Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 02:35 PM BST

PDB ID	:	1HJW
Title	:	Crystal structure of hcgp-39 in complex with chitin octamer
Authors	:	Houston, D.R.; Recklies, A.D.; Krupa, J.C.; Van Aalten, D.M.F.
Deposited on	:	2003-02-28
Resolution	:	2.30 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:

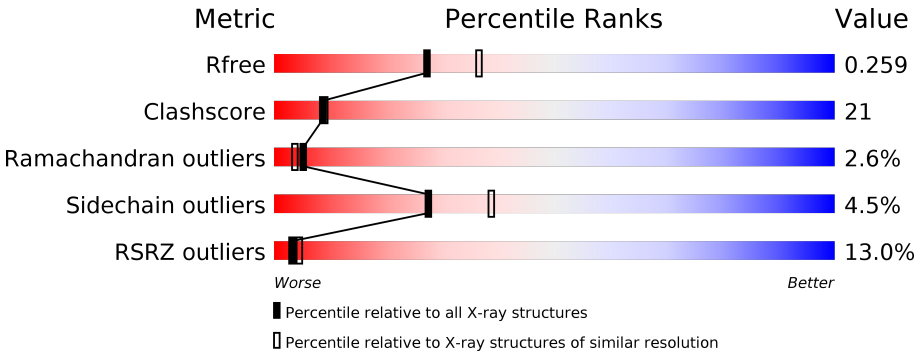
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	362	9% 72% 27%
1	B	362	17% 57% 39%
2	C	6	50% 50%
3	D	2	50% 50%
4	E	5	20% 40% 40%

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
2	NAG	C	6	-	-	-	X
3	NAG	D	2	X	-	-	-
4	NAG	E	3	-	-	X	-
5	GOL	A	1399	-	-	-	X
5	GOL	B	1385	-	-	X	-
6	SO4	A	1394	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6374 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 CHITINASE-3 LIKE PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	2	0
			2873	1835	497	530	11			
1	B	362	Total	C	N	O	S	0	9	0
			2904	1852	504	537	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	ILE	THR	variant	UNP P36222
B	311	ILE	THR	variant	UNP P36222

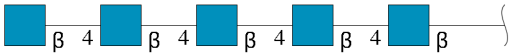
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			85	48	6	31			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

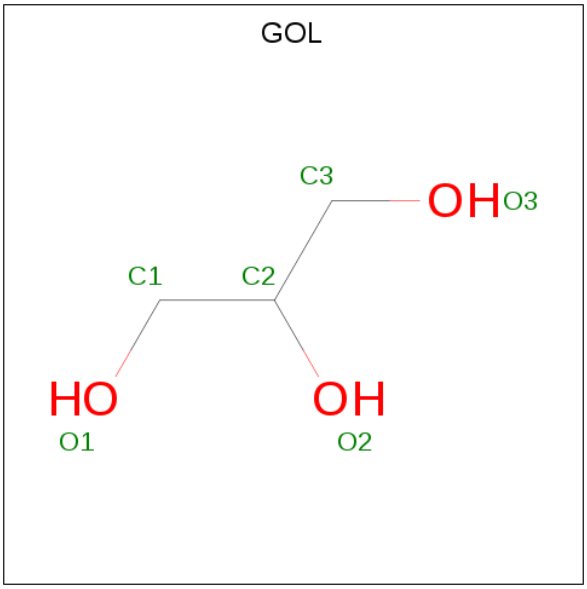
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	2	Total C N O 28 16 2 10	0	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(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	E	5	Total C N O 71 40 5 26	0	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

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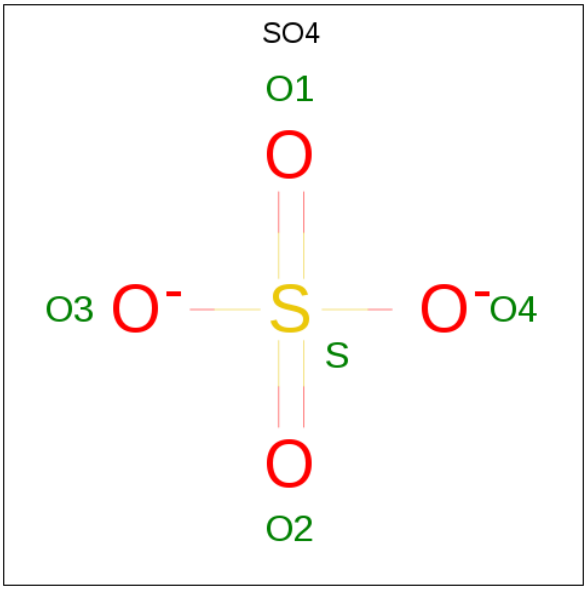
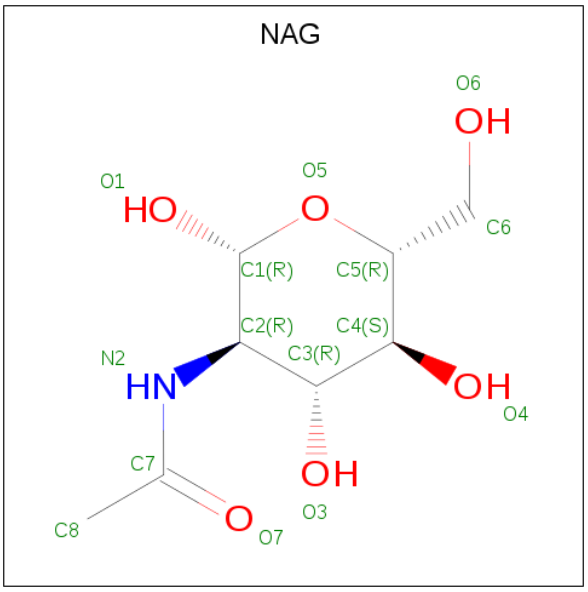
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is water.

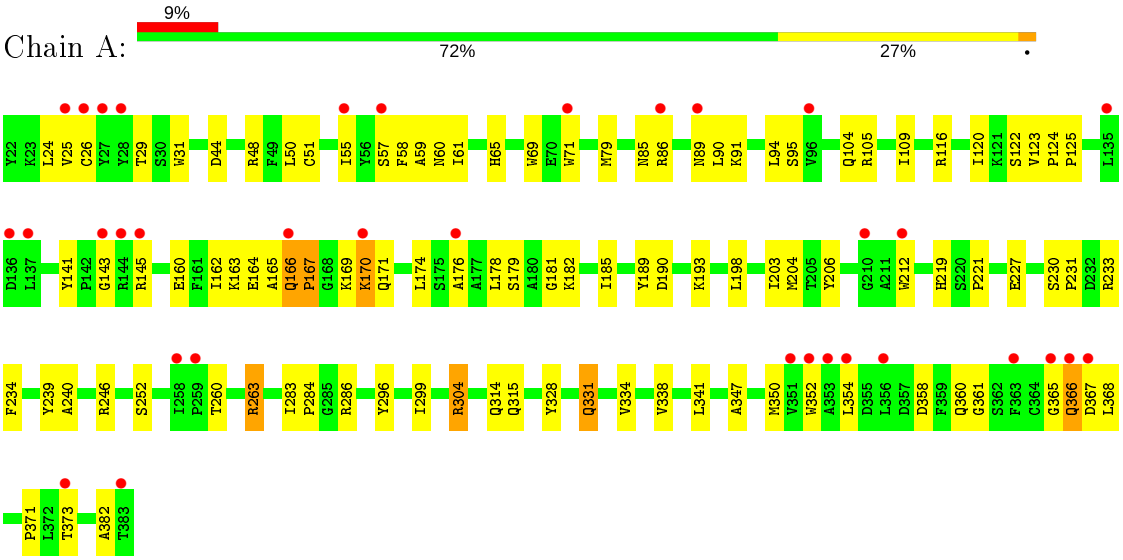
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	178	Total	O	0	0
			178	178		
8	B	159	Total	O	0	0
			159	159		

3 Residue-property plots (i)

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.

