Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 12:16 AM EDT

PDB ID	:	1TB6
Title	:	2.5A Crystal Structure of the Antithrombin-Thrombin-Heparin Ternary Complex
Authors	:	Li, W.; Johnson, D.J.; Esmon, C.T.; Huntington, J.A.
Deposited on	:	2004-05-19
Resolution	:	2.50 Å(reported)

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

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

The 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:

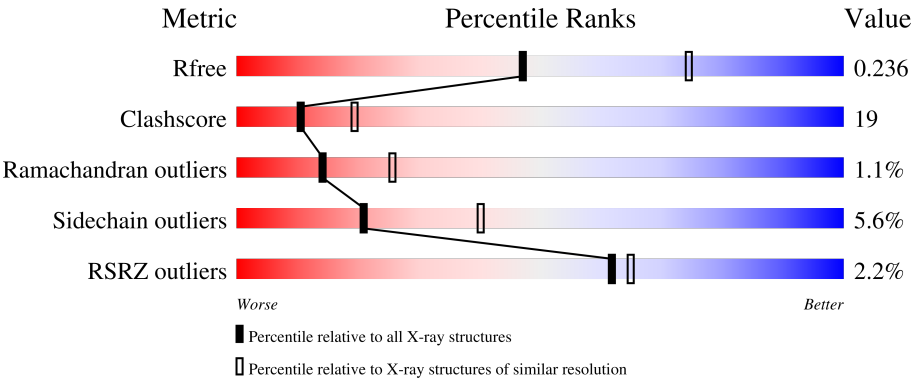
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	L	49	6%, 55%, 29%, ·, 12%
2	H	259	%, 68%, 30%, ·
3	I	432	2%, 63%, 29%, ·, 5%
4	A	3	33%, 67%
5	B	16	44%, 50%, 6%

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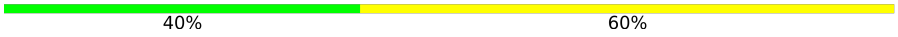
Mol	Chain	Length	Quality of chain
6	C	5	
7	D	3	

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
4	NAG	A	1	X	-	-	-
4	NAG	A	2	-	-	-	X
5	GU6	B	15	X	-	-	-
6	MAN	C	4	-	-	-	X
6	MAN	C	5	-	-	-	X
7	NAG	D	2	-	-	-	X
7	BMA	D	3	-	-	-	X
8	MPD	H	782	-	-	X	X
9	NAG	I	801	X	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 6324 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 thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	43	Total	C	N	O	S	0	0	0
			343	219	52	71	1			

- Molecule 2 is a protein called thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	259	Total	C	N	O	S	0	0	0
			2070	1324	362	370	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	195	ALA	SER	engineered mutation	UNP P00734

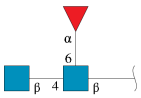
- Molecule 3 is a protein called Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	412	Total	C	N	O	S	0	0	0
			3271	2091	553	607	20			

There are 3 discrepancies between the modelled and reference sequences:

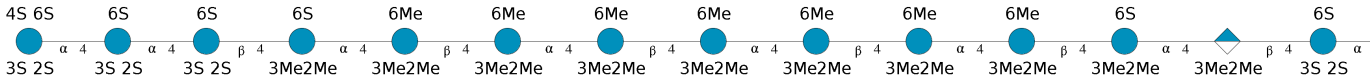
Chain	Residue	Modelled	Actual	Comment	Reference
I	137	ALA	SER	engineered mutation	UNP P01008
I	317	CYS	VAL	engineered mutation	UNP P01008
I	401	CYS	THR	engineered mutation	UNP P01008

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



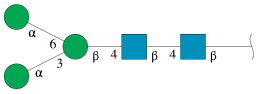
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	A	3	38	22	2	14	0	0	0

- Molecule 5 is an oligosaccharide called 2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-sulfonato-beta-D-glucopyranose-(1-4)-2,3-di-O-methyl-6-O-sulfonato-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3-di-O-methyl-6-O-sulfonato-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-alpha-L-idopyranuronic acid-(1-4)-methyl 3-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranoside.



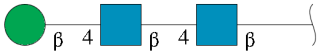
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O	S			
5	B	16	278	127	134	17	0	0	0

- Molecule 6 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.



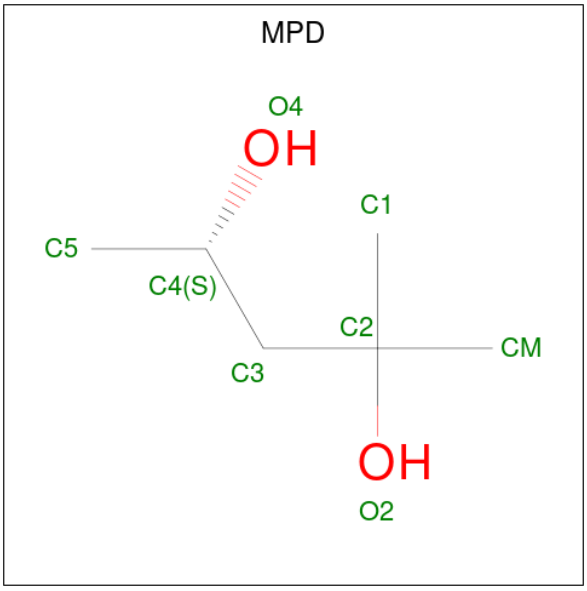
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	C	5	61	34	2	25	0	0	0

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



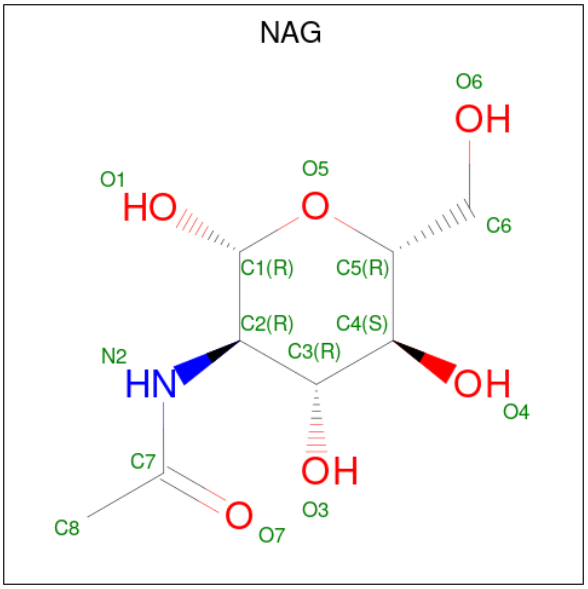
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	D	3	Total C N O 39 22 2 15	0	0	0

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total C O 8 6 2	0	0
8	H	1	Total C O 8 6 2	0	0
8	H	1	Total C O 8 6 2	0	0
8	H	1	Total C O 8 6 2	0	0
8	I	1	Total C O 8 6 2	0	0
8	I	1	Total C O 8 6 2	0	0
8	I	1	Total C O 8 6 2	0	0
8	I	1	Total C O 8 6 2	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

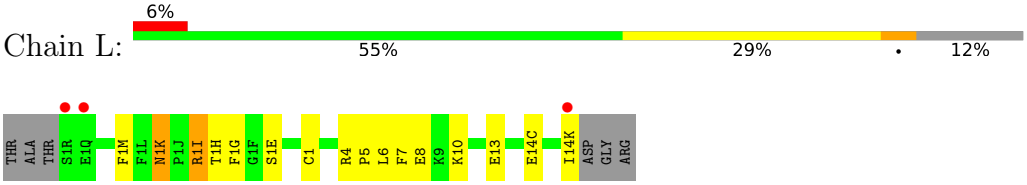
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	3	Total O 3 3	0	0
10	H	47	Total O 47 47	0	0
10	I	96	Total O 96 96	0	0

