Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2020 – 03:37 PM BST

PDB ID	:	5HDH
Title	:	Crystal structure of human TLR8 with an uncleaved Z-loop
Authors	:	Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on	:	2016-01-05
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

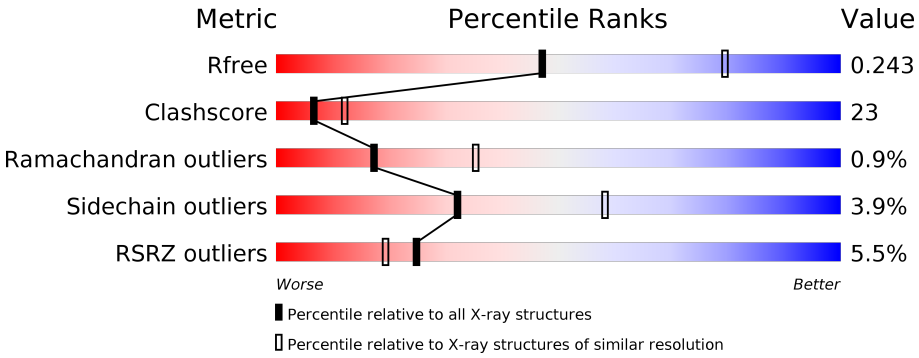
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.60 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)
RSRZ outliers	127900	3104 (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 <=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	801	5%, 62%, 28%, 6%
2	B	4	75%, 25%
3	C	2	50%, 50%
4	D	5	100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6371 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 Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	751	6042	3865	1029	1128	20	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	ASN	ARG	engineered mutation	UNP Q9NR97
A	453	GLN	LYS	engineered mutation	UNP Q9NR97
A	454	SER	ARG	engineered mutation	UNP Q9NR97
A	455	ASN	ARG	engineered mutation	UNP Q9NR97

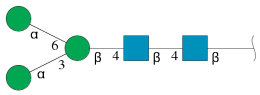
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	4	50	28	2	20	0	0	0

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

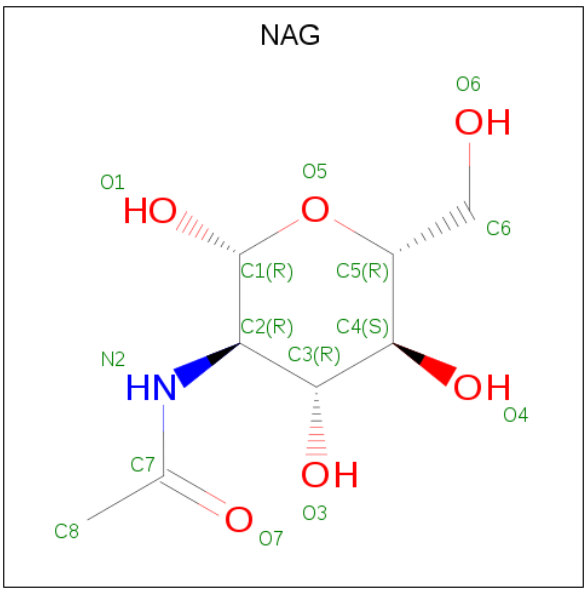
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	C	2	Total C N O 28 16 2 10	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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	D	5	Total C N O 61 34 2 25	0	0	0

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



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

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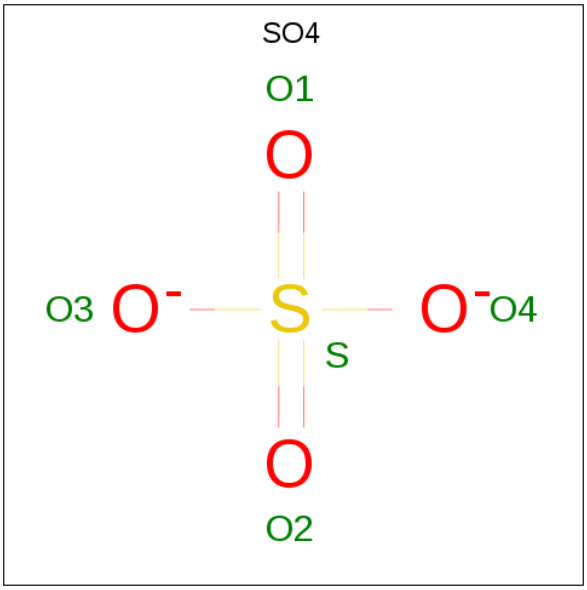
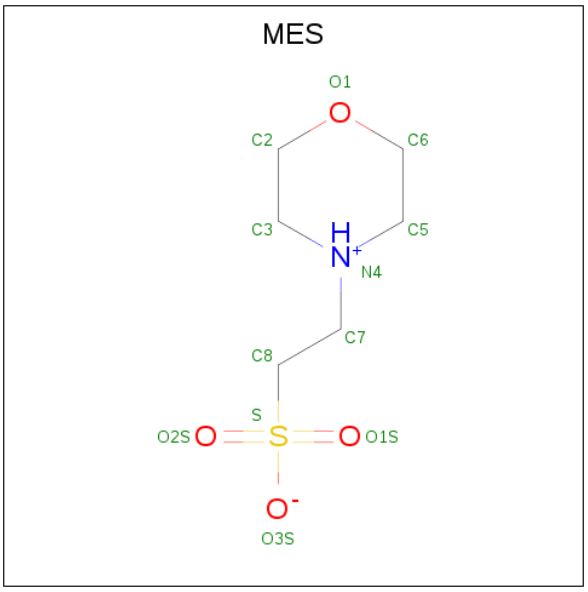
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0

- 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

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 8 is water.

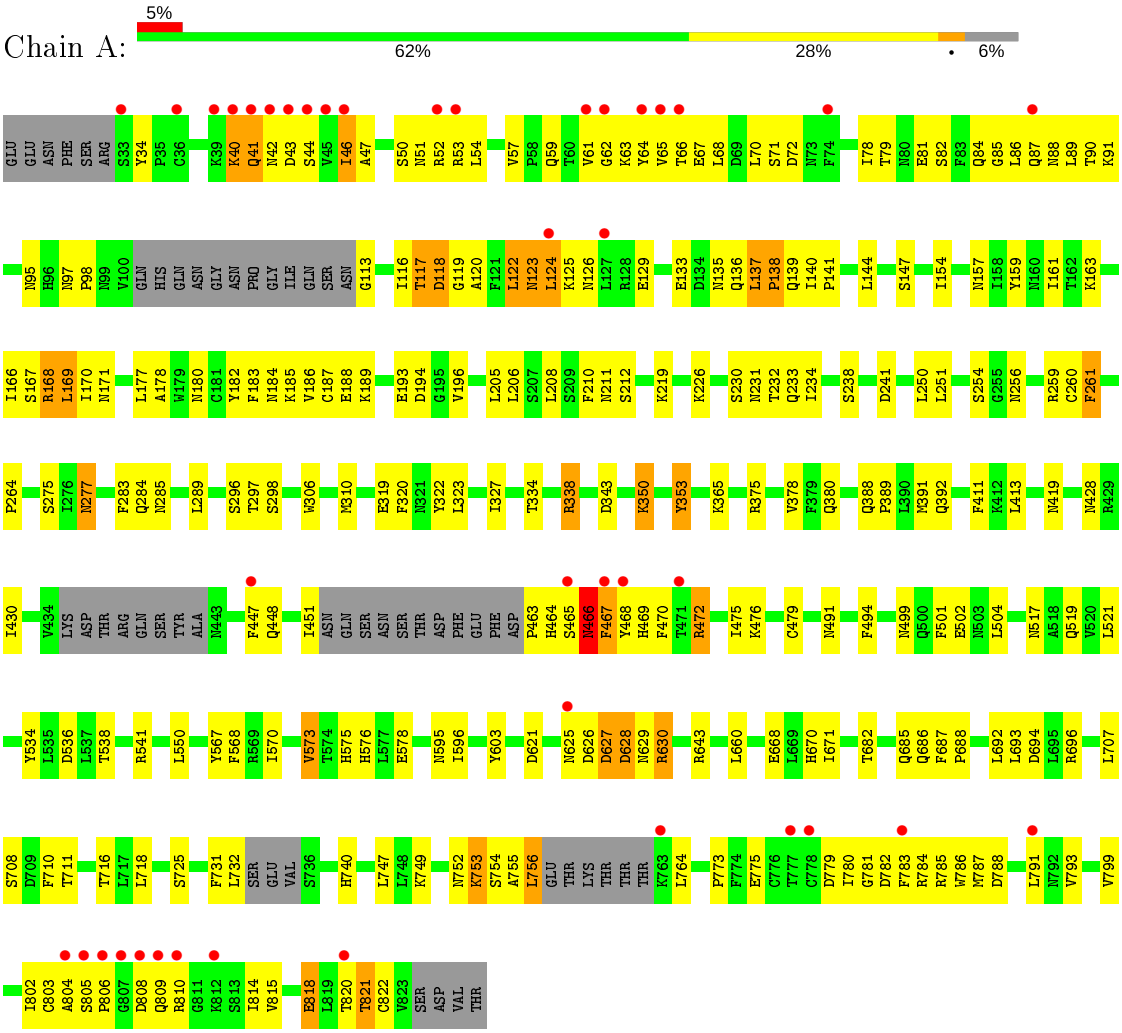
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	79	Total	O	0	0
			79	79		