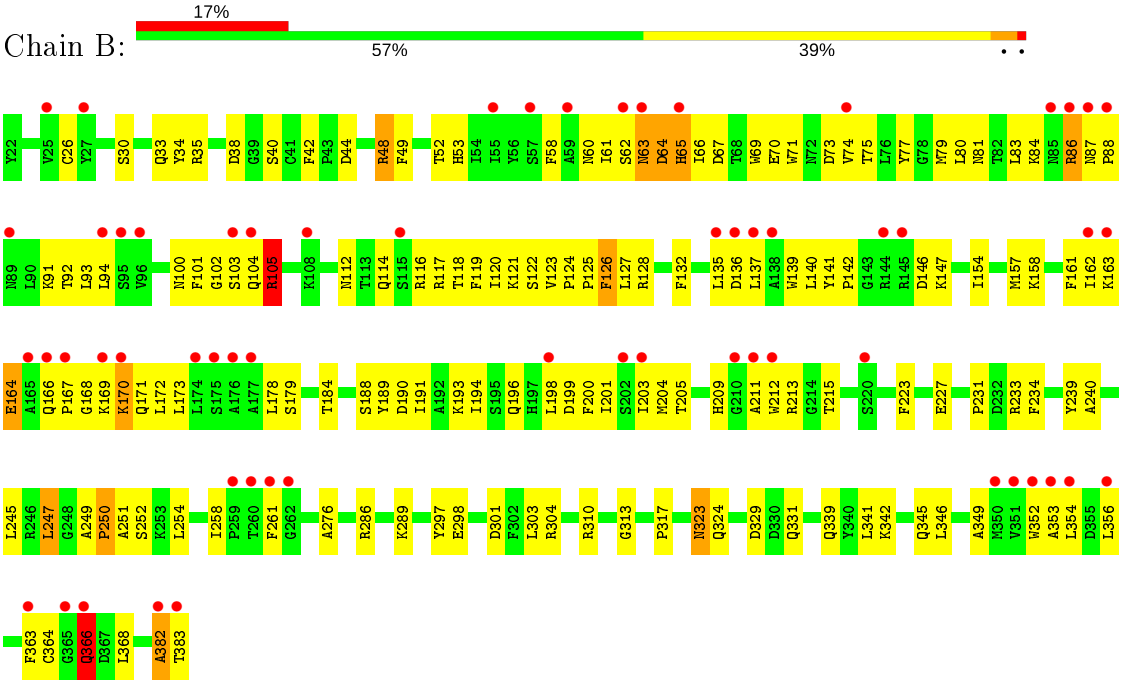
- Molecule 1: CHITINASE-3 LIKE PROTEIN 1

Chain A:



- Molecule 1: CHITINASE-3 LIKE PROTEIN 1

Chain B:



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

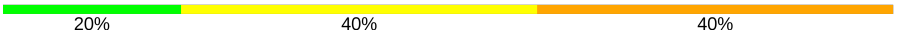
Chain C:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

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

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	109.48Å 123.63Å 136.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.88 – 2.30 25.03 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.7 (24.88-2.30) 95.8 (25.03-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.257 0.204 , 0.259	Depositor DCC
R_{free} test set	611 reflections (1.55%)	wwPDB-VP
Wilson B-factor (Å^2)	58.2	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6374	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: GOL, NAG, SO4

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	0.57	0/2957	0.73	0/4003
1	B	0.49	0/3019	0.71	0/4086
All	All	0.53	0/5976	0.72	0/8089

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	TYR	Sidechain

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	2873	0	2799	85	0
1	B	2904	0	2816	156	0
2	C	85	0	75	8	0
3	D	28	0	25	0	0
4	E	71	0	63	11	0
5	A	30	0	40	4	0
5	B	12	0	16	6	0
6	A	15	0	0	1	1
6	B	5	0	0	0	0
7	B	14	0	13	0	0
8	A	178	0	0	16	0
8	B	159	0	0	14	0
All	All	6374	0	5847	245	1

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 21.