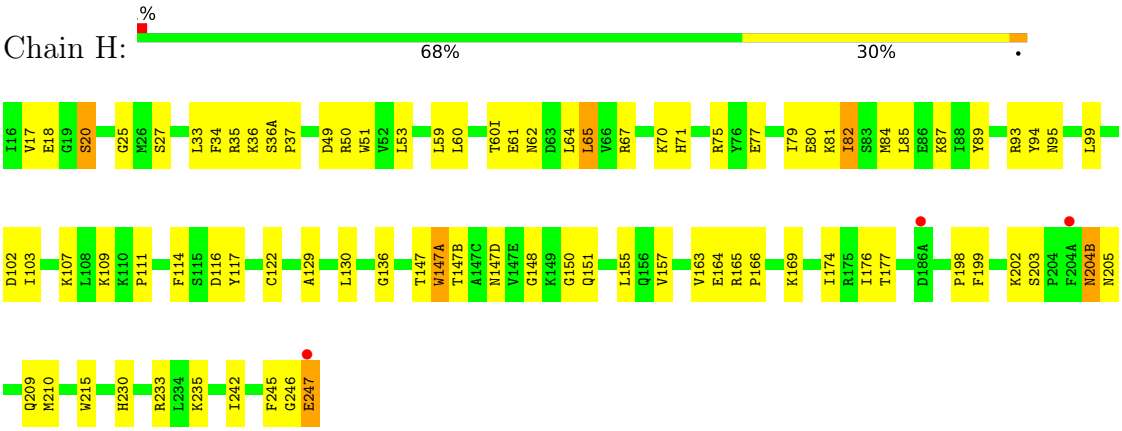
3 Residue-property plots (i)

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.

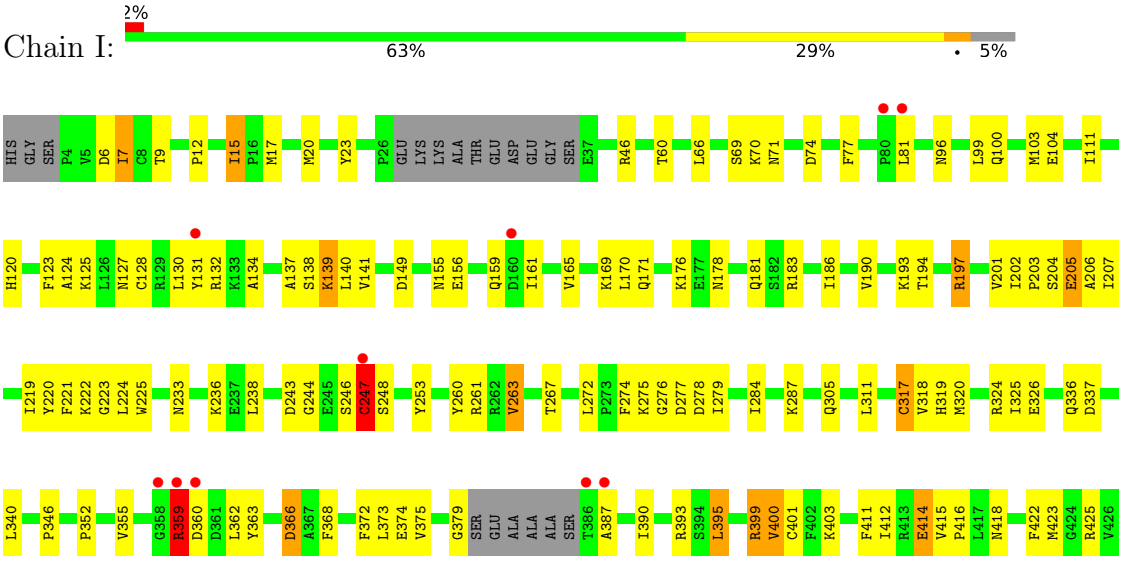
- Molecule 1: thrombin

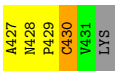


- Molecule 2: thrombin



- Molecule 3: Antithrombin-III





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

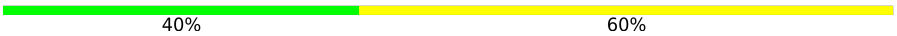
Chain A:

• Molecule 5: 2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-sulfonato-beta-D-glucopyranose-(1-4)-2,3-di-O-methyl-6-O-sulfonato-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3-di-O-methyl-6-O-sulfonato-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-alpha-L-idopyranuronic acid-(1-4)-methyl 3-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranoside

Chain B:

• Molecule 6: 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 C:



• Molecule 7: 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	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.41Å 88.40Å 117.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.46 – 2.50 37.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (37.46-2.50) 99.4 (37.46-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.208 , 0.245 0.201 , 0.236	Depositor DCC
R_{free} test set	1301 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å^2)	46.3	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6324	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: BMA, GU6, GU2, GU4, NAG, GU9, GU8, MPD, MAN, FUC, GU1, GU5, GU0, GU3

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	L	0.34	0/350	0.60	0/470
2	H	0.36	0/2125	0.67	1/2876 (0.0%)
3	I	0.40	0/3337	0.67	1/4508 (0.0%)
All	All	0.38	0/5812	0.67	2/7854 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	317	CYS	CA-CB-SG	6.18	125.12	114.00
2	H	247	GLU	N-CA-C	5.56	126.00	111.00

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	L	343	0	315	26	0
2	H	2070	0	2022	76	0
3	I	3271	0	3248	116	1
4	A	38	0	34	3	0
5	B	278	0	190	25	0
6	C	61	0	52	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	39	0	34	0	0
8	H	32	0	56	9	0
8	I	32	0	56	5	0
9	I	14	0	13	1	0
10	H	47	0	0	3	0
10	I	96	0	0	5	0
10	L	3	0	0	0	0
All	All	6324	0	6020	226	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 19.