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: Toll-like receptor 8

Chain A:



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

Chain B:

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

Chain C:

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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	171.52Å 171.52Å 301.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.02 – 2.60 45.02 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.02-2.60) 100.0 (45.02-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.20 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.206 , 0.239 0.212 , 0.243	Depositor DCC
R_{free} test set	2610 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	66.7	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 65.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6371	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: MAN, BMA, NAG, MES, 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	0.65	0/6164	0.83	6/8355 (0.1%)

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	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	137	LEU	C-N-CD	6.63	142.32	128.40
1	A	472	ARG	C-N-CD	6.03	141.06	128.40
1	A	57	VAL	C-N-CD	5.92	140.82	128.40
1	A	144	LEU	C-N-CD	5.57	140.10	128.40
1	A	138	PRO	CA-N-CD	-5.25	104.15	111.50
1	A	419	ASN	N-CA-C	5.03	124.57	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	TYR	Sidechain
1	A	466	ASN	Peptide

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	6042	0	6035	293	0
2	B	50	0	43	5	0
3	C	28	0	25	0	0
4	D	61	0	52	0	0
5	A	84	0	78	2	0
6	A	15	0	0	0	0
7	A	12	0	13	1	0
8	A	79	0	0	5	0
All	All	6371	0	6246	294	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 23.