All (245) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLN:HG3	1:A:367:ASP:H	1.35	0.88
1:B:103:SER:HB2	8:B:2028:HOH:O	1.73	0.88
1:A:204:MET:HE2	2:C:2:NAG:H62	1.55	0.87
1:B:86:ARG:NH1	1:B:86:ARG:HB3	1.89	0.86
1:A:48:ARG:HH21	1:A:86:ARG:H	1.22	0.85
1:B:86:ARG:HH11	1:B:86:ARG:HB3	1.42	0.84
1:B:105:ARG:HB3	1:B:105:ARG:HH11	1.42	0.82
1:B:117:ARG:HB2	8:B:2031:HOH:O	1.82	0.79
1:B:44:ASP:HB2	1:B:79:MET:CE	2.14	0.78
1:A:204:MET:CE	2:C:2:NAG:H62	2.14	0.77
1:B:162:ILE:HA	1:B:171:GLN:NE2	2.00	0.77
1:B:162:ILE:HA	1:B:171:GLN:HE21	1.50	0.76
1:A:145:ARG:HG2	8:A:2068:HOH:O	1.85	0.75
1:B:196:GLN:HG3	8:B:2055:HOH:O	1.87	0.74
1:A:203:ILE:HD11	1:A:240:ALA:HB1	1.71	0.72
1:B:147[B]:LYS:HE3	1:B:189:TYR:O	1.88	0.72
1:A:162:ILE:HA	1:A:171:GLN:NE2	2.03	0.72
5:B:1385:GOL:H12	4:E:5:NAG:H62	1.70	0.72
1:A:331:GLN:HE22	1:A:371:PRO:HB2	1.55	0.72
1:B:117:ARG:HH22	1:B:121:LYS:HD3	1.53	0.72
1:B:48[B]:ARG:HB3	1:B:83:LEU:HB3	1.71	0.71
1:B:123:VAL:HB	1:B:124:PRO:HD3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ARG:HH21	1:B:172:LEU:HG	1.56	0.71
1:A:331:GLN:HB2	8:A:2152:HOH:O	1.91	0.70
1:B:105:ARG:NH1	1:B:105:ARG:HB3	2.07	0.69
1:B:127:LEU:HD12	1:B:172:LEU:HD13	1.73	0.69
1:B:117:ARG:NH2	5:B:1384:GOL:H12	2.07	0.69
1:B:167:PRO:HD2	1:B:169:LYS:NZ	2.08	0.68
1:B:112:ASN:OD1	1:B:114:GLN:HG2	1.94	0.67
1:B:209:HIS:HE1	1:B:213:ARG:HH21	1.40	0.67
1:B:35:ARG:HE	5:B:1385:GOL:H32	1.61	0.66
1:B:65[A]:HIS:HB2	1:B:122:SER:CB	2.26	0.66
1:B:352:TRP:CE2	4:E:3:NAG:H5	2.31	0.65
1:B:139:TRP:O	1:B:142:PRO:HD3	1.95	0.65
1:A:368:LEU:HD12	8:A:2166:HOH:O	1.97	0.65
1:B:141:TYR:HH	4:E:2:NAG:HO6	1.44	0.64
1:B:352:TRP:CZ2	4:E:3:NAG:H3	2.32	0.64
1:A:163:LYS:O	1:A:166:GLN:HB2	1.98	0.64
1:B:382:ALA:HA	8:B:2156:HOH:O	1.97	0.64
1:B:128:ARG:NH2	1:B:172:LEU:HG	2.11	0.64
1:B:341:LEU:HD12	1:B:342:LYS:N	2.13	0.64
1:A:166:GLN:HB3	1:A:167:PRO:HD3	1.79	0.63
1:B:69:TRP:HD1	1:B:70:GLU:HG3	1.63	0.63
1:B:158:LYS:O	1:B:162:ILE:HG13	1.99	0.63
1:B:163:LYS:O	1:B:166:GLN:HG2	1.99	0.62
1:B:44:ASP:HB2	1:B:79:MET:HE2	1.81	0.62
1:A:71:TRP:NE1	5:A:1389:GOL:H2	2.15	0.62
1:A:105:ARG:O	1:A:109:ILE:HG13	1.99	0.62
1:B:135:LEU:HG	1:B:136:ASP:N	2.14	0.62
1:B:117:ARG:NH2	1:B:121:LYS:HD3	2.14	0.61
1:A:170[B]:LYS:HE3	8:A:2078:HOH:O	2.01	0.61
1:B:213:ARG:HB2	8:B:2060:HOH:O	1.99	0.61
1:B:204:MET:HE3	4:E:3:NAG:C7	2.30	0.61
1:A:162:ILE:HA	1:A:171:GLN:HE21	1.65	0.60
1:B:213:ARG:NE	8:B:2062:HOH:O	2.34	0.60
1:B:233:ARG:HG2	1:B:233:ARG:HH11	1.67	0.60
1:B:352:TRP:CH2	4:E:3:NAG:H3	2.37	0.59
1:A:44:ASP:H	1:A:79:MET:HE2	1.68	0.58
1:A:204:MET:HG2	1:A:206:TYR:OH	2.03	0.58
1:A:212:TRP:NE1	5:A:1387:GOL:H2	2.19	0.58
1:B:166:GLN:CG	1:B:167:PRO:HD3	2.34	0.57
1:B:368:LEU:HD23	8:B:2133:HOH:O	2.03	0.57
2:C:5:NAG:H61	2:C:6:NAG:H83	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:LEU:HA	1:B:199:ASP:OD2	2.04	0.57
1:A:304:ARG:HB2	1:A:304:ARG:HH11	1.69	0.57
1:B:154:ILE:HD12	1:B:198:LEU:HD21	1.87	0.57
1:B:65[B]:HIS:CD2	1:B:122:SER:HB3	2.41	0.56
1:B:301[A]:ASP:OD1	8:B:2106:HOH:O	2.18	0.56
1:A:182:LYS:HE3	6:A:1394:SO4:O4	2.06	0.56
1:A:61:ILE:HG21	1:A:109:ILE:HD13	1.86	0.56
4:E:4:NAG:H62	4:E:5:NAG:C7	2.37	0.55
1:B:167:PRO:HD2	1:B:169:LYS:HZ2	1.69	0.55
1:A:181:GLY:O	1:A:185:ILE:HG13	2.06	0.55
1:B:191:ILE:HG13	1:B:247:LEU:HD13	1.88	0.55
1:A:65:HIS:HB2	8:A:2029:HOH:O	2.07	0.55
1:B:137:LEU:HD12	1:B:154:ILE:CD1	2.37	0.54
1:A:366:GLN:HG3	1:A:367:ASP:N	2.15	0.54
1:B:128:ARG:NH1	1:B:169:LYS:HD2	2.23	0.54
1:B:141:TYR:CE1	1:B:179:SER:HB2	2.43	0.54
1:A:176:ALA:HB1	8:A:2064:HOH:O	2.07	0.54
1:B:63[B]:ASN:OD1	1:B:65[B]:HIS:ND1	2.41	0.54
1:B:366:GLN:NE2	1:B:366:GLN:H	2.05	0.54
1:A:233:ARG:HB2	8:A:2098:HOH:O	2.08	0.53
1:B:48[A]:ARG:HD3	1:B:49:PHE:CE2	2.43	0.53
1:B:298:GLU:O	1:B:301[A]:ASP:HB2	2.08	0.53
1:B:67:ASP:HA	1:B:126:PHE:HE2	1.73	0.53
1:B:128:ARG:NH1	1:B:169:LYS:CD	2.72	0.52
1:A:212:TRP:CE2	5:A:1387:GOL:H2	2.43	0.52
1:A:252:SER:O	1:A:347:ALA:HB2	2.10	0.52
1:B:137:LEU:HD12	1:B:154:ILE:HD13	1.92	0.52
1:B:310:ARG:HG3	8:B:2037:HOH:O	2.09	0.52
1:A:178:LEU:HD22	1:A:189:TYR:CE1	2.44	0.52
1:A:165:ALA:HA	1:A:169:LYS:HB2	1.91	0.51
1:B:44:ASP:HB2	1:B:79:MET:HE1	1.90	0.51
1:A:233:ARG:HG2	8:A:2105:HOH:O	2.09	0.51
1:A:122:SER:O	1:A:125:PRO:HG2	2.10	0.51
1:B:84:LYS:HE2	1:B:92:THR:HG23	1.92	0.51
1:B:166:GLN:HG2	1:B:167:PRO:HD3	1.93	0.51
1:B:140:LEU:HD22	1:B:141:TYR:CE1	2.46	0.51
1:B:209:HIS:CE1	1:B:213:ARG:HH21	2.26	0.51
1:B:233:ARG:HG2	1:B:233:ARG:NH1	2.25	0.51
1:B:53:HIS:HA	1:B:91:LYS:O	2.11	0.51
1:B:304[A]:ARG:HD3	8:B:2110:HOH:O	2.11	0.51
1:A:116:ARG:O	1:A:120:ILE:HG13	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:THR:O	1:B:188:SER:HB2	2.11	0.50
1:B:66:ILE:HG23	1:B:126:PHE:CD2	2.47	0.50
1:B:66:ILE:HB	1:B:119:PHE:HE1	1.77	0.50
1:B:48[A]:ARG:HD2	1:B:49:PHE:H	1.76	0.50
1:B:170:LYS:HD2	1:B:170:LYS:H	1.77	0.50
1:A:143:GLY:HA3	8:A:2068:HOH:O	2.12	0.50
1:B:139:TRP:CZ2	1:B:142:PRO:HA	2.47	0.49
1:B:382:ALA:O	1:B:383:THR:HB	2.11	0.49
1:B:200:PHE:C	1:B:200:PHE:CD1	2.85	0.49
1:B:204:MET:CE	4:E:3:NAG:C7	2.91	0.49
1:A:190:ASP:CG	1:A:193:LYS:HG3	2.33	0.49
1:B:204:MET:HE3	4:E:3:NAG:C8	2.42	0.49
1:A:204:MET:CE	2:C:3:NAG:C1	2.90	0.49