All (226) 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)
3:I:324:ARG:HH12	3:I:374:GLU:HG3	1.21	1.02
3:I:7:ILE:HD13	3:I:7:ILE:H	1.25	0.98
1:L:1(I):ARG:HG2	1:L:1(I):ARG:HH11	1.39	0.85
2:H:71:HIS:HB2	8:H:782:MPD:H11	1.59	0.84
3:I:355:VAL:HG21	3:I:360:ASP:HB3	1.59	0.83
2:H:60:LEU:HD11	4:A:1:NAG:H82	1.65	0.79
5:B:12:GU8:H62	5:B:13:GU5:H5	1.64	0.78
2:H:61:GLU:HG2	2:H:87:LYS:HA	1.64	0.77
1:L:1(I):ARG:HG2	1:L:1(I):ARG:NH1	1.98	0.77
3:I:324:ARG:NH1	3:I:374:GLU:HG3	1.99	0.76
3:I:324:ARG:HG3	3:I:324:ARG:HH11	1.51	0.76
2:H:93:ARG:NH1	5:B:15:GU6:H6	2.00	0.76
3:I:414:GLU:OE1	3:I:416:PRO:HD2	1.85	0.76
5:B:4:GU1:H83	5:B:4:GU1:H72	1.66	0.75
3:I:326:GLU:O	3:I:326:GLU:HG3	1.87	0.75
2:H:61:GLU:CG	2:H:87:LYS:HA	2.16	0.74
3:I:96:ASN:OD1	9:I:801:NAG:H5	1.88	0.73
3:I:139:LYS:O	3:I:221:PHE:HA	1.88	0.73
3:I:7:ILE:H	3:I:7:ILE:CD1	2.02	0.72
3:I:81:LEU:HD11	3:I:127:ASN:HD21	1.55	0.69
3:I:246:SER:O	3:I:247:CYS:HB2	1.93	0.69
1:L:1(I):ARG:HH21	2:H:247:GLU:C	1.95	0.68
2:H:67:ARG:HG2	2:H:82:ILE:HG12	1.76	0.67
1:L:1(K):ASN:HD21	1:L:1(I):ARG:CB	2.09	0.65
1:L:1(H):THR:HG22	2:H:247:GLU:HA	1.78	0.65
5:B:5:GU5:H61	5:B:6:GU8:H73	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1(K):ASN:HD21	1:L:1(I):ARG:HB3	1.61	0.64
2:H:59:LEU:HD22	2:H:64:LEU:HD11	1.79	0.64
3:I:415:VAL:HB	3:I:416:PRO:HD3	1.79	0.64
3:I:23:TYR:CE2	3:I:100:GLN:HG3	2.33	0.64
3:I:15:ILE:HD13	3:I:15:ILE:N	2.13	0.63
3:I:159:GLN:HB3	3:I:169:LYS:HD2	1.80	0.63
2:H:53:LEU:HD11	2:H:103:ILE:HD11	1.81	0.63
3:I:127:ASN:HB3	8:I:864:MPD:H11	1.80	0.62
3:I:60:THR:HA	8:I:865:MPD:H31	1.81	0.62
1:L:1(K):ASN:OD1	1:L:1(I):ARG:HB2	1.99	0.62
3:I:120:HIS:H	3:I:120:HIS:CD2	2.18	0.62
3:I:186:ILE:HG21	3:I:202:ILE:HD12	1.81	0.62
1:L:1(I):ARG:HH11	1:L:1(I):ARG:CG	2.13	0.61
2:H:67:ARG:NH2	2:H:82:ILE:HD11	2.15	0.60
3:I:7:ILE:HD13	3:I:7:ILE:N	2.08	0.60
1:L:5:PRO:HB2	2:H:116:ASP:HA	1.82	0.60
3:I:128:CYS:HB3	3:I:132:ARG:HH21	1.67	0.60
3:I:425:ARG:HD3	3:I:427:ALA:HB2	1.82	0.59
3:I:190:VAL:HG11	3:I:201:VAL:HG21	1.84	0.59
2:H:34:PHE:HB2	2:H:65:LEU:HD22	1.85	0.59
1:L:5:PRO:CB	2:H:116:ASP:HA	2.33	0.58
2:H:81:LYS:HE3	10:H:801:HOH:O	2.03	0.58
3:I:170:LEU:C	3:I:170:LEU:HD23	2.24	0.58
2:H:174:ILE:HD13	3:I:390:ILE:HB	1.85	0.58
3:I:399:ARG:HH11	3:I:399:ARG:CG	2.16	0.58
2:H:27:SER:H	8:H:782:MPD:H53	1.69	0.57
3:I:100:GLN:O	3:I:104:GLU:HG3	2.03	0.57
3:I:319:HIS:HB2	3:I:403:LYS:HA	1.85	0.57
3:I:276:GLY:O	3:I:277:ASP:HB2	2.05	0.56
3:I:125:LYS:HE3	10:I:912:HOH:O	2.05	0.56
2:H:35:ARG:HD2	2:H:37:PRO:O	2.05	0.56
2:H:80:GLU:O	2:H:81:LYS:HD2	2.06	0.56
5:B:10:GU8:O4	5:B:11:GU9:H72	2.06	0.56
3:I:272:LEU:N	3:I:272:LEU:HD12	2.21	0.55
2:H:164:GLU:HB3	2:H:166:PRO:HD2	1.89	0.55
3:I:134:ALA:O	3:I:138:SER:HB2	2.07	0.55
3:I:238:LEU:HD22	3:I:246:SER:OG	2.07	0.55
3:I:206:ALA:HB1	3:I:368:PHE:HZ	1.72	0.55
3:I:355:VAL:HG13	3:I:362:LEU:HD22	1.89	0.55
5:B:7:GU9:H61	5:B:8:GU8:C7	2.37	0.55
3:I:99:LEU:O	3:I:103:MET:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:25:GLY:H	8:H:782:MPD:H31	1.71	0.54
2:H:176:ILE:HG22	2:H:177:THR:N	2.23	0.54
3:I:305:GLN:OE1	3:I:418:ASN:ND2	2.41	0.54
3:I:66:LEU:O	3:I:70:LYS:HG3	2.08	0.54
3:I:400:VAL:CG1	3:I:401:CYS:N	2.70	0.54
3:I:12:PRO:HB2	5:B:3:GU6:O15	2.08	0.53
1:L:1(G):PHE:CD1	2:H:242:ILE:HD13	2.44	0.53
2:H:129:ALA:O	2:H:130:LEU:HB2	2.09	0.53
3:I:149:ASP:OD2	3:I:176:LYS:HG3	2.08	0.53
4:A:1:NAG:H61	4:A:3:FUC:O2	2.09	0.53
3:I:81:LEU:HD11	3:I:127:ASN:ND2	2.22	0.53
2:H:67:ARG:CZ	2:H:82:ILE:HD11	2.39	0.53
3:I:77:PHE:CE2	3:I:373:LEU:HB2	2.44	0.53
3:I:141:VAL:HG22	3:I:220:TYR:HB3	1.90	0.53
5:B:6:GU8:O4	5:B:7:GU9:H72	2.08	0.53
3:I:278:ASP:C	3:I:279:ILE:HD12	2.30	0.52
3:I:204:SER:O	3:I:205:GLU:CB	2.57	0.52
2:H:80:GLU:OE2	8:H:783:MPD:H51	2.10	0.52
5:B:5:GU5:H61	5:B:6:GU8:C7	2.40	0.52
2:H:49:ASP:HB3	2:H:114:PHE:CZ	2.45	0.52
2:H:147:THR:HG21	2:H:147(D):ASN:HB3	1.92	0.51
3:I:204:SER:O	3:I:205:GLU:HB3	2.10	0.51
2:H:155:LEU:CD2	8:H:782:MPD:H51	2.41	0.51
2:H:65:LEU:C	2:H:65:LEU:HD23	2.32	0.51
2:H:233:ARG:HG2	2:H:233:ARG:HH21	1.76	0.51
3:I:236:LYS:HE3	3:I:248:SER:OG	2.11	0.50
3:I:197:ARG:HG3	10:I:953:HOH:O	2.11	0.50
5:B:4:GU1:H72	5:B:4:GU1:C8	2.38	0.50
3:I:71:ASN:HB3	3:I:74:ASP:OD2	2.12	0.50
5:B:7:GU9:H61	5:B:8:GU8:H73	1.92	0.50
2:H:64:LEU:HB2	2:H:85:LEU:HD12	1.93	0.50
3:I:399:ARG:HH11	3:I:399:ARG:HG2	1.76	0.50
3:I:359:ARG:HG3	10:I:931:HOH:O	2.11	0.50
3:I:400:VAL:HG13	3:I:401:CYS:N	2.27	0.50
2:H:136:GLY:HA3	2:H:199:PHE:CE1	2.46	0.50
3:I:355:VAL:HG21	3:I:360:ASP:CB	2.36	0.49
2:H:169:LYS:HA	2:H:176:ILE:HD12	1.94	0.49
3:I:77:PHE:HB2	3:I:325:ILE:HG21	1.95	0.49
3:I:260:TYR:CZ	3:I:400:VAL:HG11	2.48	0.49
2:H:165:ARG:N	2:H:166:PRO:CD	2.76	0.49
3:I:399:ARG:CG	3:I:399:ARG:NH1	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1:CYS:C	2:H:122:CYS:SG	2.92	0.49
2:H:50:ARG:HH11	2:H:111:PRO:HG2	1.77	0.49
1:L:1:CYS:O	2:H:122:CYS:SG	2.70	0.48
2:H:36:LYS:HE3	2:H:64:LEU:O	2.12	0.48
8:H:781:MPD:H13	10:I:955:HOH:O	2.12	0.48
3:I:20:MET:SD	3:I:352:PRO:HB2	2.53	0.48
3:I:324:ARG:HD3	3:I:372:PHE:HZ	1.78	0.48
2:H:169:LYS:HE3	10:H:805:HOH:O	2.12	0.48
5:B:11:GU9:O4	5:B:12:GU8:H73	2.13	0.48
3:I:225:TRP:CD1	3:I:379:GLY:HA2	2.48	0.48