All (294) 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:79:THR:HA	1:A:117:THR:CG2	1.49	1.42
1:A:79:THR:HA	1:A:117:THR:HG21	1.28	1.14
1:A:79:THR:HA	1:A:117:THR:HG22	1.30	1.12
1:A:755:ALA:HA	1:A:786:TRP:HZ3	1.07	1.11
1:A:755:ALA:HA	1:A:786:TRP:CZ3	1.89	1.07
1:A:59:GLN:N	1:A:59:GLN:OE1	1.88	1.06
1:A:388:GLN:HA	1:A:391:MET:CE	1.88	1.03
1:A:91:LYS:HG3	1:A:129:GLU:HB3	1.43	1.00
1:A:261:PHE:HE2	1:A:350:LYS:HG2	1.27	0.98
1:A:388:GLN:HA	1:A:391:MET:HE2	1.44	0.98
1:A:708:SER:HB2	1:A:732:LEU:CD1	1.96	0.96
1:A:261:PHE:HE2	1:A:350:LYS:CG	1.80	0.95
1:A:79:THR:CA	1:A:117:THR:CG2	2.44	0.95
1:A:626:ASP:O	1:A:627:ASP:HB2	1.67	0.94
1:A:193:GLU:O	1:A:196:VAL:HG23	1.70	0.91
1:A:79:THR:CA	1:A:117:THR:HG21	2.02	0.90
1:A:694:ASP:OD2	1:A:696:ARG:NH1	2.02	0.90
1:A:185:LYS:H	1:A:186:VAL:HA	1.35	0.89
1:A:375:ARG:NH2	1:A:470:PHE:CE2	2.40	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ASP:O	1:A:625:ASN:HB2	1.73	0.88
1:A:467:PHE:CE1	2:B:1:NAG:O6	2.27	0.87
1:A:708:SER:CB	1:A:732:LEU:HD13	2.04	0.87
1:A:319:GLU:OE2	1:A:468:TYR:HB3	1.74	0.86
1:A:46:ILE:HD13	1:A:47:ALA:N	1.92	0.84
1:A:627:ASP:OD1	1:A:630:ARG:HB2	1.79	0.83
1:A:708:SER:HB2	1:A:732:LEU:HD13	1.59	0.83
1:A:692:LEU:HD23	1:A:693:LEU:N	1.94	0.83
1:A:392:GLN:HB3	8:A:1013:HOH:O	1.79	0.82
1:A:338:ARG:HD3	1:A:338:ARG:O	1.80	0.82
1:A:626:ASP:O	1:A:627:ASP:CB	2.28	0.81
1:A:261:PHE:CE2	1:A:350:LYS:HG2	2.15	0.81
1:A:753:LYS:H	1:A:753:LYS:CD	1.94	0.80
1:A:753:LYS:HD3	1:A:753:LYS:H	1.44	0.80
1:A:463:PRO:HA	1:A:464:HIS:CB	2.10	0.80
1:A:694:ASP:OD1	1:A:696:ARG:HD3	1.81	0.79
1:A:95:ASN:OD1	1:A:133:GLU:N	2.16	0.78
1:A:193:GLU:O	1:A:196:VAL:CG2	2.31	0.78
1:A:350:LYS:HD2	1:A:350:LYS:H	1.49	0.77
1:A:185:LYS:N	1:A:186:VAL:HA	2.00	0.76
1:A:157:ASN:O	1:A:159:TYR:CE2	2.39	0.75
1:A:731:PHE:HB3	1:A:732:LEU:HG	1.69	0.75
1:A:183:PHE:HB2	1:A:184:ASN:HD22	1.52	0.75
1:A:67:GLU:CB	1:A:91:LYS:HB2	2.17	0.74
1:A:78:ILE:O	1:A:117:THR:HG22	1.86	0.74
1:A:40:LYS:O	1:A:41:GLN:HB2	1.85	0.74
1:A:44:SER:HB2	1:A:66:THR:OG1	1.88	0.74
1:A:752:ASN:HB3	1:A:753:LYS:HE2	1.68	0.73
1:A:463:PRO:HA	1:A:464:HIS:HB3	1.70	0.72
1:A:86:LEU:O	1:A:88:ASN:N	2.21	0.71
1:A:261:PHE:CZ	1:A:350:LYS:HE2	2.26	0.71
1:A:350:LYS:N	1:A:350:LYS:HD2	2.05	0.70
1:A:168:ARG:O	1:A:170:ILE:HG12	1.91	0.70
1:A:467:PHE:O	1:A:468:TYR:HB2	1.91	0.70
1:A:159:TYR:CD1	1:A:187:CYS:SG	2.86	0.69
1:A:756:LEU:O	1:A:756:LEU:HD13	1.92	0.69
1:A:135:ASN:O	1:A:137:LEU:HD23	1.92	0.69
1:A:809:GLN:OE1	1:A:809:GLN:HA	1.91	0.69
1:A:465:SER:O	1:A:466:ASN:HB2	1.93	0.69
1:A:185:LYS:H	1:A:186:VAL:CA	2.06	0.69
1:A:168:ARG:HG2	1:A:168:ARG:NH1	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LYS:CD	1:A:350:LYS:H	2.01	0.68
1:A:67:GLU:HB3	1:A:91:LYS:HB2	1.73	0.68
1:A:168:ARG:HH11	1:A:168:ARG:HG2	1.57	0.67
1:A:86:LEU:HD22	1:A:86:LEU:N	2.08	0.67
1:A:388:GLN:HB3	1:A:389:PRO:HD3	1.77	0.67
1:A:793:VAL:O	1:A:793:VAL:HG23	1.95	0.67
1:A:261:PHE:CE2	1:A:350:LYS:CG	2.70	0.67
1:A:470:PHE:O	1:A:472:ARG:HG2	1.96	0.66
1:A:467:PHE:HE1	2:B:1:NAG:O6	1.78	0.66
1:A:466:ASN:HB3	2:B:1:NAG:O7	1.97	0.65
1:A:183:PHE:HB2	1:A:184:ASN:ND2	2.13	0.64
1:A:90:THR:HA	1:A:126:ASN:O	1.97	0.64
1:A:40:LYS:H	1:A:40:LYS:HD3	1.60	0.64
1:A:375:ARG:NH2	1:A:470:PHE:CD2	2.62	0.64
1:A:65:VAL:O	1:A:89:LEU:HD23	1.98	0.63
1:A:79:THR:HG23	1:A:81:GLU:HB3	1.80	0.63
1:A:168:ARG:HH11	1:A:168:ARG:CG	2.12	0.63
1:A:137:LEU:HD23	1:A:137:LEU:N	2.13	0.63
1:A:34:TYR:CE1	1:A:815:VAL:HG21	2.34	0.63
1:A:125:LYS:HD2	1:A:147:SER:HB3	1.81	0.63
1:A:627:ASP:CG	1:A:628:ASP:H	2.03	0.62
1:A:818:GLU:N	1:A:818:GLU:OE1	2.33	0.62
1:A:117:THR:HG23	1:A:120:ALA:HB2	1.82	0.62
1:A:205:LEU:HD23	1:A:206:LEU:N	2.15	0.61
1:A:708:SER:HB2	1:A:732:LEU:HD12	1.79	0.61
1:A:696:ARG:HD2	1:A:718:LEU:HB3	1.82	0.61
1:A:451:ILE:C	1:A:451:ILE:HD12	2.20	0.61
1:A:117:THR:O	1:A:120:ALA:HB2	2.01	0.61
1:A:756:LEU:H	1:A:786:TRP:HH2	1.48	0.61
1:A:84:GLN:O	1:A:86:LEU:HD22	2.01	0.61
1:A:708:SER:CB	1:A:732:LEU:CD1	2.68	0.61
1:A:166:ILE:HA	1:A:169:LEU:HD23	1.83	0.60
1:A:205:LEU:C	1:A:205:LEU:HD23	2.21	0.60
1:A:284:GLN:OE1	5:A:901:NAG:H61	2.02	0.60
1:A:259:ARG:HD2	1:A:322:TYR:CZ	2.36	0.60
1:A:40:LYS:N	1:A:40:LYS:HD3	2.16	0.60
1:A:467:PHE:CD1	2:B:1:NAG:O6	2.54	0.60
1:A:707:LEU:CD2	1:A:711:THR:HG22	2.31	0.60
1:A:334:THR:HG22	1:A:365:LYS:HD2	1.83	0.60
1:A:41:GLN:OE1	1:A:42:ASN:HB3	2.01	0.60
1:A:694:ASP:CG	1:A:696:ARG:HH11	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LYS:HG3	1:A:129:GLU:CB	2.23	0.60
1:A:250:LEU:HD23	1:A:250:LEU:C	2.21	0.59
1:A:671:ILE:O	1:A:671:ILE:HG22	2.02	0.59
1:A:212:SER:HB3	1:A:233:GLN:NE2	2.17	0.59
1:A:51:ASN:HA	1:A:72:ASP:O	2.02	0.59
1:A:125:LYS:O	1:A:125:LYS:HG3	2.03	0.59
1:A:62:GLY:O	1:A:65:VAL:HG23	2.02	0.59
1:A:576:HIS:HB3	1:A:578:GLU:OE1	2.03	0.59
1:A:188:GLU:C	1:A:189:LYS:HD2	2.23	0.59
1:A:238:SER:N	1:A:241:ASP:OD2	2.25	0.58
1:A:682:THR:HA	1:A:710:PHE:CD1	2.37	0.58
1:A:805:SER:HB2	1:A:806:PRO:HA	1.85	0.58
1:A:113:GLY:HA2	1:A:136:GLN:HB3	1.85	0.58
1:A:118:ASP:N	1:A:118:ASP:OD1	2.37	0.58
1:A:53:ARG:NH2	1:A:799:VAL:HG12	2.19	0.58
1:A:277:ASN:HD22	1:A:277:ASN:C	2.08	0.57
1:A:79:THR:CA	1:A:117:THR:HG22	2.18	0.57
1:A:725:SER:HA	1:A:747:LEU:O	2.05	0.57
1:A:46:ILE:HD13	1:A:47:ALA:C	2.25	0.57
1:A:79:THR:O	1:A:82:SER:HB2	2.05	0.56
1:A:219:LYS:HE2	1:A:219:LYS:HA	1.87	0.56
1:A:388:GLN:CA	1:A:391:MET:HE2	2.27	0.56
1:A:137:LEU:O	1:A:157:ASN:HB2	2.04	0.56
1:A:782:ASP:O	1:A:785:ARG:HB3	2.05	0.56
1:A:84:GLN:C	1:A:86:LEU:HD22	2.26	0.56
1:A:68:LEU:HD21	1:A:70:LEU:HD11	1.87	0.56
1:A:184:ASN:O	1:A:185:LYS:HD2	2.06	0.56
1:A:708:SER:HB3	1:A:732:LEU:HD13	1.85	0.56
1:A:123:ASN:O	1:A:123:ASN:ND2	2.39	0.56
1:A:628:ASP:O	1:A:629:ASN:HB2	2.06	0.56
1:A:86:LEU:C	1:A:87:GLN:HG3	2.25	0.55
1:A:64:TYR:HA	1:A:88:ASN:OD1	2.06	0.55
1:A:289:LEU:HD23	1:A:310:MET:SD	2.46	0.55
1:A:157:ASN:O	1:A:159:TYR:CD2	2.60	0.55
1:A:707:LEU:CD2	1:A:711:THR:CG2	2.84	0.55
1:A:692:LEU:HD23	1:A:692:LEU:C	2.27	0.55
1:A:749:LYS:O	1:A:775:GLU:N	2.24	0.54
1:A:53:ARG:HH21	1:A:799:VAL:HG12	1.72	0.54
1:A:212:SER:CB	1:A:233:GLN:HE21	2.20	0.54
1:A:261:PHE:HE2	1:A:350:LYS:HG3	1.69	0.54
1:A:138:PRO:HD2	1:A:139:GLN:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:SER:HB2	1:A:71:SER:O	2.08	0.54
1:A:784:ARG:NH2	1:A:814:ILE:O	2.41	0.54
1:A:319:GLU:OE2	1:A:468:TYR:CB	2.52	0.53
1:A:140:ILE:HD13	1:A:166:ILE:HG12	1.91	0.53
1:A:125:LYS:CG	1:A:125:LYS:O	2.56	0.53
1:A:185:LYS:N	1:A:186:VAL:CA	2.70	0.53
1:A:660:LEU:HD22	1:A:686:GLN:HG3	1.91	0.53