1:B:366:GLN:CD	1:B:366:GLN:H	2.15	0.49
1:B:35:ARG:HG2	5:B:1385:GOL:H32	1.95	0.49
1:B:178:LEU:O	1:B:204:MET:HG3	2.12	0.49
1:A:25:VAL:O	1:A:350:MET:HA	2.12	0.49
1:B:42:PHE:C	1:B:44:ASP:N	2.66	0.49
1:B:35:ARG:O	1:B:40:SER:HB2	2.13	0.48
1:A:141:TYR:CE1	1:A:179:SER:HB2	2.48	0.48
1:A:334:VAL:O	1:A:338:VAL:HG23	2.13	0.48
1:A:90:LEU:HD12	1:A:91:LYS:N	2.29	0.47
1:B:116:ARG:O	1:B:120:ILE:HG13	2.14	0.47
1:A:85:ASN:ND2	8:A:2043:HOH:O	2.47	0.47
1:B:139:TRP:CH2	1:B:146:ASP:HB3	2.49	0.47
1:B:48[A]:ARG:HB3	1:B:83:LEU:HB3	1.95	0.47
1:B:26:CYS:HB3	1:B:354:LEU:HG	1.97	0.47
1:A:50:LEU:HD21	1:A:373:THR:HB	1.97	0.47
1:A:57:SER:HA	1:A:58:PHE:HA	1.53	0.47
1:B:209:HIS:CE1	8:B:2062:HOH:O	2.67	0.47
1:B:86:ARG:O	1:B:88:PRO:HD3	2.14	0.47
1:A:61:ILE:HG21	1:A:109:ILE:CD1	2.45	0.46
1:B:65[A]:HIS:HB2	1:B:122:SER:HB2	1.97	0.46
1:B:157:MET:SD	1:B:161:PHE:CE1	3.08	0.46
1:A:260:THR:O	1:A:296:TYR:HB2	2.15	0.46
1:B:167:PRO:HG2	1:B:169:LYS:HZ1	1.80	0.46
1:B:74:VAL:HG23	1:B:75:THR:N	2.31	0.46
1:A:55:ILE:CG2	1:A:95:SER:HB2	2.46	0.46
1:B:122:SER:O	1:B:125:PRO:HG2	2.15	0.46
1:A:352:TRP:CE2	2:C:3:NAG:H5	2.51	0.46
1:B:298:GLU:O	1:B:301[B]:ASP:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:LEU:HD12	1:B:93:LEU:N	2.31	0.46
1:A:160:GLU:OE1	1:A:160:GLU:HA	2.15	0.46
1:A:60:ASN:HB2	1:A:69:TRP:HE3	1.80	0.46
1:A:44:ASP:HB3	1:A:79:MET:HE3	1.97	0.45
1:B:77:TYR:O	1:B:81:ASN:ND2	2.49	0.45
1:A:219:HIS:CB	1:A:263:ARG:HG3	2.47	0.45
1:A:124:PRO:N	1:A:125:PRO:HD2	2.31	0.45
1:A:246:ARG:NH2	8:A:2111:HOH:O	2.47	0.45
1:B:223:PHE:HB2	1:B:313:GLY:O	2.16	0.45
1:B:30:SER:O	1:B:33:GLN:HG2	2.17	0.45
1:A:190:ASP:OD1	1:A:193:LYS:HG3	2.17	0.45
1:A:328:TYR:N	1:A:328:TYR:CD1	2.84	0.45
1:A:104:GLN:HG2	8:A:2050:HOH:O	2.16	0.45
1:A:24:LEU:O	1:A:51:CYS:HB3	2.17	0.45
1:B:157:MET:O	1:B:161:PHE:CD1	2.70	0.45
1:B:215:THR:HA	1:B:276:ALA:O	2.17	0.44
1:B:48[A]:ARG:HD3	1:B:49:PHE:CD2	2.52	0.44
1:B:94:LEU:HB2	1:B:132:PHE:CD2	2.52	0.44
1:A:358:ASP:HB3	1:A:371:PRO:CD	2.48	0.44
1:B:301[A]:ASP:OD1	1:B:304[A]:ARG:NH2	2.51	0.44
1:B:38:ASP:N	1:B:38:ASP:OD2	2.51	0.44
1:B:84:LYS:HA	1:B:87:ASN:O	2.17	0.44
1:A:26:CYS:HB3	1:A:354:LEU:HG	1.98	0.44
1:A:352:TRP:CZ3	2:C:3:NAG:H83	2.52	0.44
1:B:100:ASN:HD22	4:E:4:NAG:H62	1.81	0.44
1:B:139:TRP:CE2	1:B:142:PRO:HA	2.53	0.44
1:B:203:ILE:HD11	1:B:240:ALA:HB1	2.00	0.44
1:A:59:ALA:HB2	1:A:94:LEU:HD21	1.99	0.44
1:A:219:HIS:CG	1:A:263:ARG:HG3	2.52	0.44
1:A:304:ARG:HH11	1:A:304:ARG:CB	2.31	0.44
1:B:139:TRP:O	1:B:141:TYR:HA	2.18	0.44
1:B:245:LEU:HA	1:B:249:ALA:HB3	2.00	0.43
1:A:71:TRP:CE2	5:A:1389:GOL:H2	2.53	0.43
1:A:124:PRO:HB3	1:A:164:GLU:HG3	1.99	0.43
1:B:178:LEU:CD1	1:B:201:ILE:HD13	2.49	0.43
1:A:221:PRO:HB2	1:A:314:GLN:HB3	2.01	0.43
1:B:65[B]:HIS:CE1	1:B:118:THR:CG2	3.02	0.43
1:A:162:ILE:HG12	1:A:171:GLN:NE2	2.33	0.43
1:A:170[B]:LYS:HD2	8:A:2079:HOH:O	2.18	0.43
1:B:139:TRP:CD1	1:B:139:TRP:C	2.91	0.43
1:A:174:LEU:HG	1:A:198:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:THR:OG1	1:B:53:HIS:HD2	2.01	0.43
1:A:338:VAL:O	1:A:341:LEU:HG	2.19	0.42
1:B:124:PRO:HB3	1:B:164:GLU:HG3	2.01	0.42
1:B:234:PHE:CD2	1:B:239:TYR:CZ	3.07	0.42
1:A:204:MET:HE2	2:C:3:NAG:C1	2.50	0.42
1:A:29:THR:HB	1:A:31:TRP:CE3	2.55	0.42
1:B:117:ARG:HH21	5:B:1384:GOL:H31	1.84	0.42
1:B:166:GLN:HG3	1:B:167:PRO:HD3	2.02	0.42
1:B:61:ILE:O	1:B:61:ILE:HG22	2.20	0.42
1:A:246:ARG:NE	8:A:2111:HOH:O	2.43	0.42
1:A:91:LYS:HD2	8:A:2042:HOH:O	2.20	0.42
1:B:258:ILE:HD12	1:B:349:ALA:HB1	2.02	0.42
1:A:361:GLY:HA2	1:A:368:LEU:O	2.19	0.42
1:B:80:LEU:HD23	1:B:132:PHE:HE1	1.84	0.42
1:A:91:LYS:HE3	1:A:170[A]:LYS:HE3	2.01	0.42
1:B:190:ASP:OD2	1:B:193:LYS:HB3	2.20	0.42
1:A:283:ILE:HA	1:A:284:PRO:HD3	1.95	0.42
1:B:303:LEU:HD23	1:B:303:LEU:HA	1.85	0.42
1:B:383:THR:HG22	1:B:383:THR:OXT	2.18	0.42
1:A:190:ASP:OD1	1:A:193:LYS:CG	2.68	0.41
1:B:254:LEU:HB3	1:B:346:LEU:HD22	2.02	0.41
1:B:331:GLN:NE2	8:B:2134:HOH:O	2.52	0.41
1:B:352:TRP:HA	1:B:353:ALA:HA	1.79	0.41
1:B:60:ASN:HB2	1:B:69:TRP:HE3	1.85	0.41
1:B:103:SER:HB3	1:B:139:TRP:HE1	1.84	0.41
1:B:323:ASN:ND2	1:B:324:GLN:HE21	2.18	0.41
1:B:35:ARG:CG	5:B:1385:GOL:H32	2.50	0.41
1:A:299:ILE:HD13	1:A:328:TYR:CG	2.55	0.41
1:B:166:GLN:N	1:B:167:PRO:CD	2.84	0.41
1:B:193:LYS:HG3	1:B:196:GLN:HE22	1.86	0.41
1:B:297:TYR:HB2	1:B:363:PHE:CG	2.56	0.41
2:C:3:NAG:H61	2:C:4:NAG:H82	2.02	0.41
1:B:33:GLN:HG3	1:B:34:TYR:CD1	2.55	0.41
1:B:135:LEU:HG	1:B:136:ASP:H	1.85	0.41
1:B:249:ALA:HA	1:B:250:PRO:HD3	1.75	0.41
1:B:140:LEU:HA	1:B:141:TYR:HA	1.77	0.41
1:B:178:LEU:HD11	1:B:201:ILE:HD13	2.03	0.41
1:B:261:PHE:HB3	1:B:356:LEU:HD13	2.02	0.41
1:B:233:ARG:HG2	8:B:2072:HOH:O	2.19	0.41
1:B:190:ASP:O	1:B:194:ILE:HG12	2.21	0.41
1:B:190:ASP:N	8:B:2053:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ALA:HB1	1:B:345:GLN:O	2.21	0.40
1:B:352:TRP:NE1	4:E:3:NAG:H5	2.37	0.40
1:A:123:VAL:HB	1:A:124:PRO:HD3	2.03	0.40
1:A:230:SER:HA	1:A:231:PRO:HD3	1.92	0.40
1:A:315:GLN:NE2	8:A:2145:HOH:O	2.53	0.40
1:B:126:PHE:C	1:B:126:PHE:CD1	2.95	0.40
1:B:163:LYS:HA	1:B:166:GLN:OE1	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1394:SO4:O2	6:A:1394:SO4:O2[8_565]	2.19	0.01