5:B:5:GU5:O2	5:B:5:GU5:H82	2.14	0.48
1:L:1(H):THR:HG22	2:H:247:GLU:N	2.29	0.47
10:I:944:HOH:O	5:B:13:GU5:C7	2.62	0.47
5:B:10:GU8:H83	5:B:10:GU8:O2	2.14	0.47
3:I:77:PHE:CZ	3:I:373:LEU:HB2	2.50	0.47
2:H:84:MET:HB2	2:H:109:LYS:HG3	1.97	0.47
2:H:99:LEU:O	2:H:102:ASP:HB2	2.14	0.47
8:H:781:MPD:H12	3:I:233:ASN:O	2.14	0.47
3:I:139:LYS:HB2	3:I:222:LYS:O	2.14	0.47
3:I:190:VAL:HG11	3:I:201:VAL:CG2	2.44	0.47
3:I:324:ARG:HH11	3:I:324:ARG:CG	2.22	0.47
1:L:1(K):ASN:ND2	1:L:1(I):ARG:CB	2.78	0.47
3:I:161:ILE:O	3:I:165:VAL:HG12	2.14	0.47
3:I:128:CYS:HB3	3:I:132:ARG:NH2	2.30	0.46
3:I:20:MET:HE3	6:C:1:NAG:H2	1.96	0.46
3:I:183:ARG:NH2	3:I:204:SER:HB2	2.30	0.46
5:B:9:GU9:O4	5:B:10:GU8:H73	2.15	0.46
5:B:7:GU9:O4	5:B:8:GU8:H73	2.15	0.46
1:L:14(C):GLU:OE1	2:H:202:LYS:NZ	2.38	0.46
2:H:36:LYS:HD2	2:H:62:ASN:O	2.16	0.45
2:H:148:GLY:HA2	2:H:151:GLN:NE2	2.31	0.45
3:I:261:ARG:CB	3:I:311:LEU:HD23	2.47	0.45
2:H:20:SER:O	2:H:157:VAL:HG12	2.16	0.45
3:I:131:TYR:HB2	8:I:864:MPD:H13	1.97	0.45
3:I:138:SER:HB3	3:I:223:GLY:HA2	1.98	0.45
3:I:346:PRO:HG3	3:I:363:TYR:CZ	2.52	0.45
3:I:130:LEU:CD2	3:I:414:GLU:HG3	2.46	0.45
3:I:287:LYS:HE3	3:I:287:LYS:HB2	1.81	0.45
1:L:1(M):PHE:CD2	2:H:235:LYS:HE2	2.52	0.45
1:L:1(G):PHE:HD1	2:H:242:ILE:HD13	1.82	0.45
2:H:129:ALA:HA	2:H:210:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:163:VAL:HG12	2:H:164:GLU:N	2.33	0.45
3:I:46:ARG:NH2	5:B:2:GU2:O6	2.50	0.45
2:H:25:GLY:H	8:H:782:MPD:C3	2.29	0.44
3:I:243:ASP:OD1	3:I:244:GLY:N	2.49	0.44
2:H:61:GLU:CD	2:H:61:GLU:H	2.20	0.44
3:I:186:ILE:HG21	3:I:202:ILE:CD1	2.48	0.44
3:I:253:TYR:HA	3:I:318:VAL:O	2.18	0.44
3:I:261:ARG:HB3	3:I:311:LEU:HD23	2.00	0.44
1:L:13:GLU:HA	1:L:14(C):GLU:OE2	2.17	0.44
2:H:36(A):SER:HA	2:H:37:PRO:C	2.37	0.44
3:I:124:ALA:HB2	3:I:165:VAL:CG2	2.48	0.44
2:H:164:GLU:CB	2:H:166:PRO:HD2	2.48	0.44
3:I:203:PRO:HG3	8:I:867:MPD:O2	2.18	0.44
4:A:1:NAG:C6	4:A:3:FUC:O2	2.65	0.44
5:B:1:GU3:H7B	5:B:1:GU3:O4	2.18	0.44
1:L:1(H):THR:HG22	2:H:247:GLU:CA	2.46	0.43
1:L:7:PHE:O	1:L:8:GLU:C	2.56	0.43
3:I:17:MET:O	3:I:120:HIS:HE1	2.01	0.43
3:I:260:TYR:CG	3:I:261:ARG:N	2.86	0.43
1:L:1(K):ASN:HD21	1:L:1(I):ARG:HB2	1.80	0.43
2:H:49:ASP:O	2:H:111:PRO:HA	2.18	0.43
3:I:137:ALA:CB	3:I:275:LYS:HE2	2.48	0.43
1:L:1(K):ASN:ND2	1:L:1(I):ARG:HB2	2.33	0.43
2:H:107:LYS:NZ	2:H:246:GLY:HA2	2.33	0.43
3:I:324:ARG:HD3	3:I:372:PHE:CZ	2.54	0.43
5:B:4:GU1:H83	5:B:4:GU1:C7	2.41	0.43
2:H:215:TRP:CE3	3:I:390:ILE:HG12	2.54	0.43
3:I:284:ILE:HD13	3:I:411:PHE:HE2	1.84	0.43
3:I:12:PRO:HG2	5:B:3:GU6:O17	2.18	0.43
3:I:125:LYS:NZ	5:B:4:GU1:O6A	2.50	0.43
3:I:206:ALA:HB1	3:I:368:PHE:CZ	2.52	0.43
2:H:215:TRP:HA	3:I:393:ARG:HG3	2.00	0.43
3:I:284:ILE:HD13	3:I:411:PHE:CE2	2.54	0.43
1:L:4:ARG:HA	1:L:5:PRO:HD3	1.91	0.43
3:I:320:MET:CE	3:I:375:VAL:HG11	2.49	0.43
3:I:346:PRO:HG3	3:I:363:TYR:CE2	2.54	0.43
5:B:9:GU9:H61	5:B:10:GU8:C7	2.49	0.42
2:H:80:GLU:C	2:H:81:LYS:HD2	2.40	0.42
2:H:117:TYR:CD1	8:H:782:MPD:HM3	2.54	0.42
2:H:147:THR:CG2	2:H:147(D):ASN:HD22	2.32	0.42
5:B:9:GU9:H61	5:B:10:GU8:H73	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:147:THR:CG2	2:H:147(A):TRP:N	2.82	0.42
3:I:132:ARG:HD3	3:I:132:ARG:N	2.33	0.42
3:I:178:ASN:HB3	3:I:181:GLN:HB2	2.01	0.42
3:I:355:VAL:CG1	3:I:362:LEU:HD22	2.50	0.42
3:I:366:ASP:HB3	3:I:368:PHE:CE2	2.55	0.42
3:I:412:ILE:HB	3:I:422:PHE:HB2	2.01	0.42
1:L:6:LEU:HA	1:L:10:LYS:HE2	2.02	0.42
2:H:147:THR:CG2	2:H:147(B):THR:H	2.32	0.42
2:H:70:LYS:HE3	2:H:70:LYS:HB3	1.94	0.42
3:I:155:ASN:ND2	6:C:1:NAG:C7	2.82	0.42
2:H:50:ARG:HG3	2:H:51:TRP:CD1	2.55	0.42
3:I:6:ASP:OD1	3:I:9:THR:HG23	2.20	0.42
3:I:263:VAL:HG22	3:I:267:THR:O	2.20	0.42
2:H:89:TYR:OH	2:H:245:PHE:HB3	2.20	0.41
3:I:138:SER:CB	3:I:223:GLY:HA2	2.51	0.41
1:L:8:GLU:CD	1:L:8:GLU:H	2.24	0.41
2:H:17:VAL:O	2:H:18:GLU:HB2	2.20	0.41
3:I:423:MET:HE1	8:I:865:MPD:HM1	2.02	0.41
2:H:75:ARG:O	2:H:77:GLU:HG3	2.21	0.41
2:H:203:SER:O	2:H:205:ASN:HA	2.21	0.41
3:I:140:LEU:HD11	3:I:219:ILE:HD11	2.03	0.41
2:H:79:ILE:HG23	2:H:117:TYR:CD2	2.56	0.41
3:I:15:ILE:HG12	3:I:15:ILE:O	2.20	0.41
3:I:324:ARG:NH1	3:I:324:ARG:CG	2.81	0.41
2:H:198:PRO:HB3	2:H:209:GLN:NE2	2.36	0.41
5:B:4:GU1:O6B	5:B:5:GU5:H5	2.21	0.41
2:H:130:LEU:HD21	2:H:230:HIS:CE1	2.56	0.41
3:I:274:PHE:CD2	3:I:279:ILE:HG22	2.56	0.41
3:I:320:MET:HE1	3:I:375:VAL:HG11	2.02	0.41
3:I:324:ARG:HH12	3:I:374:GLU:CG	2.10	0.41
3:I:336:GLN:HA	3:I:340:LEU:O	2.21	0.41
3:I:194:THR:O	3:I:197:ARG:HB2	2.20	0.41
3:I:395:LEU:HD23	3:I:395:LEU:HA	1.82	0.40
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.37	0.40
2:H:150:GLY:HA3	10:H:792:HOH:O	2.20	0.40
3:I:181:GLN:OE1	3:I:181:GLN:N	2.51	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)
3:I:207:ILE:O	3:I:399:ARG:NH2[4_455]	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	L	41/49 (84%)	35 (85%)	6 (15%)	0	100 100
2	H	257/259 (99%)	237 (92%)	20 (8%)	0	100 100
3	I	406/432 (94%)	378 (93%)	20 (5%)	8 (2%)	7 12
All	All	704/740 (95%)	650 (92%)	46 (6%)	8 (1%)	14 26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	247	CYS
3	I	359	ARG
3	I	387	ALA
3	I	205	GLU
3	I	111	ILE
3	I	430	CYS
3	I	429	PRO
3	I	263	VAL