1:A:707:LEU:HD23	1:A:711:THR:HG22	1.89	0.53
1:A:756:LEU:C	1:A:756:LEU:HD22	2.30	0.52
1:A:78:ILE:HB	1:A:116:ILE:HG12	1.91	0.52
1:A:67:GLU:HB2	1:A:91:LYS:HB2	1.91	0.52
1:A:259:ARG:NH1	1:A:322:TYR:CD1	2.77	0.52
1:A:567:TYR:O	1:A:575:HIS:HE1	1.92	0.52
1:A:250:LEU:HD23	1:A:251:LEU:N	2.24	0.52
1:A:802:ILE:CG2	1:A:803:CYS:N	2.72	0.52
1:A:52:ARG:O	1:A:54:LEU:HD23	2.09	0.52
1:A:212:SER:CB	1:A:233:GLN:NE2	2.74	0.52
1:A:806:PRO:O	1:A:809:GLN:N	2.43	0.52
1:A:188:GLU:HG3	1:A:189:LYS:H	1.75	0.51
1:A:189:LYS:HA	1:A:212:SER:OG	2.10	0.51
1:A:323:LEU:O	1:A:327:ILE:HG13	2.10	0.51
1:A:275:SER:HB3	1:A:298:SER:O	2.10	0.51
1:A:731:PHE:CB	1:A:732:LEU:HG	2.40	0.51
1:A:448:GLN:HA	1:A:448:GLN:HE21	1.74	0.51
1:A:54:LEU:N	1:A:54:LEU:HD23	2.26	0.51
1:A:731:PHE:HB3	1:A:732:LEU:CG	2.40	0.51
1:A:86:LEU:N	1:A:86:LEU:CD2	2.73	0.51
1:A:212:SER:HB3	1:A:233:GLN:HE21	1.74	0.51
1:A:169:LEU:O	1:A:171:ASN:N	2.40	0.51
1:A:350:LYS:N	1:A:350:LYS:CD	2.70	0.51
1:A:65:VAL:HB	1:A:89:LEU:HD21	1.92	0.50
1:A:756:LEU:N	1:A:786:TRP:HH2	2.10	0.50
1:A:138:PRO:HD2	1:A:139:GLN:N	2.27	0.50
1:A:183:PHE:CB	1:A:184:ASN:HD22	2.24	0.50
1:A:499:ASN:HA	1:A:502:GLU:HG2	1.93	0.50
1:A:285:ASN:OD1	5:A:901:NAG:O5	2.23	0.50
1:A:140:ILE:O	1:A:141:PRO:C	2.50	0.49
1:A:211:ASN:O	1:A:232:THR:HA	2.13	0.49
1:A:595:ASN:HD22	1:A:595:ASN:N	2.10	0.49
1:A:277:ASN:ND2	1:A:277:ASN:C	2.66	0.49
1:A:411:PHE:CD1	1:A:504:LEU:HD21	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ARG:CD	1:A:338:ARG:O	2.56	0.49
1:A:43:ASP:N	1:A:43:ASP:OD2	2.45	0.49
1:A:773:PRO:HA	1:A:804:ALA:HB2	1.95	0.49
1:A:413:LEU:HD12	1:A:413:LEU:C	2.33	0.49
1:A:85:GLY:C	1:A:87:GLN:HG3	2.33	0.49
1:A:122:LEU:N	1:A:122:LEU:CD1	2.76	0.49
1:A:463:PRO:CA	1:A:464:HIS:CB	2.88	0.49
1:A:63:LYS:H	1:A:63:LYS:HD3	1.78	0.49
1:A:820:THR:C	1:A:822:CYS:H	2.14	0.49
1:A:136:GLN:HG3	1:A:157:ASN:ND2	2.28	0.48
1:A:86:LEU:HD22	1:A:86:LEU:H	1.76	0.48
1:A:466:ASN:O	1:A:467:PHE:HB2	2.13	0.48
1:A:180:ASN:HD22	1:A:180:ASN:N	2.12	0.48
1:A:161:ILE:HG22	1:A:196:VAL:HG11	1.94	0.48
1:A:177:LEU:HB2	1:A:208:LEU:HD23	1.95	0.48
1:A:501:PHE:HB3	1:A:504:LEU:HD12	1.95	0.48
1:A:494:PHE:O	1:A:517:ASN:HA	2.14	0.48
1:A:643:ARG:HG3	1:A:668:GLU:HB3	1.96	0.48
1:A:136:GLN:HG3	1:A:157:ASN:HD21	1.77	0.48
1:A:469:HIS:HD2	8:A:1012:HOH:O	1.96	0.47
1:A:764:LEU:O	1:A:764:LEU:HD12	2.13	0.47
1:A:788:ASP:O	1:A:791:LEU:CD1	2.63	0.47
1:A:79:THR:O	1:A:82:SER:CB	2.62	0.47
1:A:466:ASN:HD22	1:A:466:ASN:HA	1.45	0.47
1:A:86:LEU:CD2	1:A:86:LEU:H	2.27	0.47
1:A:50:SER:O	1:A:52:ARG:HD2	2.15	0.47
1:A:753:LYS:N	1:A:753:LYS:HD3	2.21	0.47
1:A:163:LYS:HA	1:A:167:SER:OG	2.15	0.47
1:A:731:PHE:HA	1:A:732:LEU:HD23	1.96	0.47
1:A:447:PHE:O	1:A:447:PHE:CD2	2.69	0.47
1:A:731:PHE:HB3	1:A:732:LEU:CD2	2.45	0.47
1:A:793:VAL:O	1:A:793:VAL:CG2	2.60	0.46
1:A:319:GLU:HG2	1:A:343:ASP:CG	2.36	0.46
1:A:84:GLN:N	1:A:86:LEU:CD2	2.78	0.46
1:A:536:ASP:OD1	1:A:538:THR:HG23	2.16	0.46
1:A:388:GLN:N	1:A:389:PRO:CD	2.78	0.46
1:A:124:LEU:N	1:A:124:LEU:HD23	2.30	0.46
1:A:205:LEU:CD2	1:A:205:LEU:C	2.84	0.46
1:A:139:GLN:O	1:A:141:PRO:HD3	2.16	0.46
1:A:183:PHE:HA	1:A:184:ASN:HA	1.49	0.45
1:A:283:PHE:HD2	1:A:306:TRP:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PRO:CD	1:A:139:GLN:N	2.80	0.45
1:A:392:GLN:CB	8:A:1013:HOH:O	2.52	0.45
1:A:296:SER:HA	1:A:320:PHE:O	2.17	0.45
1:A:79:THR:N	1:A:82:SER:OG	2.38	0.45
7:A:921:MES:H82	7:A:921:MES:H31	1.88	0.45
1:A:260:CYS:O	1:A:261:PHE:C	2.55	0.45
1:A:716:THR:HG23	1:A:740:HIS:HB3	1.98	0.45
1:A:802:ILE:HG22	1:A:803:CYS:N	2.32	0.45
1:A:570:ILE:HB	1:A:573:VAL:CG1	2.48	0.44
1:A:696:ARG:HD2	1:A:718:LEU:CB	2.47	0.44
1:A:780:ILE:O	1:A:780:ILE:HG23	2.17	0.44
1:A:806:PRO:HD2	1:A:809:GLN:HB2	1.99	0.44
1:A:85:GLY:O	1:A:87:GLN:HG3	2.17	0.44
1:A:466:ASN:O	1:A:467:PHE:CD2	2.70	0.44
1:A:353:TYR:CZ	1:A:380:GLN:HG2	2.52	0.44
1:A:708:SER:N	1:A:732:LEU:HD11	2.31	0.44
1:A:621:ASP:O	1:A:625:ASN:CB	2.57	0.44
1:A:97:ASN:HA	1:A:98:PRO:HA	1.68	0.44
1:A:475:ILE:O	1:A:476:LYS:C	2.52	0.43
1:A:166:ILE:HA	1:A:169:LEU:CD2	2.48	0.43
1:A:230:SER:HA	1:A:254:SER:O	2.18	0.43
1:A:821:THR:HG22	1:A:821:THR:O	2.18	0.43
1:A:67:GLU:OE1	1:A:91:LYS:HB2	2.18	0.43
1:A:780:ILE:O	1:A:784:ARG:HB2	2.17	0.43
1:A:783:PHE:O	1:A:786:TRP:HB3	2.18	0.43
1:A:570:ILE:HB	1:A:573:VAL:HG11	2.00	0.43
1:A:219:LYS:CA	1:A:219:LYS:HE2	2.49	0.43
1:A:154:ILE:HG23	1:A:178:ALA:O	2.18	0.43
1:A:430:ILE:HD12	1:A:430:ILE:N	2.34	0.43
1:A:182:TYR:O	1:A:183:PHE:C	2.58	0.42
1:A:476:LYS:HD2	8:A:1075:HOH:O	2.17	0.42
1:A:319:GLU:HG3	1:A:319:GLU:H	1.51	0.42
1:A:79:THR:O	1:A:82:SER:N	2.52	0.42
1:A:122:LEU:H	1:A:122:LEU:CD1	2.32	0.42
1:A:234:ILE:O	1:A:256:ASN:HB3	2.20	0.42
1:A:79:THR:HG23	1:A:82:SER:H	1.83	0.42
1:A:568:PHE:CD1	1:A:596:ILE:HG12	2.55	0.42
1:A:466:ASN:HB3	1:A:467:PHE:H	1.64	0.42
1:A:125:LYS:CD	1:A:147:SER:HB3	2.49	0.42
1:A:692:LEU:C	1:A:692:LEU:CD2	2.88	0.42
1:A:79:THR:CG2	1:A:81:GLU:HB3	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LYS:HG2	1:A:250:LEU:HB3	2.02	0.41
1:A:261:PHE:CE2	1:A:350:LYS:HG3	2.48	0.41
1:A:521:LEU:HD13	1:A:550:LEU:HD21	2.02	0.41
1:A:119:GLY:HA2	1:A:122:LEU:HD13	2.02	0.41
1:A:137:LEU:O	1:A:157:ASN:N	2.47	0.41
1:A:163:LYS:HG3	8:A:1035:HOH:O	2.20	0.41
1:A:42:ASN:O	1:A:43:ASP:HB2	2.19	0.41
1:A:820:THR:C	1:A:822:CYS:N	2.73	0.41
1:A:670:HIS:HA	1:A:694:ASP:HB3	2.03	0.41
1:A:428:ASN:O	1:A:491:ASN:HA	2.20	0.41
1:A:517:ASN:OD1	1:A:519:GLN:HG2	2.21	0.41
1:A:773:PRO:CA	1:A:804:ALA:HB2	2.51	0.41
1:A:627:ASP:CG	1:A:628:ASP:N	2.73	0.41
1:A:749:LYS:HA	1:A:773:PRO:O	2.20	0.41
1:A:467:PHE:HA	2:B:1:NAG:H2	2.02	0.41
1:A:193:GLU:O	1:A:196:VAL:HG22	2.18	0.41
1:A:256:ASN:O	1:A:297:THR:HA	2.21	0.41
1:A:685:GLN:HG2	1:A:710:PHE:HA	2.02	0.41
1:A:779:ASP:C	1:A:781:GLY:H	2.23	0.41
1:A:40:LYS:O	1:A:41:GLN:CB	2.58	0.41
1:A:479:CYS:SG	1:A:534:TYR:CD1	3.14	0.41
1:A:625:ASN:N	1:A:625:ASN:HD22	2.18	0.41
1:A:603:TYR:CZ	1:A:630:ARG:NH1	2.89	0.41
1:A:687:PHE:HA	1:A:688:PRO:HD2	1.93	0.41
1:A:210:PHE:CE2	1:A:231:ASN:OD1	2.74	0.41
1:A:451:ILE:CD1	1:A:451:ILE:C	2.89	0.40
1:A:375:ARG:NH2	1:A:470:PHE:HE2	2.10	0.40
1:A:470:PHE:N	1:A:470:PHE:CD1	2.88	0.40
1:A:818:GLU:H	1:A:818:GLU:CD	2.24	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	739/801 (92%)	675 (91%)	57 (8%)	7 (1%)	17 35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	PHE
1	A	466	ASN
1	A	627	ASP
1	A	467	PHE
1	A	378	VAL
1	A	821	THR
1	A	264	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	698/745 (94%)	671 (96%)	27 (4%)	32 58

