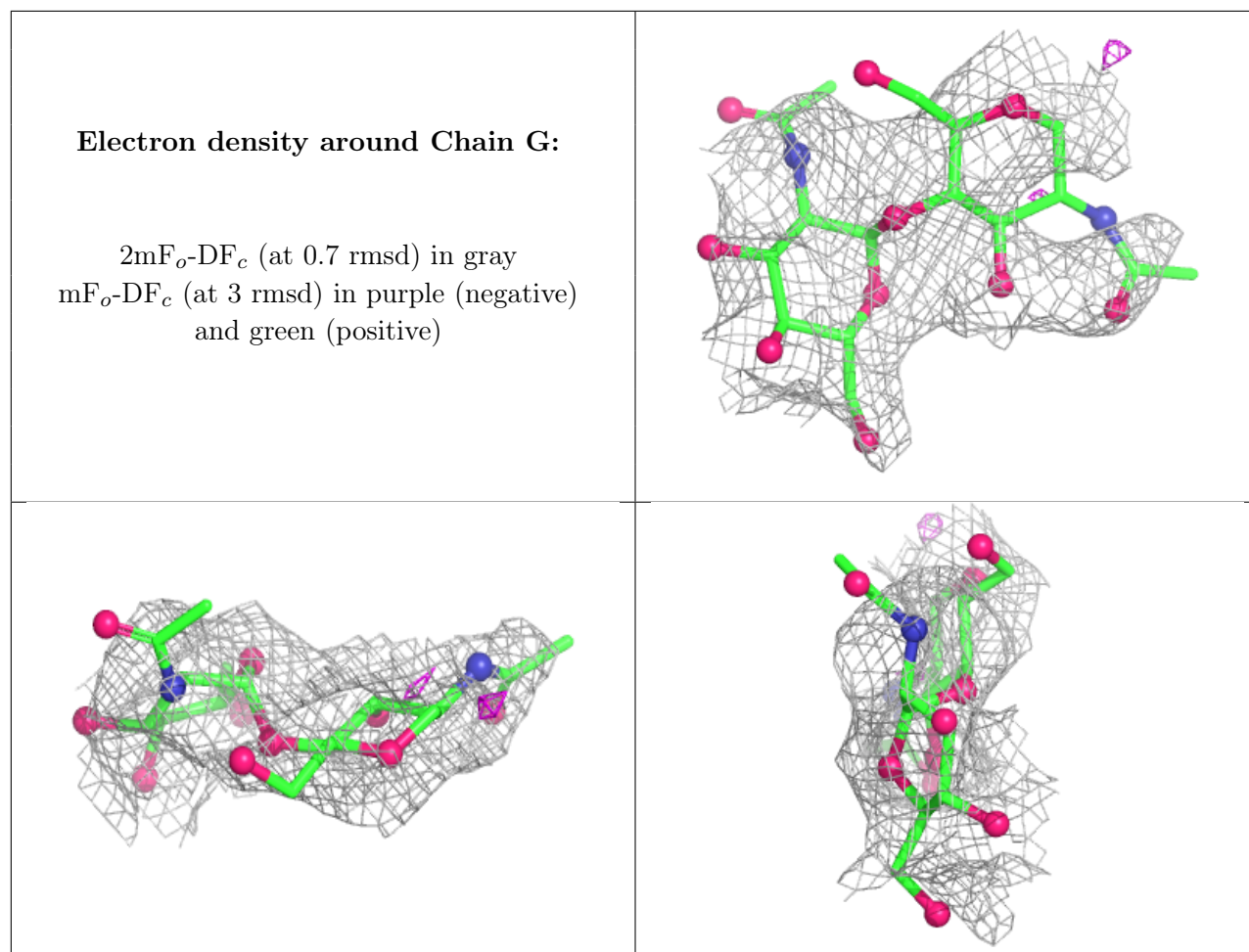
Electron density around Chain E:

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

**Electron density around Chain F:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	A	5441	14/15	0.36	0.18	51,53,54,54	0
6	NAG	A	5041	14/15	0.39	0.21	48,49,50,50	0
6	NAG	A	625	14/15	0.39	0.16	41,44,44,46	0
6	NAG	D	881	14/15	0.66	0.13	57,59,62,62	0
6	NAG	A	3891	14/15	0.74	0.12	48,51,52,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.