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	L	36/43 (84%)	32 (89%)	4 (11%)	6 11
2	H	218/224 (97%)	209 (96%)	9 (4%)	30 55
3	I	358/382 (94%)	337 (94%)	21 (6%)	19 37
All	All	612/649 (94%)	578 (94%)	34 (6%)	21 40

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1(K)	ASN
1	L	1(I)	ARG
1	L	1(E)	SER
1	L	14(K)	ILE
2	H	20	SER
2	H	33	LEU
2	H	60(I)	THR
2	H	65	LEU
2	H	82	ILE
2	H	94	TYR
2	H	95	ASN
2	H	147(A)	TRP
2	H	204(B)	ASN
3	I	7	ILE
3	I	15	ILE
3	I	69	SER
3	I	123	PHE
3	I	139	LYS
3	I	156	GLU
3	I	171	GLN
3	I	193	LYS
3	I	197	ARG
3	I	224	LEU
3	I	247	CYS
3	I	317	CYS
3	I	337	ASP
3	I	359	ARG
3	I	366	ASP
3	I	395	LEU
3	I	399	ARG
3	I	400	VAL
3	I	414	GLU
3	I	428	ASN
3	I	430	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	95	ASN
2	H	151	GLN
2	H	204(B)	ASN
2	H	239	GLN
3	I	55	ASN
3	I	65	HIS
3	I	120	HIS
3	I	127	ASN
3	I	171	GLN
3	I	305	GLN
3	I	319	HIS
3	I	418	ASN
3	I	428	ASN

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

27 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	A	1	2,4	14,14,15	0.66	0	17,19,21	1.19	3 (17%)
4	NAG	A	2	4	14,14,15	0.60	0	17,19,21	0.59	0
4	FUC	A	3	4	10,10,11	0.67	0	14,14,16	0.82	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GU3	B	1	5	22,22,22	1.67	3 (13%)	28,33,33	1.11	2 (7%)
5	GU8	B	10	5	14,14,15	0.41	0	18,18,20	0.64	0
5	GU9	B	11	5	14,14,15	0.55	0	18,18,20	1.17	2 (11%)
5	GU8	B	12	5	14,14,15	0.39	0	18,18,20	0.81	1 (5%)
5	GU5	B	13	5	17,17,18	1.34	1 (5%)	22,24,26	0.94	1 (4%)
5	GU0	B	14	5	23,23,24	1.93	4 (17%)	25,36,38	1.05	2 (8%)
5	GU6	B	15	5	23,23,24	3.37	10 (43%)	25,36,38	3.93	10 (40%)
5	GU4	B	16	5	27,27,28	2.04	5 (18%)	29,43,45	1.38	4 (13%)
5	GU2	B	2	5	14,14,15	0.75	1 (7%)	15,19,21	0.91	0
5	GU6	B	3	5	23,23,24	1.93	4 (17%)	25,36,38	1.28	4 (16%)
5	GU1	B	4	5	14,14,15	0.68	1 (7%)	15,19,21	0.95	0
5	GU5	B	5	5	17,17,18	1.33	1 (5%)	22,24,26	0.82	0
5	GU8	B	6	5	14,14,15	0.42	0	18,18,20	0.70	0
5	GU9	B	7	5	14,14,15	0.42	0	18,18,20	0.68	0
5	GU8	B	8	5	14,14,15	0.41	0	18,18,20	0.59	0
5	GU9	B	9	5	14,14,15	0.42	0	18,18,20	0.63	0
6	NAG	C	1	3,6	14,14,15	0.66	0	17,19,21	0.71	0
6	NAG	C	2	6	14,14,15	0.60	0	17,19,21	0.84	0
6	BMA	C	3	6	11,11,12	0.67	0	15,15,17	1.16	2 (13%)
6	MAN	C	4	6	11,11,12	0.63	0	15,15,17	0.53	0
6	MAN	C	5	6	11,11,12	0.61	0	15,15,17	0.62	1 (6%)
7	NAG	D	1	3,7	14,14,15	0.55	0	17,19,21	0.69	1 (5%)
7	NAG	D	2	7	14,14,15	0.68	0	17,19,21	0.67	0
7	BMA	D	3	7	11,11,12	0.60	0	15,15,17	0.48	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
4	NAG	A	1	2,4	1/1/5/7	1/6/23/26	0/1/1/1
4	NAG	A	2	4	-	5/6/23/26	0/1/1/1
4	FUC	A	3	4	-	-	0/1/1/1
5	GU3	B	1	5	-	0/15/35/35	0/1/1/1
5	GU8	B	10	5	-	2/7/24/27	0/1/1/1
5	GU9	B	11	5	-	3/7/24/27	0/1/1/1
5	GU8	B	12	5	-	2/7/24/27	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GU5	B	13	5	-	3/10/27/30	0/1/1/1
5	GU0	B	14	5	-	0/16/33/36	0/1/1/1
5	GU6	B	15	5	4/4/7/8	10/16/33/36	0/1/1/1
5	GU4	B	16	5	-	2/21/38/41	0/1/1/1
5	GU2	B	2	5	-	2/8/25/28	0/1/1/1
5	GU6	B	3	5	-	4/16/33/36	0/1/1/1
5	GU1	B	4	5	-	2/8/25/28	0/1/1/1
5	GU5	B	5	5	-	0/10/27/30	0/1/1/1
5	GU8	B	6	5	-	1/7/24/27	0/1/1/1
5	GU9	B	7	5	-	3/7/24/27	0/1/1/1
5	GU8	B	8	5	-	2/7/24/27	0/1/1/1
5	GU9	B	9	5	-	2/7/24/27	0/1/1/1
6	NAG	C	1	3,6	-	4/6/23/26	0/1/1/1
6	NAG	C	2	6	-	3/6/23/26	0/1/1/1
6	BMA	C	3	6	-	2/2/19/22	0/1/1/1
6	MAN	C	4	6	-	2/2/19/22	1/1/1/1
6	MAN	C	5	6	-	2/2/19/22	1/1/1/1
7	NAG	D	1	3,7	-	4/6/23/26	0/1/1/1
7	NAG	D	2	7	-	3/6/23/26	0/1/1/1
7	BMA	D	3	7	-	2/2/19/22	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	15	GU6	O2-C2	-6.97	1.36	1.47
5	B	15	GU6	C4-C5	-6.69	1.39	1.53
5	B	15	GU6	C3-C2	-5.07	1.39	1.52
5	B	15	GU6	O6-S6	-5.04	1.43	1.56
5	B	13	GU5	O6-S6	-4.98	1.43	1.56
5	B	5	GU5	O6-S6	-4.94	1.43	1.56
5	B	15	GU6	C4-C3	-4.92	1.39	1.52
5	B	14	GU0	O6-S6	-4.92	1.43	1.56
5	B	16	GU4	O6-S6	-4.92	1.43	1.56
5	B	3	GU6	O6-S6	-4.89	1.43	1.56
5	B	1	GU3	O6-S6	-4.88	1.43	1.56
5	B	15	GU6	O3-C3	-4.86	1.36	1.46
5	B	16	GU4	O2-S2	-4.64	1.43	1.57
5	B	14	GU0	O2-S2	-4.63	1.43	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1	GU3	O2-S2	-4.63	1.43	1.57
5	B	3	GU6	O2-S2	-4.62	1.43	1.57
5	B	3	GU6	O3-S3	-4.61	1.43	1.57
5	B	16	GU4	O4-S4	-4.57	1.43	1.57
5	B	15	GU6	O2-S2	-4.54	1.43	1.57
5	B	16	GU4	O3-S3	-4.54	1.43	1.57
5	B	14	GU0	O3-S3	-4.52	1.43	1.57
5	B	15	GU6	O3-S3	-4.49	1.44	1.57
5	B	15	GU6	O5-C5	-3.25	1.36	1.43
5	B	15	GU6	O4-C4	-2.76	1.36	1.43
5	B	16	GU4	O2-C2	-2.46	1.43	1.47
5	B	14	GU0	O2-C2	-2.44	1.43	1.47
5	B	3	GU6	O2-C2	-2.31	1.43	1.47
5	B	2	GU2	O6-C6	-2.30	1.23	1.30
5	B	1	GU3	O1-C1	2.24	1.44	1.40
5	B	4	GU1	O6B-C6	-2.07	1.23	1.30