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	41	GLN
1	A	46	ILE
1	A	61	VAL
1	A	117	THR
1	A	118	ASP
1	A	122	LEU
1	A	123	ASN
1	A	124	LEU
1	A	168	ARG
1	A	169	LEU
1	A	194	ASP
1	A	277	ASN
1	A	338	ARG

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Mol	Chain	Res	Type
1	A	350	LYS
1	A	466	ASN
1	A	541	ARG
1	A	573	VAL
1	A	628	ASP
1	A	630	ARG
1	A	753	LYS
1	A	754	SER
1	A	756	LEU
1	A	787	MET
1	A	808	ASP
1	A	810	ARG
1	A	818	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	77	HIS
1	A	84	GLN
1	A	99	ASN
1	A	157	ASN
1	A	184	ASN
1	A	231	ASN
1	A	233	GLN
1	A	277	ASN
1	A	388	GLN
1	A	448	GLN
1	A	466	ASN
1	A	575	HIS
1	A	595	ASN
1	A	625	ASN
1	A	629	ASN
1	A	752	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

11 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	B	1	1,2	14,14,15	1.02	2 (14%)	17,19,21	1.83	2 (11%)
2	NAG	B	2	2	14,14,15	1.02	1 (7%)	17,19,21	1.20	3 (17%)
2	BMA	B	3	2	11,11,12	0.35	0	15,15,17	0.94	1 (6%)
2	MAN	B	4	2	11,11,12	0.64	0	15,15,17	0.92	1 (6%)
3	NAG	C	1	1,3	14,14,15	0.60	0	17,19,21	1.43	5 (29%)
3	NAG	C	2	3	14,14,15	0.29	0	17,19,21	0.61	0
4	NAG	D	1	1,4	14,14,15	0.69	0	17,19,21	1.42	3 (17%)
4	NAG	D	2	4	14,14,15	0.83	1 (7%)	17,19,21	1.69	3 (17%)
4	BMA	D	3	4	11,11,12	0.64	0	15,15,17	1.73	3 (20%)
4	MAN	D	4	4	11,11,12	0.43	0	15,15,17	1.05	2 (13%)
4	MAN	D	5	4	11,11,12	0.77	0	15,15,17	1.20	2 (13%)

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	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	1/2/19/22	0/1/1/1
4	MAN	D	5	4	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	-2.69	1.39	1.43
4	D	2	NAG	O5-C1	-2.21	1.40	1.43
2	B	1	NAG	O5-C1	-2.14	1.40	1.43
2	B	1	NAG	O5-C5	-2.10	1.39	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	O5-C1-C2	-5.14	103.17	111.29
4	D	3	BMA	O3-C3-C2	4.93	119.43	109.99
4	D	2	NAG	O5-C1-C2	-4.06	104.89	111.29
4	D	2	NAG	C2-N2-C7	-3.48	117.95	122.90
2	B	1	NAG	C1-O5-C5	-3.28	107.74	112.19
4	D	1	NAG	O5-C5-C6	3.22	112.26	107.20
2	B	2	NAG	O5-C1-C2	-2.87	106.75	111.29
3	C	1	NAG	C1-O5-C5	-2.82	108.38	112.19
4	D	5	MAN	O5-C1-C2	-2.79	106.47	110.77
4	D	3	BMA	O5-C5-C6	2.71	111.46	107.20
4	D	1	NAG	O5-C1-C2	-2.68	107.05	111.29
2	B	4	MAN	C1-C2-C3	2.65	112.92	109.67
4	D	3	BMA	O5-C1-C2	-2.44	107.00	110.77
2	B	2	NAG	O4-C4-C3	-2.33	104.95	110.35
3	C	1	NAG	O7-C7-N2	2.33	126.24	121.95
3	C	1	NAG	O7-C7-C8	-2.33	117.73	122.06
2	B	3	BMA	O5-C5-C6	2.22	110.68	107.20
4	D	4	MAN	O5-C5-C6	2.20	110.66	107.20
3	C	1	NAG	O4-C4-C3	-2.20	105.26	110.35
4	D	4	MAN	C1-O5-C5	2.17	115.14	112.19
4	D	1	NAG	O3-C3-C4	2.15	115.32	110.35
4	D	5	MAN	O3-C3-C2	2.11	114.03	109.99
4	D	2	NAG	C1-C2-N2	2.05	113.99	110.49
2	B	2	NAG	O5-C5-C6	2.03	110.38	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	NAG	O5-C1-C2	-2.01	108.11	111.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	MAN	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
4	D	5	MAN	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

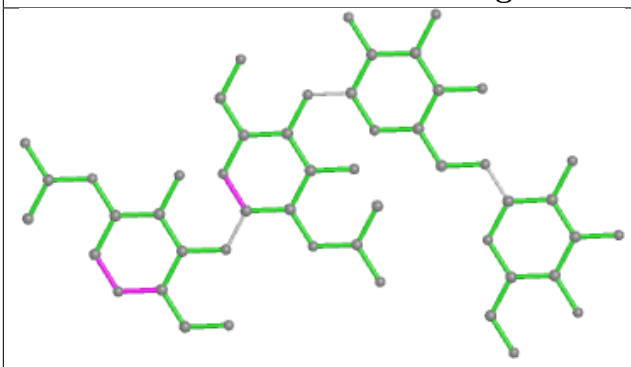
There are no ring outliers.