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	362/362 (100%)	345 (95%)	12 (3%)	5 (1%)	11 11
1	B	369/362 (102%)	316 (86%)	39 (11%)	14 (4%)	3 1
All	All	731/724 (101%)	661 (90%)	51 (7%)	19 (3%)	5 4

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	PRO
1	B	64	ASP
1	A	365	GLY
1	A	366	GLN
1	B	101	PHE
1	B	105	ARG

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Mol	Chain	Res	Type
1	B	211	ALA
1	B	231	PRO
1	B	366	GLN
1	A	382	ALA
1	B	102	GLY
1	B	168	GLY
1	B	289	LYS
1	B	71	TRP
1	B	382	ALA
1	B	164	GLU
1	B	364	CYS
1	A	166	GLN
1	B	250	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	304/302 (101%)	295 (97%)	9 (3%)	41 57
1	B	311/302 (103%)	289 (93%)	22 (7%)	14 19
All	All	615/604 (102%)	584 (95%)	31 (5%)	27 34

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	170[A]	LYS
1	A	170[B]	LYS
1	A	227	GLU
1	A	234	PHE
1	A	263	ARG
1	A	304	ARG
1	A	331	GLN
1	A	360	GLN
1	B	48[A]	ARG

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Mol	Chain	Res	Type
1	B	48[B]	ARG
1	B	63[A]	ASN
1	B	63[B]	ASN
1	B	65[A]	HIS
1	B	65[B]	HIS
1	B	73	ASP
1	B	86	ARG
1	B	105	ARG
1	B	126	PHE
1	B	170	LYS
1	B	205	THR
1	B	212	TRP
1	B	227	GLU
1	B	247	LEU
1	B	252	SER
1	B	286	ARG
1	B	317	PRO
1	B	323	ASN
1	B	329	ASP
1	B	339	GLN
1	B	366	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	85	ASN
1	A	89	ASN
1	A	104	GLN
1	A	130	HIS
1	A	171	GLN
1	A	196	GLN
1	A	209	HIS
1	A	331	GLN
1	B	53	HIS
1	B	85	ASN
1	B	100	ASN
1	B	130	HIS
1	B	171	GLN
1	B	196	GLN
1	B	209	HIS
1	B	323	ASN

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Mol	Chain	Res	Type
1	B	366	GLN

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

13 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	2	15,15,15	0.69	0	21,21,21	1.01	3 (14%)
2	NAG	C	2	2	14,14,15	0.74	0	17,19,21	1.00	1 (5%)
2	NAG	C	3	2	14,14,15	0.87	1 (7%)	17,19,21	0.99	2 (11%)
2	NAG	C	4	2	14,14,15	0.90	0	17,19,21	0.83	0
2	NAG	C	5	2	14,14,15	0.65	0	17,19,21	0.65	0
2	NAG	C	6	2	14,14,15	0.97	1 (7%)	17,19,21	0.65	0
3	NAG	D	1	1,3	14,14,15	0.73	0	17,19,21	0.79	0
3	NAG	D	2	3	14,14,15	0.92	1 (7%)	17,19,21	0.60	0
4	NAG	E	1	4	15,15,15	0.72	0	21,21,21	0.70	0
4	NAG	E	2	4	14,14,15	0.65	0	17,19,21	0.74	1 (5%)
4	NAG	E	3	4	14,14,15	0.84	0	17,19,21	1.12	2 (11%)
4	NAG	E	4	4	14,14,15	0.74	0	17,19,21	0.76	0
4	NAG	E	5	4	14,14,15	0.72	0	17,19,21	0.60	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	2	-	0/6/26/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	C	3	2	-	0/6/23/26	0/1/1/1
2	NAG	C	4	2	-	2/6/23/26	0/1/1/1
2	NAG	C	5	2	-	4/6/23/26	0/1/1/1
2	NAG	C	6	2	-	5/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	E	1	4	-	3/6/26/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	3	4	-	0/6/23/26	0/1/1/1
4	NAG	E	4	4	-	0/6/23/26	0/1/1/1
4	NAG	E	5	4	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	NAG	C1-C2	2.39	1.55	1.52
3	D	2	NAG	C1-C2	2.19	1.55	1.52
2	C	3	NAG	C1-C2	2.06	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	3	NAG	C1-O5-C5	2.76	115.94	112.19
2	C	2	NAG	C2-N2-C7	-2.66	119.11	122.90
4	E	3	NAG	C2-N2-C7	-2.62	119.17	122.90
2	C	3	NAG	C2-N2-C7	-2.47	119.39	122.90
2	C	3	NAG	C1-O5-C5	2.37	115.41	112.19
2	C	1	NAG	C4-C3-C2	2.36	113.79	110.34
2	C	1	NAG	C1-C2-N2	-2.13	108.25	110.73
4	E	2	NAG	C2-N2-C7	-2.03	120.01	122.90
2	C	1	NAG	C1-C2-C3	2.02	113.30	110.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	2	NAG	C1

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C3-C2-N2-C7
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2
2	C	6	NAG	O5-C5-C6-O6
3	D	1	NAG	C8-C7-N2-C2
2	C	5	NAG	O5-C5-C6-O6
2	C	6	NAG	C4-C5-C6-O6
3	D	1	NAG	O7-C7-N2-C2
2	C	5	NAG	C4-C5-C6-O6
2	C	6	NAG	C8-C7-N2-C2
2	C	6	NAG	C1-C2-N2-C7
2	C	6	NAG	O7-C7-N2-C2
4	E	5	NAG	O5-C5-C6-O6
2	C	4	NAG	C8-C7-N2-C2
4	E	1	NAG	O5-C5-C6-O6
2	C	4	NAG	O7-C7-N2-C2
2	C	5	NAG	C8-C7-N2-C2
2	C	5	NAG	O7-C7-N2-C2

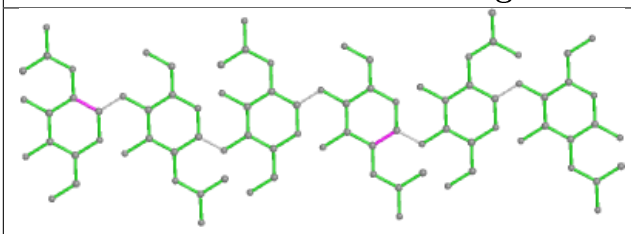
There are no ring outliers.

9 monomers are involved in 19 short contacts:

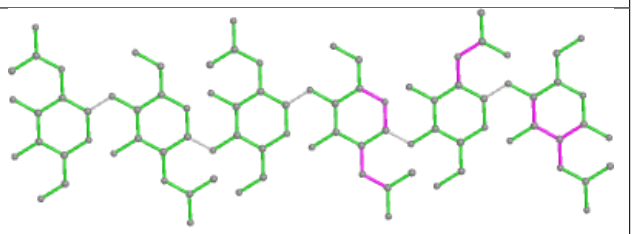
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6	NAG	1	0
2	C	2	NAG	2	0
2	C	3	NAG	5	0
4	E	3	NAG	7	0
2	C	4	NAG	1	0
4	E	4	NAG	2	0
4	E	5	NAG	2	0
2	C	5	NAG	1	0
4	E	2	NAG	1	0