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	15	GU6	O2-C2-C3	14.15	122.31	106.65
5	B	15	GU6	C6-C5-C4	5.45	123.48	112.09
5	B	15	GU6	C1-C2-C3	5.22	117.20	109.40
5	B	15	GU6	O4-C4-C5	4.80	121.22	109.30
5	B	15	GU6	O4-C4-C3	4.78	122.62	109.94
5	B	15	GU6	O5-C5-C6	4.58	117.75	107.61
5	B	16	GU4	C2-O2-S2	-4.32	112.27	117.91
5	B	15	GU6	C2-O2-S2	-4.02	112.67	117.91
5	B	1	GU3	C2-O2-S2	-3.97	111.20	118.88
5	B	15	GU6	C1-O5-C5	3.73	117.25	112.19
5	B	3	GU6	C3-O3-S3	-3.23	112.64	118.88
5	B	15	GU6	O5-C5-C4	3.22	118.65	110.83
5	B	14	GU0	C2-O2-S2	-3.18	113.77	117.91
5	B	3	GU6	C2-O2-S2	-3.03	113.96	117.91
4	A	1	NAG	C4-C3-C2	-3.02	106.59	111.02
5	B	3	GU6	O2-C2-C3	2.98	109.95	106.65
5	B	11	GU9	C6-C5-C4	-2.91	106.01	112.09
5	B	15	GU6	C3-C4-C5	2.81	115.64	109.66
5	B	11	GU9	O4-C4-C3	-2.79	102.56	109.94
5	B	16	GU4	C4-O4-S4	-2.70	113.66	118.88
5	B	16	GU4	C3-O3-S3	-2.63	113.79	118.88
5	B	12	GU8	C1-C2-C3	-2.55	105.58	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	16	GU4	O2-C2-C3	2.53	109.45	106.65
6	C	3	BMA	C1-O5-C5	2.51	115.59	112.19
6	C	3	BMA	O5-C5-C6	-2.50	103.28	107.20
4	A	1	NAG	C2-N2-C7	-2.38	119.51	122.90
5	B	3	GU6	O6-C6-C5	2.20	111.72	107.62
5	B	14	GU0	O2-C2-C3	2.15	109.03	106.65
6	C	5	MAN	C1-O5-C5	2.14	115.09	112.19
7	D	1	NAG	C2-N2-C7	-2.12	119.89	122.90
4	A	3	FUC	O5-C1-C2	-2.11	107.51	110.77
4	A	1	NAG	C1-O5-C5	2.10	115.03	112.19
5	B	1	GU3	C8-O1-C1	-2.09	110.05	113.27
5	B	13	GU5	C6-C5-C4	-2.06	107.79	112.09

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1	NAG	C1
5	B	15	GU6	C4
5	B	15	GU6	C5
5	B	15	GU6	C2
5	B	15	GU6	C3

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	NAG	C3-C2-N2-C7
4	A	2	NAG	C3-C2-N2-C7
4	A	2	NAG	C8-C7-N2-C2
4	A	2	NAG	O7-C7-N2-C2
5	B	3	GU6	C1-C2-O2-S2
5	B	3	GU6	C3-C2-O2-S2
5	B	11	GU9	C3-C2-O2-C7
5	B	15	GU6	C3-C2-O2-S2
5	B	15	GU6	C2-C3-O3-S3
5	B	15	GU6	C3-O3-S3-O18
5	B	15	GU6	C6-O6-S6-O19
5	B	15	GU6	C6-O6-S6-O20
5	B	15	GU6	C6-O6-S6-O21
7	D	1	NAG	C8-C7-N2-C2
7	D	1	NAG	O7-C7-N2-C2
7	D	2	NAG	C8-C7-N2-C2
7	D	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	B	10	GU8	C2-C3-O3-C8
5	B	6	GU8	C2-C3-O3-C8
4	A	2	NAG	O5-C5-C6-O6
7	D	1	NAG	O5-C5-C6-O6
6	C	3	BMA	O5-C5-C6-O6
6	C	5	MAN	O5-C5-C6-O6
7	D	1	NAG	C4-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6
6	C	5	MAN	C4-C5-C6-O6
6	C	1	NAG	C4-C5-C6-O6
7	D	3	BMA	C4-C5-C6-O6
5	B	4	GU1	C2-C3-O3-C8
6	C	3	BMA	C4-C5-C6-O6
6	C	1	NAG	C8-C7-N2-C2
5	B	8	GU8	C2-C3-O3-C8
6	C	1	NAG	O5-C5-C6-O6
5	B	13	GU5	C2-C3-O3-C8
5	B	11	GU9	C4-C3-O3-C8
7	D	3	BMA	O5-C5-C6-O6
5	B	7	GU9	C4-C3-O3-C8
5	B	12	GU8	C2-C3-O3-C8
5	B	15	GU6	C3-O3-S3-O16
5	B	2	GU2	C4-C3-O3-C8
5	B	11	GU9	C2-C3-O3-C8
5	B	9	GU9	C4-C3-O3-C8
5	B	9	GU9	C2-C3-O3-C8
5	B	2	GU2	C2-C3-O3-C8
5	B	7	GU9	C3-C2-O2-C7
5	B	7	GU9	C2-C3-O3-C8
6	C	4	MAN	C4-C5-C6-O6
6	C	1	NAG	O7-C7-N2-C2
5	B	16	GU4	C6-O6-S6-O22
5	B	12	GU8	C4-C3-O3-C8
5	B	13	GU5	C4-C3-O3-C8
5	B	15	GU6	C4-C5-C6-O6
5	B	3	GU6	C2-O2-S2-O13
5	B	8	GU8	C4-C3-O3-C8
5	B	4	GU1	C4-C3-O3-C8
5	B	16	GU4	C6-O6-S6-O23
7	D	2	NAG	O5-C5-C6-O6
6	C	2	NAG	C8-C7-N2-C2
5	B	3	GU6	C2-O2-S2-O15