1 monomer is involved in 5 short contacts:

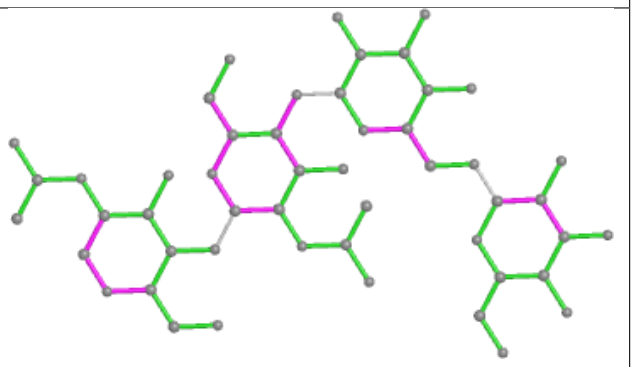
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	5	0

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

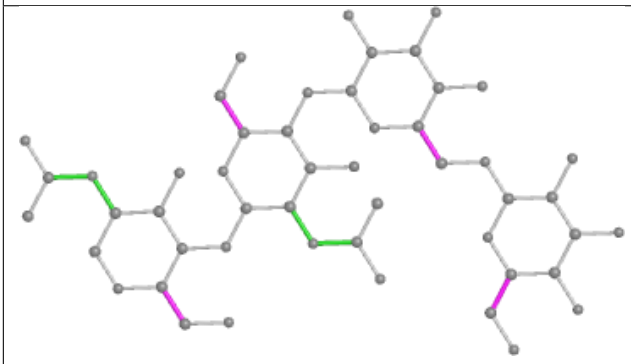
Oligosaccharide Chain B



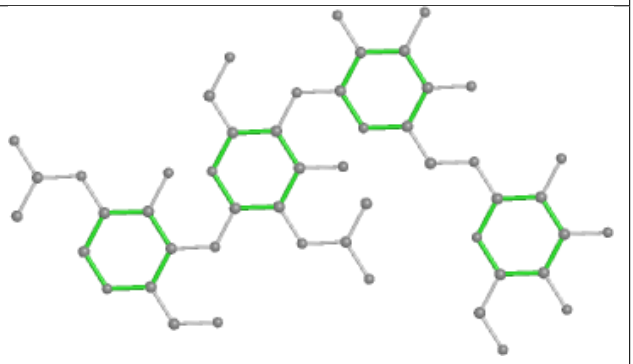
Bond lengths



Bond angles

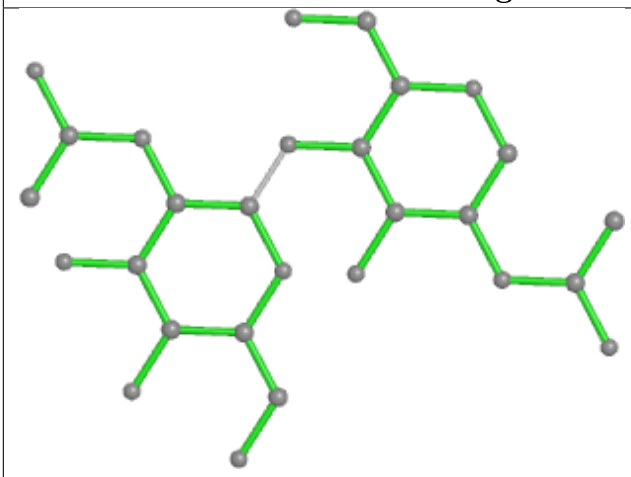


Torsions

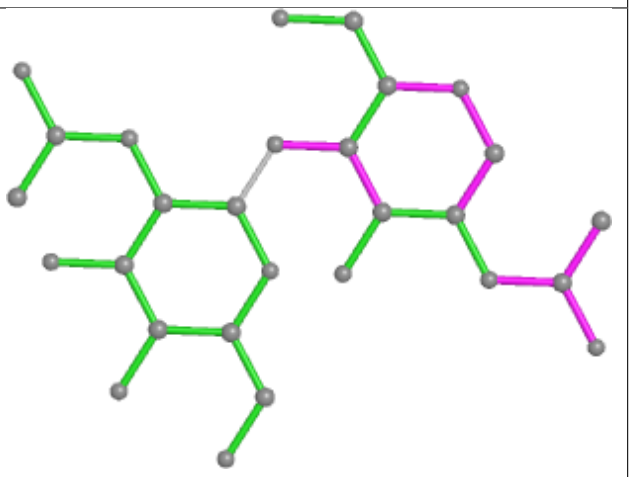


Rings

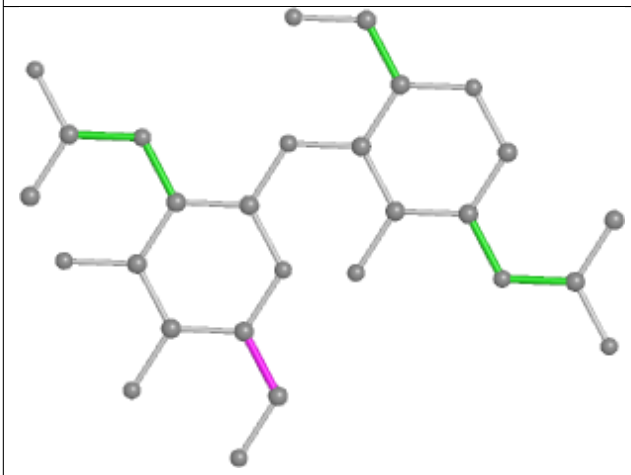
Oligosaccharide Chain C



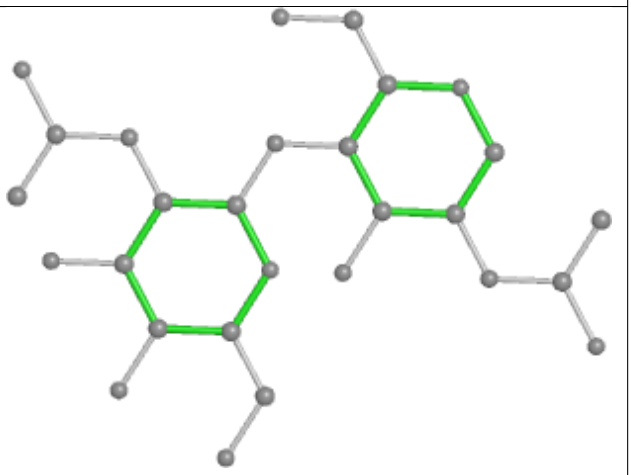
Bond lengths



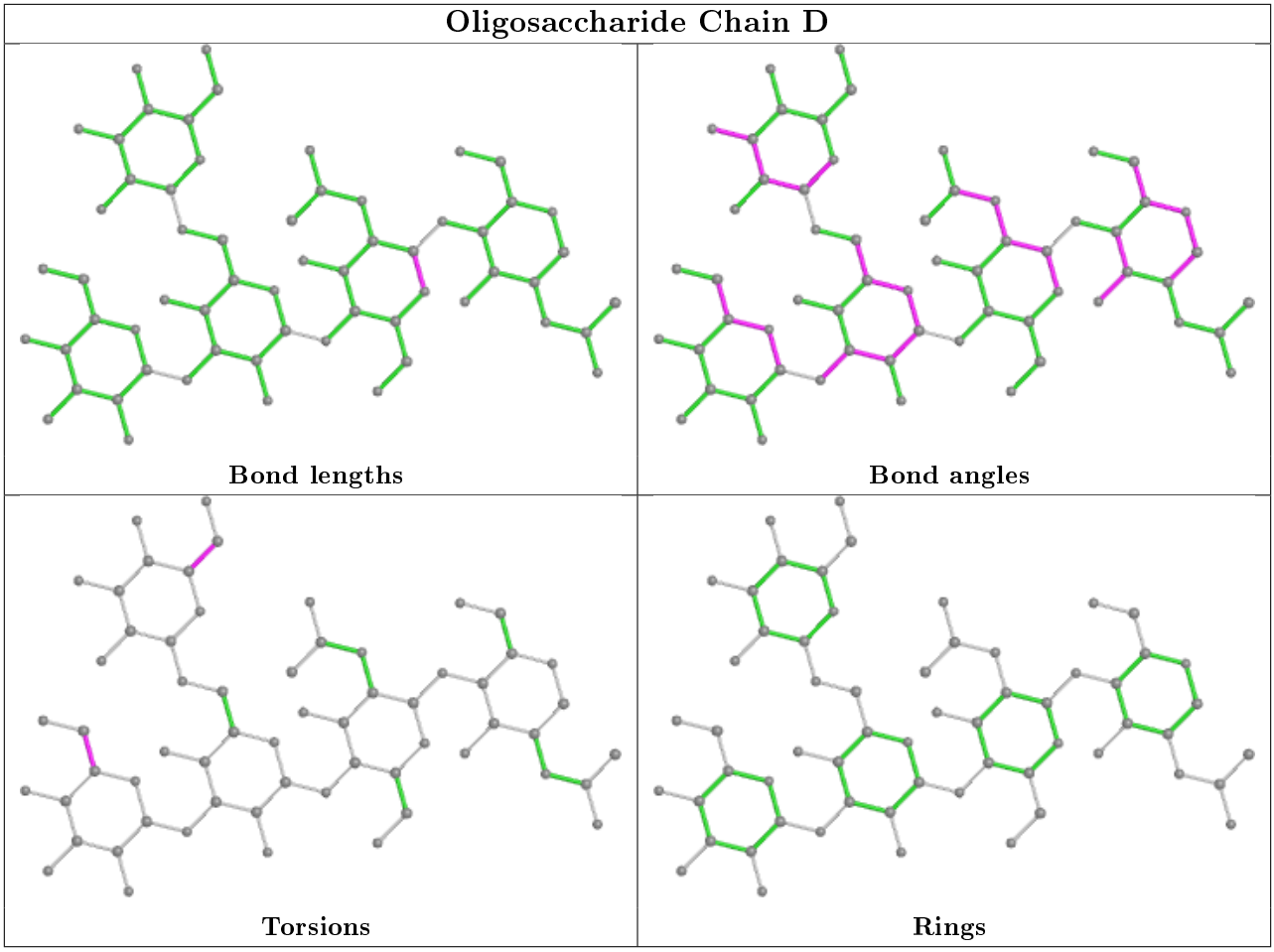
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
7	MES	A	921	-	12,12,12	2.32	1 (8%)	14,16,16	1.63	4 (28%)
5	NAG	A	917	1	14,14,15	0.64	0	17,19,21	1.32	3 (17%)
5	NAG	A	910	1	14,14,15	0.89	1 (7%)	17,19,21	1.49	2 (11%)
6	SO4	A	920	-	4,4,4	0.39	0	6,6,6	0.28	0
5	NAG	A	901	1	14,14,15	0.30	0	17,19,21	0.62	0
5	NAG	A	906	1	14,14,15	0.62	0	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	911	1	14,14,15	0.57	0	17,19,21	1.07	1 (5%)
6	SO4	A	919	-	4,4,4	0.32	0	6,6,6	0.25	0
6	SO4	A	918	-	4,4,4	0.30	0	6,6,6	0.32	0
5	NAG	A	907	1	14,14,15	0.60	0	17,19,21	1.09	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MES	A	921	-	-	5/6/14/14	0/1/1/1
5	NAG	A	917	1	-	0/6/23/26	0/1/1/1
5	NAG	A	910	1	-	1/6/23/26	0/1/1/1
5	NAG	A	901	1	-	1/6/23/26	0/1/1/1
5	NAG	A	906	1	-	0/6/23/26	0/1/1/1
5	NAG	A	911	1	-	1/6/23/26	0/1/1/1
5	NAG	A	907	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	921	MES	C8-S	-7.58	1.66	1.77
5	A	910	NAG	O5-C1	-2.31	1.40	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	921	MES	O1S-S-C8	3.14	110.70	106.92
5	A	917	NAG	C4-C3-C2	-3.00	106.61	111.02
5	A	907	NAG	C1-O5-C5	2.90	116.12	112.19
5	A	910	NAG	C6-C5-C4	-2.71	106.66	113.00
7	A	921	MES	O2S-S-C8	2.66	110.12	106.92
7	A	921	MES	O3S-S-C8	2.47	109.76	105.77
5	A	911	NAG	O5-C5-C6	2.44	111.03	107.20
7	A	921	MES	C2-C3-N4	2.39	113.72	110.10
5	A	917	NAG	O5-C5-C6	2.16	110.59	107.20
5	A	910	NAG	O3-C3-C4	-2.04	105.64	110.35
5	A	917	NAG	C1-C2-N2	-2.01	107.06	110.49