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

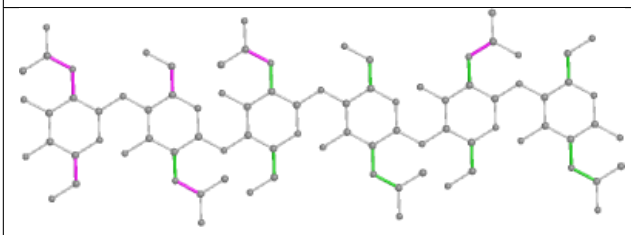
Oligosaccharide Chain C



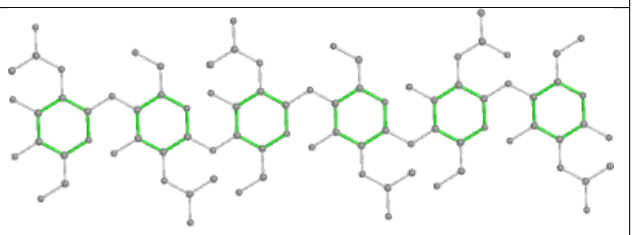
Bond lengths



Bond angles

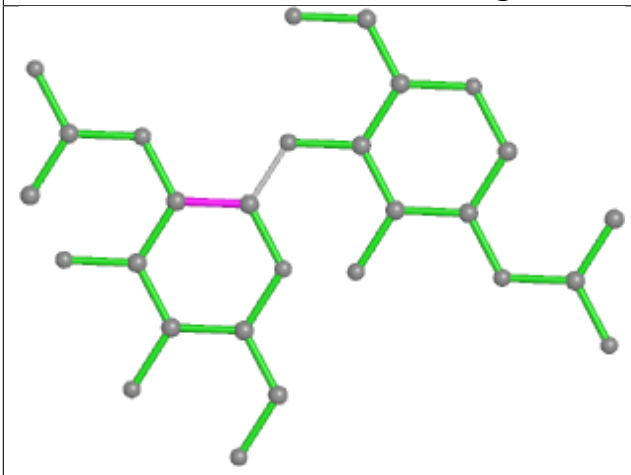


Torsions

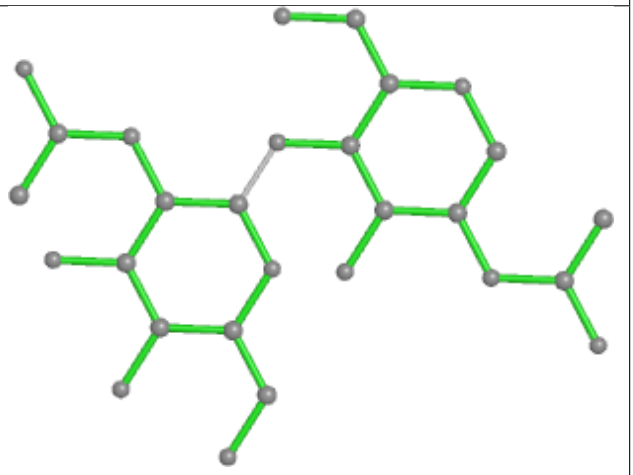


Rings

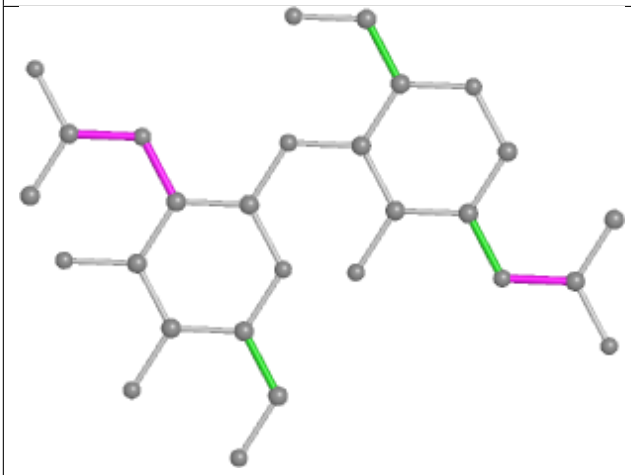
Oligosaccharide Chain D



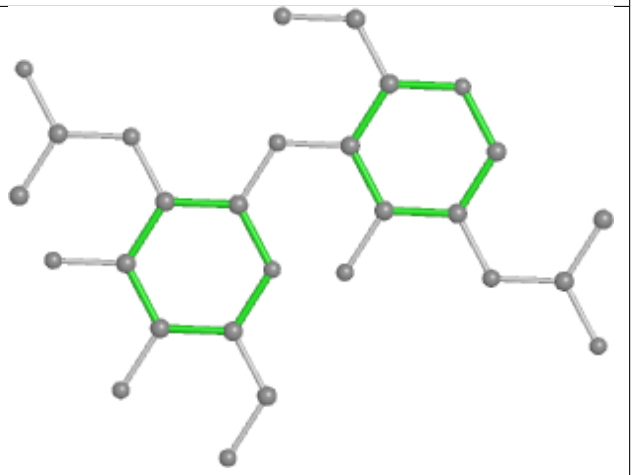
Bond lengths



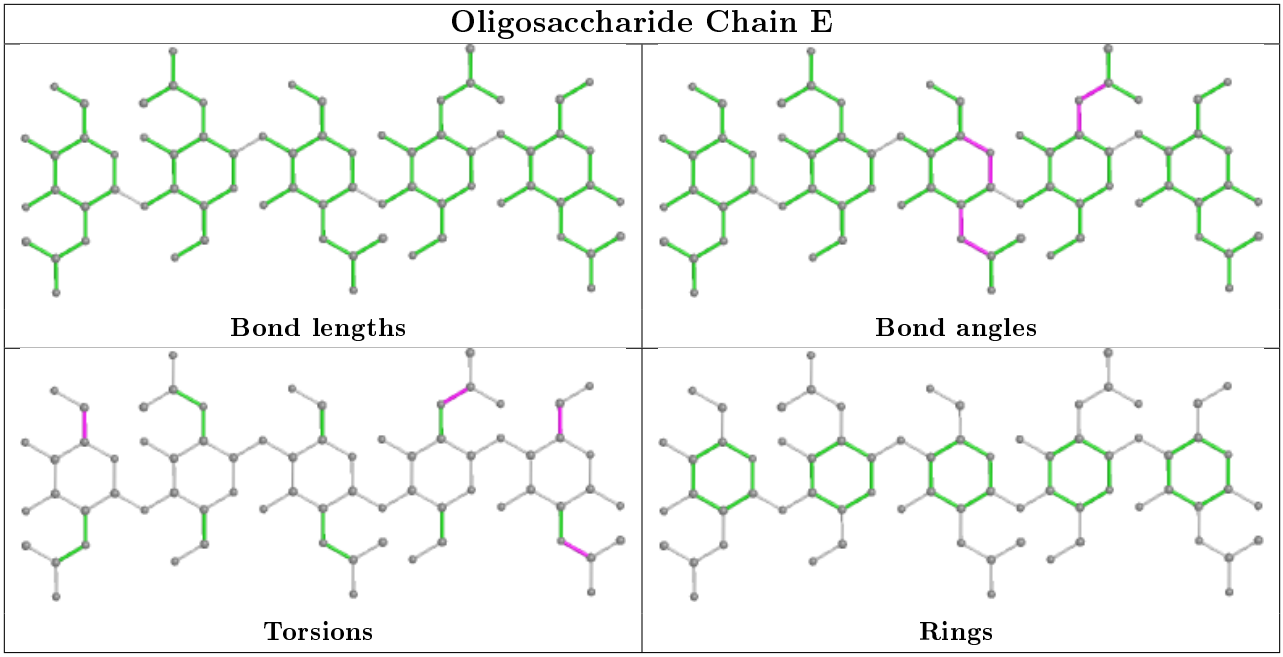
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	A	1387	-	5,5,5	0.44	0	5,5,5	0.19	0
6	SO4	A	1392	-	4,4,4	0.25	0	6,6,6	0.11	0
6	SO4	A	1396	-	4,4,4	0.25	0	6,6,6	0.09	0
5	GOL	A	1399	-	5,5,5	0.42	0	5,5,5	0.24	0
5	GOL	B	1384	-	5,5,5	0.49	0	5,5,5	0.25	0
5	GOL	A	1386	-	5,5,5	0.45	0	5,5,5	0.32	0
7	NAG	B	1383	1	14,14,15	0.55	0	17,19,21	0.60	0
5	GOL	A	1389	-	5,5,5	0.44	0	5,5,5	0.34	0
5	GOL	B	1385	-	5,5,5	0.60	0	5,5,5	0.27	0
6	SO4	A	1394	-	4,4,4	0.26	0	6,6,6	0.13	0
6	SO4	B	1386	-	4,4,4	0.23	0	6,6,6	0.09	0
5	GOL	A	1388	-	5,5,5	0.37	0	5,5,5	0.26	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
5	GOL	A	1387	-	-	0/4/4/4	-
5	GOL	A	1399	-	-	0/4/4/4	-
5	GOL	B	1384	-	-	0/4/4/4	-
5	GOL	A	1386	-	-	0/4/4/4	-
7	NAG	B	1383	1	-	5/6/23/26	0/1/1/1
5	GOL	A	1389	-	-	0/4/4/4	-
5	GOL	B	1385	-	-	0/4/4/4	-
5	GOL	A	1388	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1383	NAG	C8-C7-N2-C2
7	B	1383	NAG	O7-C7-N2-C2
7	B	1383	NAG	C1-C2-N2-C7
7	B	1383	NAG	O5-C5-C6-O6
7	B	1383	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1387	GOL	2	0
5	B	1384	GOL	2	0
5	A	1389	GOL	2	0
5	B	1385	GOL	4	0
6	A	1394	SO4	1	1