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Mol	Chain	Res	Type	Atoms
5	B	15	GU6	C3-O3-S3-O17
5	B	13	GU5	C3-C2-O2-C7
6	C	4	MAN	O5-C5-C6-O6
5	B	15	GU6	C2-O2-S2-O14
6	C	2	NAG	O5-C5-C6-O6
5	B	10	GU8	C5-C6-O6-C9
6	C	2	NAG	O7-C7-N2-C2

All (2) ring outliers are listed below:

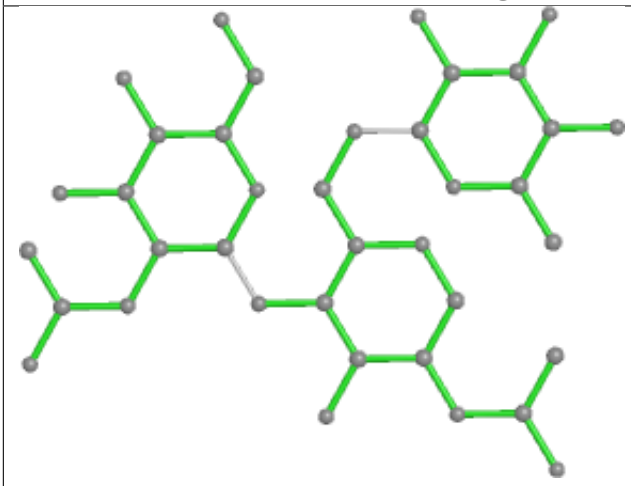
Mol	Chain	Res	Type	Atoms
6	C	5	MAN	C1-C2-C3-C4-C5-O5
6	C	4	MAN	C1-C2-C3-C4-C5-O5

17 monomers are involved in 30 short contacts:

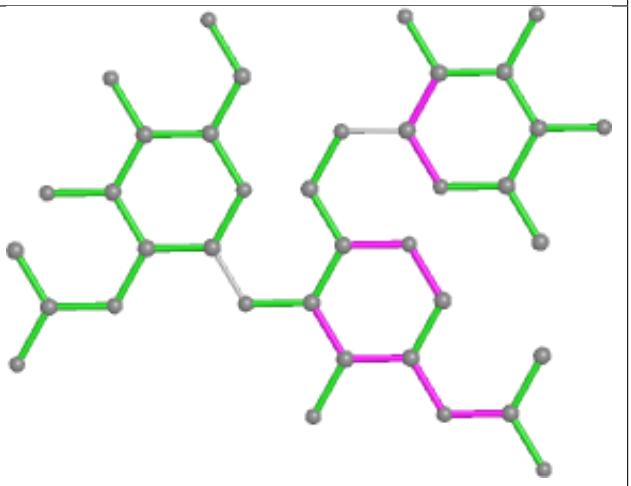
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3	FUC	2	0
5	B	8	GU8	3	0
5	B	6	GU8	3	0
5	B	15	GU6	1	0
5	B	13	GU5	2	0
5	B	1	GU3	1	0
5	B	5	GU5	4	0
5	B	3	GU6	2	0
5	B	12	GU8	2	0
5	B	7	GU9	4	0
5	B	4	GU1	5	0
5	B	11	GU9	2	0
4	A	1	NAG	3	0
5	B	2	GU2	1	0
6	C	1	NAG	2	0
5	B	9	GU9	3	0
5	B	10	GU8	5	0