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	921	MES	C8-C7-N4-C3
7	A	921	MES	N4-C7-C8-S
5	A	901	NAG	O5-C5-C6-O6
7	A	921	MES	C7-C8-S-O3S
7	A	921	MES	C7-C8-S-O1S
7	A	921	MES	C7-C8-S-O2S
5	A	910	NAG	C1-C2-N2-C7
5	A	911	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	921	MES	1	0
5	A	901	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	751/801 (93%)	0.15	41 (5%)	25	19	37, 73, 136, 171	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	64	TYR	6.3
1	A	467	PHE	5.0
1	A	74	PHE	4.9
1	A	42	ASN	4.8
1	A	46	ILE	4.8
1	A	41	GLN	4.7
1	A	808	ASP	4.6
1	A	39	LYS	4.1
1	A	45	VAL	4.0
1	A	43	ASP	3.9
1	A	36	CYS	3.9
1	A	806	PRO	3.7
1	A	447	PHE	3.6
1	A	87	GLN	3.6
1	A	40	LYS	3.5
1	A	65	VAL	3.5
1	A	810	ARG	3.5
1	A	809	GLN	3.2
1	A	783	PHE	3.1
1	A	44	SER	2.9
1	A	66	THR	2.9
1	A	778	CYS	2.9
1	A	812	LYS	2.8
1	A	52	ARG	2.7
1	A	61	VAL	2.7
1	A	33	SER	2.7
1	A	791	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	468	TYR	2.6
1	A	777	THR	2.6
1	A	625	ASN	2.6
1	A	124	LEU	2.5
1	A	804	ALA	2.5
1	A	62	GLY	2.4
1	A	471	THR	2.4
1	A	127	LEU	2.4
1	A	807	GLY	2.2
1	A	465	SER	2.2
1	A	53	ARG	2.2
1	A	805	SER	2.1
1	A	820	THR	2.1
1	A	763	LYS	2.0

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

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

6.3 Carbohydrates (i)

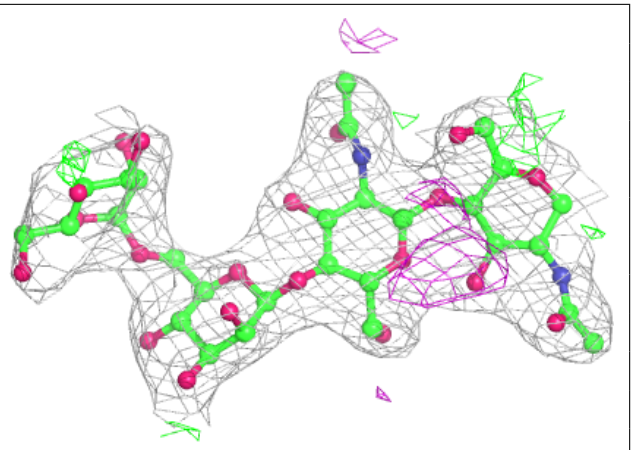
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

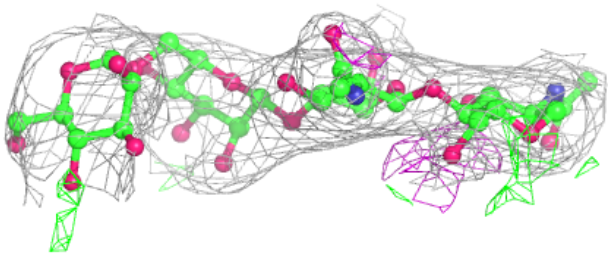
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	B	4	11/12	0.71	0.25	100,122,138,138	0
4	MAN	D	4	11/12	0.84	0.17	109,119,129,131	0
4	MAN	D	5	11/12	0.87	0.14	88,103,119,128	0
2	BMA	B	3	11/12	0.87	0.17	68,98,115,130	0
3	NAG	C	2	14/15	0.91	0.18	58,94,121,129	0
4	BMA	D	3	11/12	0.93	0.15	68,97,107,125	0
2	NAG	B	1	14/15	0.96	0.15	44,52,62,73	0
4	NAG	D	2	14/15	0.97	0.10	42,53,68,75	0
3	NAG	C	1	14/15	0.98	0.13	42,47,57,64	0
2	NAG	B	2	14/15	0.98	0.13	52,60,72,74	0
4	NAG	D	1	14/15	0.99	0.13	43,46,51,54	0

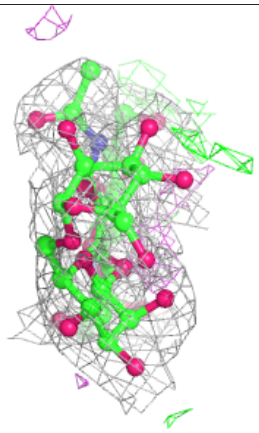
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