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, 95^{th} 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	362/362 (100%)	0.24	34 (9%) 8 11	41, 56, 80, 99	0
1	B	362/362 (100%)	0.72	60 (16%) 1 2	37, 75, 113, 125	0
All	All	724/724 (100%)	0.48	94 (12%) 3 4	37, 61, 108, 125	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65[A]	HIS	7.3
1	B	212	TRP	6.0
1	B	145	ARG	5.0
1	B	365	GLY	5.0
1	B	259	PRO	4.6
1	B	166	GLN	4.4
1	B	177	ALA	4.4
1	B	137	LEU	4.4
1	A	86	ARG	4.4
1	A	166	GLN	4.3
1	B	63[A]	ASN	4.0
1	B	95	SER	4.0
1	B	352	TRP	4.0
1	B	351	VAL	3.9
1	B	176	ALA	3.9
1	B	27	TYR	3.8
1	B	162	ILE	3.8
1	B	94	LEU	3.7
1	A	135	LEU	3.7
1	B	135	LEU	3.6
1	B	211	ALA	3.5
1	A	351	VAL	3.5
1	B	55	ILE	3.4
1	B	260	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	365	GLY	3.4
1	B	96	VAL	3.4
1	B	382	ALA	3.3
1	B	86	ARG	3.3
1	B	261	PHE	3.2
1	A	144	ARG	3.2
1	A	354	LEU	3.2
1	B	262	GLY	3.2
1	B	144	ARG	3.2
1	B	87	ASN	3.1
1	A	55	ILE	3.1
1	A	27	TYR	3.1
1	A	383	THR	3.1
1	B	59	ALA	3.0
1	B	103	SER	3.0
1	B	210	GLY	3.0
1	B	356	LEU	3.0
1	A	145	ARG	2.9
1	A	96	VAL	2.9
1	B	169	LYS	2.9
1	B	170	LYS	2.8
1	B	202	SER	2.8
1	B	366	GLN	2.8
1	A	212	TRP	2.8
1	B	57[A]	SER	2.8
1	B	136	ASP	2.8
1	B	85	ASN	2.8
1	B	383	THR	2.7
1	A	26	CYS	2.7
1	B	62	SER	2.7
1	A	25	VAL	2.7
1	A	352	TRP	2.6
1	B	167	PRO	2.6
1	B	89	ASN	2.6
1	B	220	SER	2.6
1	B	108	LYS	2.6
1	B	175	SER	2.5
1	A	71	TRP	2.5
1	B	104[A]	GLN	2.5
1	A	176	ALA	2.5
1	B	88	PRO	2.4
1	B	25	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	74	VAL	2.4
1	A	259	PRO	2.4
1	A	356	LEU	2.4
1	B	138	ALA	2.4
1	B	350	MET	2.4
1	B	203	ILE	2.3
1	A	367	ASP	2.3
1	B	363	PHE	2.3
1	B	165	ALA	2.3
1	A	363	PHE	2.2
1	A	258	ILE	2.2
1	B	354	LEU	2.2
1	B	353	ALA	2.2
1	A	366	GLN	2.1
1	A	353	ALA	2.1
1	A	89	ASN	2.1
1	A	143	GLY	2.1
1	A	57	SER	2.1
1	A	210	GLY	2.1
1	A	137	LEU	2.1
1	B	163	LYS	2.1
1	B	198	LEU	2.1
1	A	373	THR	2.1
1	A	170[A]	LYS	2.0
1	A	28	TYR	2.0
1	B	174	LEU	2.0
1	A	136	ASP	2.0
1	B	115	SER	2.0

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

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

6.3 Carbohydrates (i)

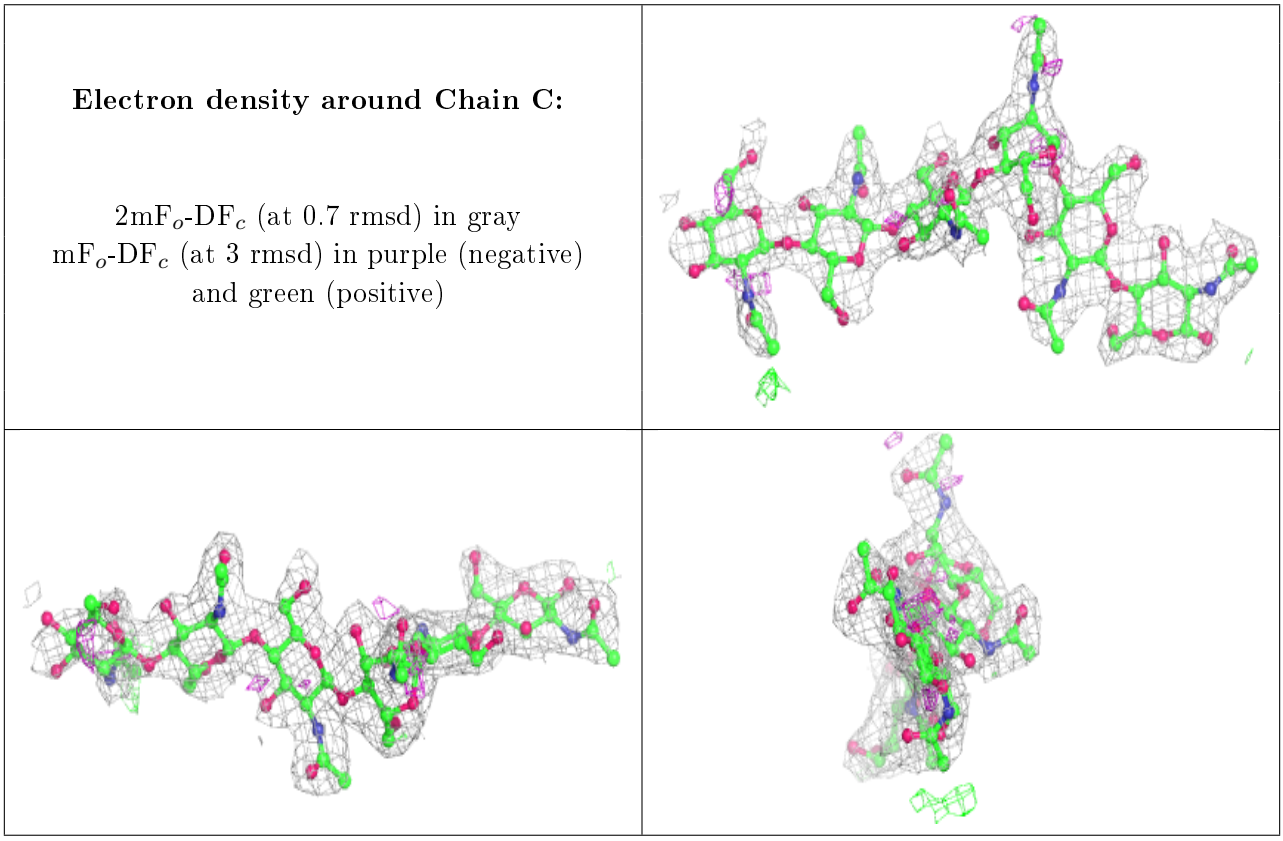
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	C	6	14/15	0.69	0.41	96,98,101,101	0
3	NAG	D	2	14/15	0.81	0.38	105,107,109,109	0
4	NAG	E	4	14/15	0.82	0.16	67,81,84,86	0
4	NAG	E	1	15/15	0.83	0.23	89,96,99,99	0
4	NAG	E	2	14/15	0.86	0.13	79,85,89,90	0
4	NAG	E	5	14/15	0.89	0.22	87,90,92,94	0
4	NAG	E	3	14/15	0.89	0.13	64,76,78,79	0
3	NAG	D	1	14/15	0.90	0.25	85,90,95,101	0
2	NAG	C	4	14/15	0.90	0.16	59,68,71,73	0
2	NAG	C	1	15/15	0.91	0.22	73,80,83,84	0
2	NAG	C	3	14/15	0.91	0.13	55,63,65,68	0
2	NAG	C	5	14/15	0.92	0.21	73,81,89,90	0
2	NAG	C	2	14/15	0.93	0.22	71,78,84,87	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.

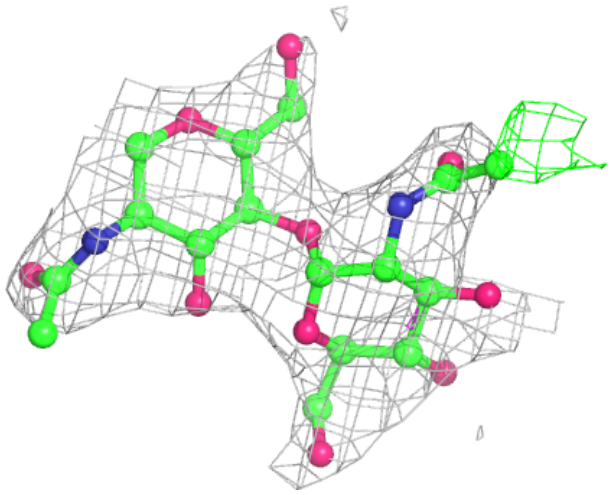
Electron density around Chain C:

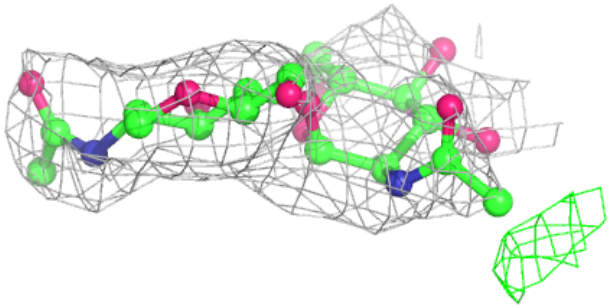
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

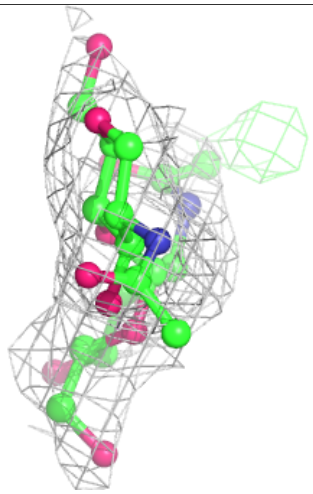


Electron density around Chain D:

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

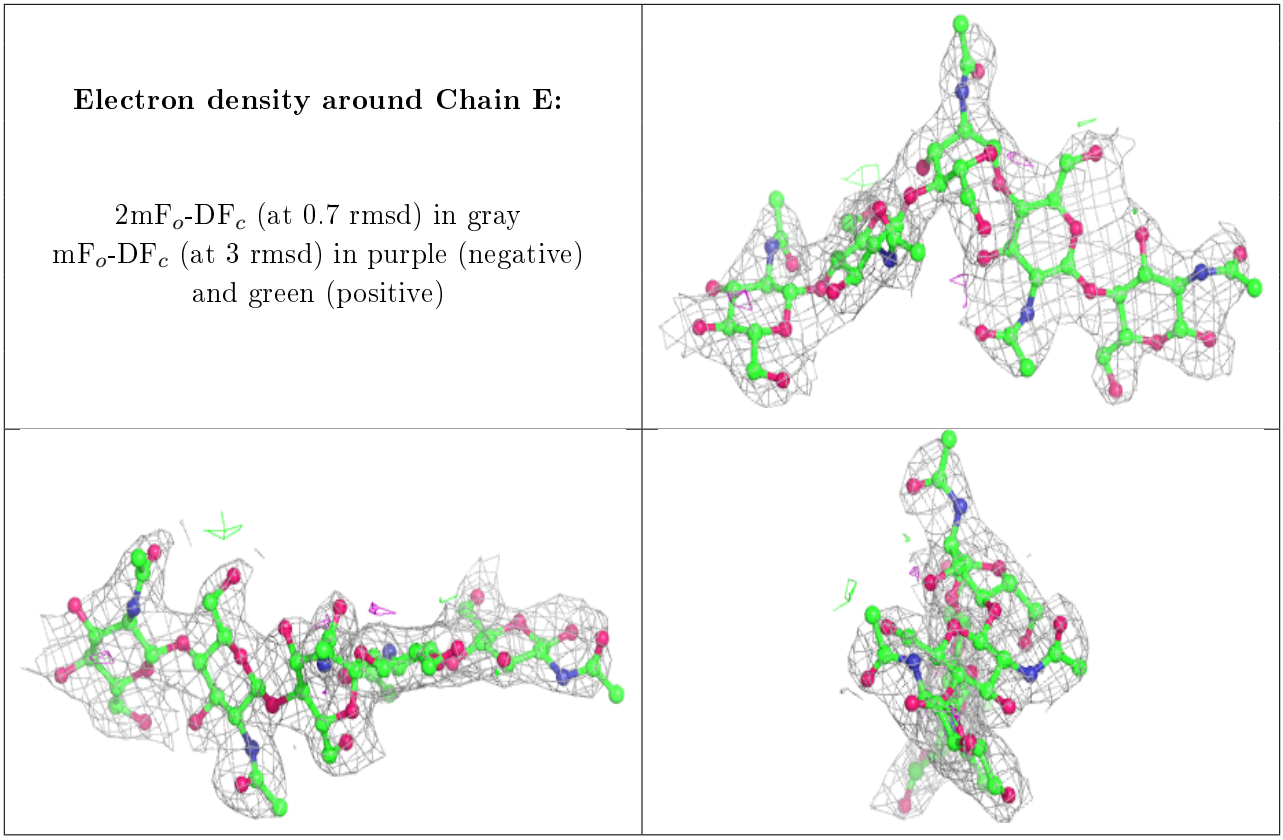






Electron density around Chain E:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
5	GOL	A	1399	6/6	0.49	0.45	122,122,123,124	0
5	GOL	A	1387	6/6	0.75	0.25	95,99,99,100	0
5	GOL	A	1389	6/6	0.78	0.33	87,89,89,90	0
5	GOL	B	1385	6/6	0.80	0.30	101,103,103,104	0
6	SO4	A	1394	5/5	0.82	0.34	155,156,156,156	0
6	SO4	B	1386	5/5	0.83	0.20	163,164,164,164	0
6	SO4	A	1396	5/5	0.86	0.19	146,146,146,146	0
5	GOL	B	1384	6/6	0.86	0.21	85,87,87,89	0
5	GOL	A	1386	6/6	0.87	0.38	92,95,95,96	0
7	NAG	B	1383	14/15	0.87	0.24	102,104,106,106	0
5	GOL	A	1388	6/6	0.90	0.13	83,85,86,86	0
6	SO4	A	1392	5/5	0.94	0.11	110,110,111,111	0

6.5 Other polymers (i)

There are no such residues in this entry.