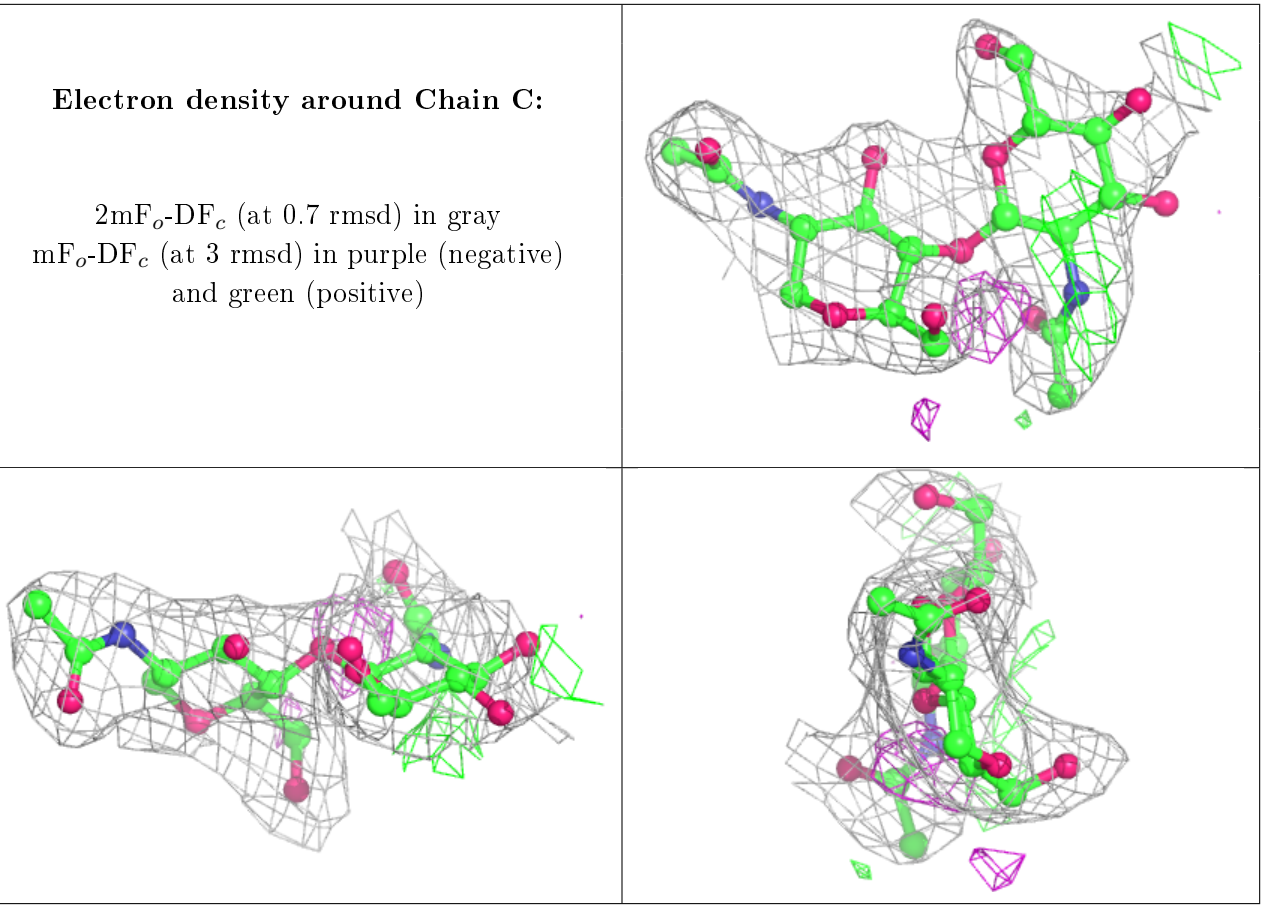






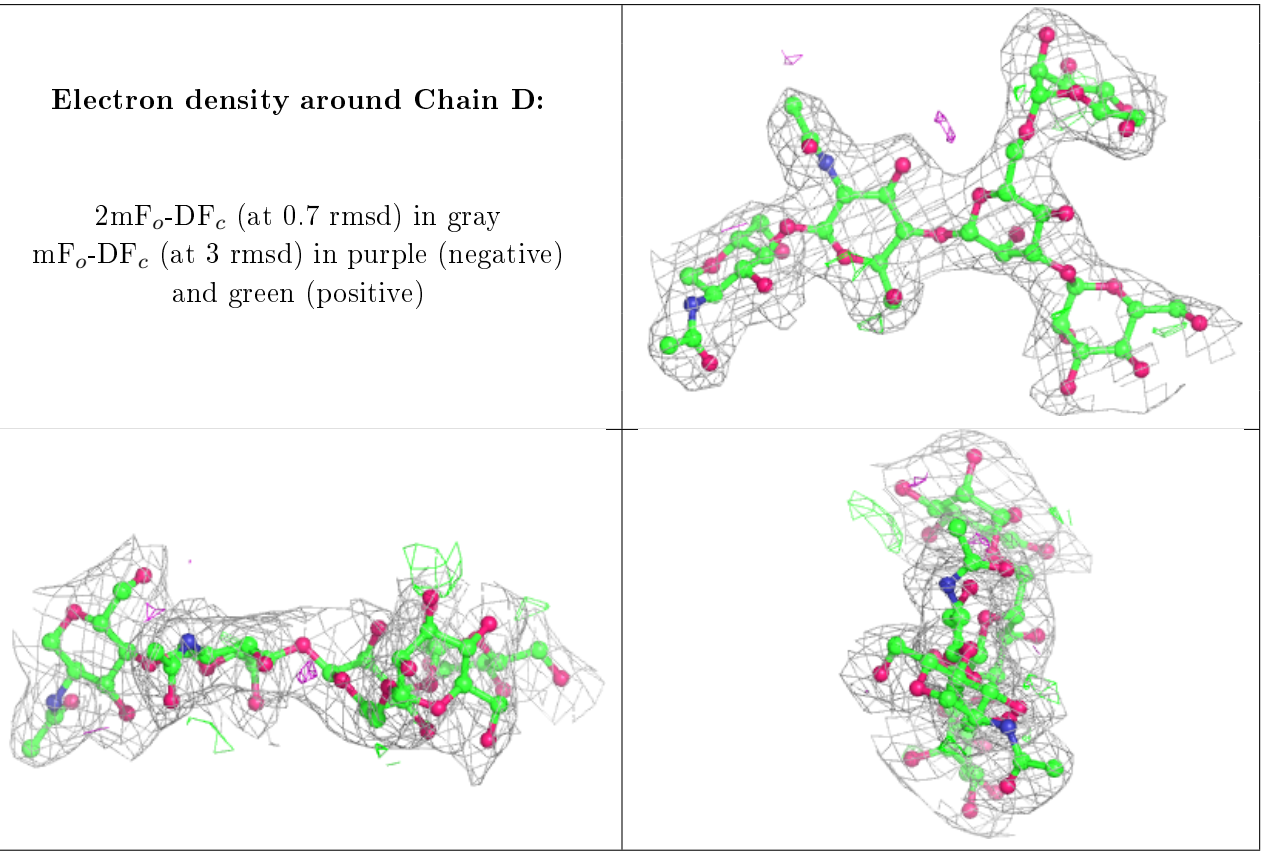
Electron density around Chain C:

$2mF_o$-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)



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	NAG	A	911	14/15	0.81	0.24	101,115,142,145	0
7	MES	A	921	12/12	0.83	0.26	58,78,82,86	12
5	NAG	A	907	14/15	0.87	0.27	81,95,108,116	0
5	NAG	A	901	14/15	0.88	0.16	83,106,122,122	0
6	SO4	A	919	5/5	0.91	0.17	94,108,132,136	0
5	NAG	A	910	14/15	0.91	0.15	77,91,103,104	0
5	NAG	A	906	14/15	0.94	0.15	64,73,81,82	0
6	SO4	A	920	5/5	0.95	0.08	97,98,109,112	0
6	SO4	A	918	5/5	0.96	0.12	71,85,90,96	0
5	NAG	A	917	14/15	0.96	0.24	64,72,85,87	0

6.5 Other polymers

There are no such residues in this entry.