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

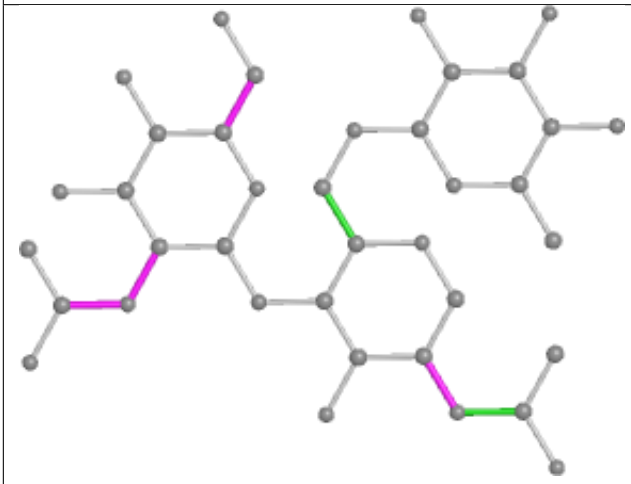
Oligosaccharide Chain A



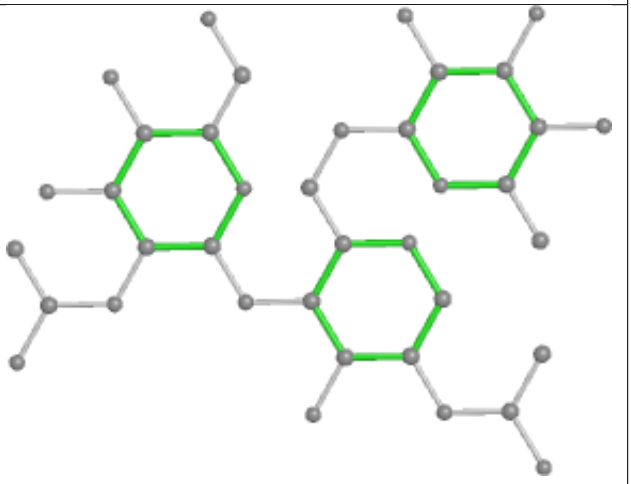
Bond lengths



Bond angles

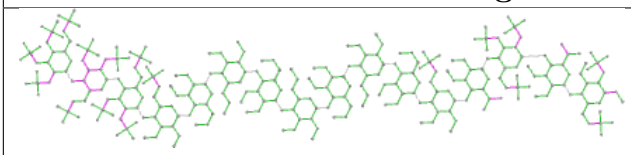


Torsions

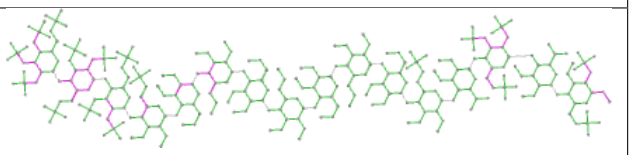


Rings

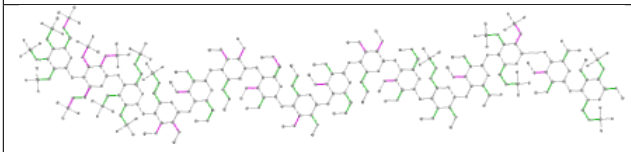
Oligosaccharide Chain B



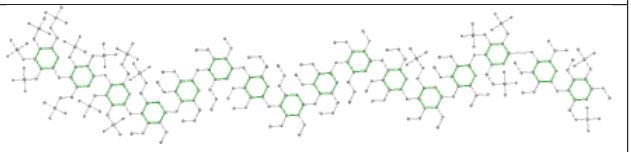
Bond lengths



Bond angles

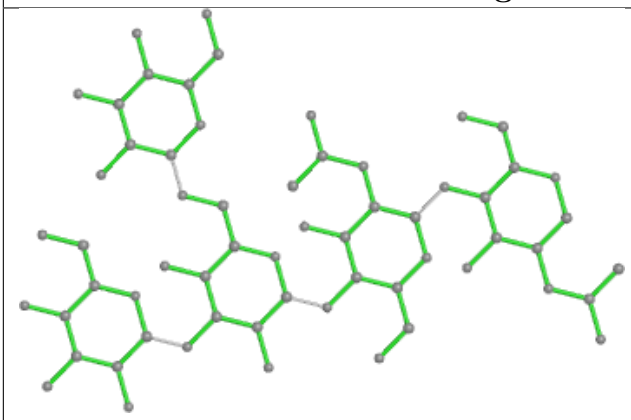


Torsions

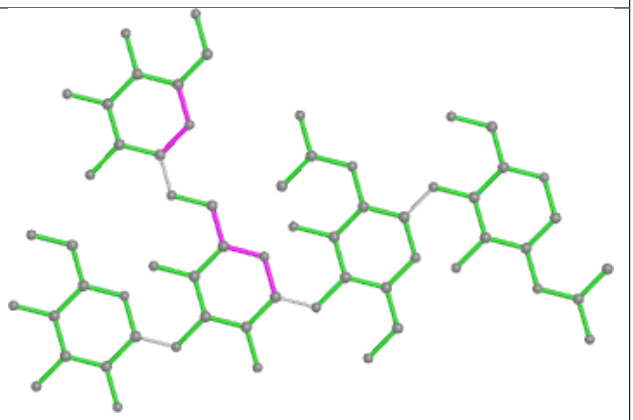


Rings

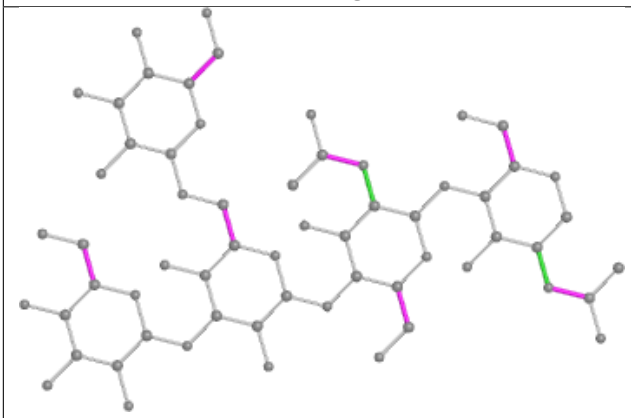
Oligosaccharide Chain C



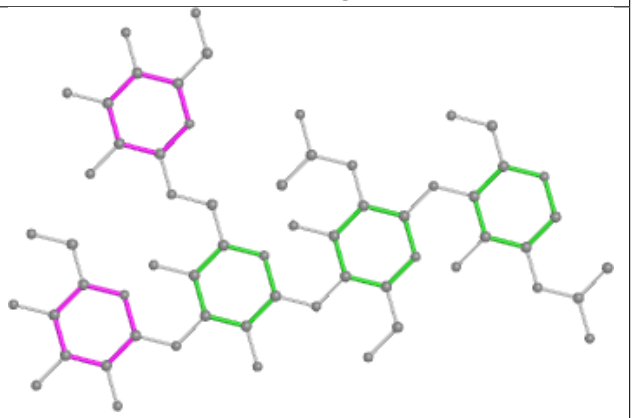
Bond lengths



Bond angles

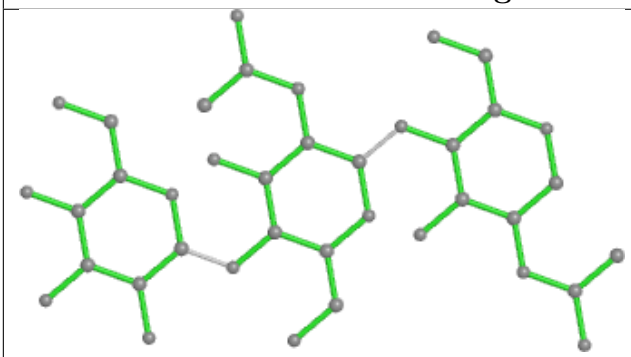


Torsions

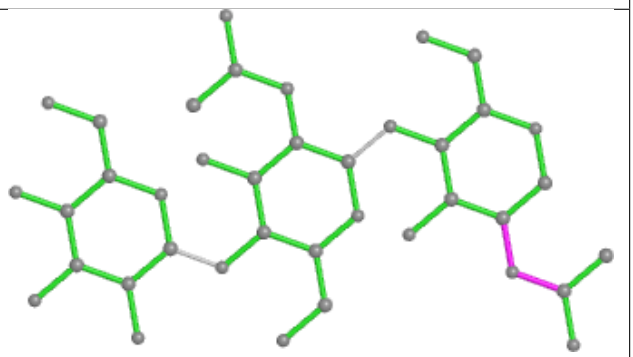


Rings

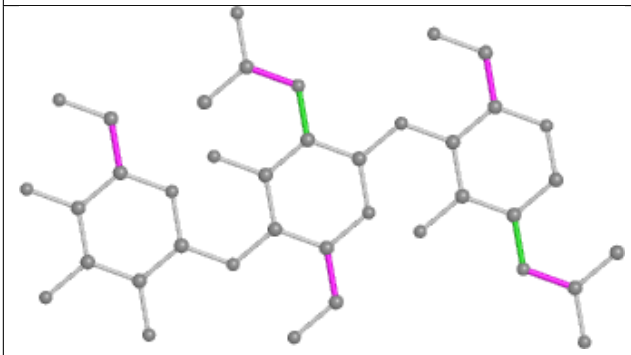
Oligosaccharide Chain D



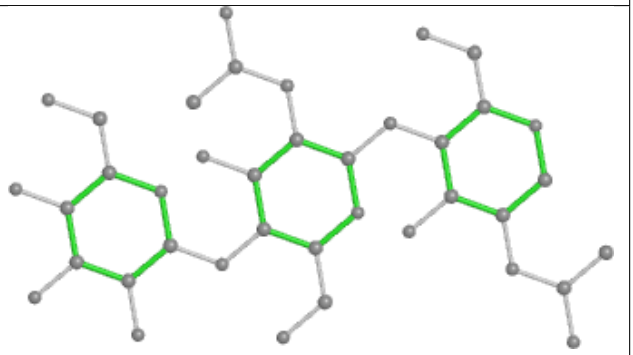
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
8	MPD	I	865	-	7,7,7	0.66	0	9,10,10	0.55	0
8	MPD	H	782	-	7,7,7	0.65	0	9,10,10	0.70	0
8	MPD	I	864	-	7,7,7	0.49	0	9,10,10	0.51	0
8	MPD	H	781	-	7,7,7	0.67	0	9,10,10	0.52	0
8	MPD	H	783	-	7,7,7	0.44	0	9,10,10	0.42	0
9	NAG	I	801	3	14,14,15	0.69	0	17,19,21	0.68	0
8	MPD	H	784	-	7,7,7	0.50	0	9,10,10	0.49	0
8	MPD	I	867	-	7,7,7	0.46	0	9,10,10	0.59	0
8	MPD	I	866	-	7,7,7	0.49	0	9,10,10	0.42	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
8	MPD	I	865	-	-	3/5/5/5	-
8	MPD	H	782	-	-	0/5/5/5	-
8	MPD	I	864	-	-	0/5/5/5	-
8	MPD	H	781	-	-	0/5/5/5	-
8	MPD	H	783	-	-	0/5/5/5	-
9	NAG	I	801	3	1/1/5/7	4/6/23/26	0/1/1/1
8	MPD	H	784	-	-	0/5/5/5	-
8	MPD	I	867	-	-	0/5/5/5	-
8	MPD	I	866	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	I	801	NAG	C1

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	865	MPD	O2-C2-C3-C4
8	I	865	MPD	CM-C2-C3-C4
9	I	801	NAG	C8-C7-N2-C2
9	I	801	NAG	O7-C7-N2-C2
9	I	801	NAG	C4-C5-C6-O6
9	I	801	NAG	O5-C5-C6-O6
8	I	865	MPD	C1-C2-C3-C4
8	I	866	MPD	O2-C2-C3-C4

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	865	MPD	2	0
8	H	782	MPD	6	0
8	I	864	MPD	2	0
8	H	781	MPD	2	0
8	H	783	MPD	1	0
9	I	801	NAG	1	0
8	I	867	MPD	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	L	43/49 (87%)	0.22	3 (6%)	16	16	47, 64, 77, 90	0
2	H	259/259 (100%)	-0.04	3 (1%)	79	80	22, 42, 60, 83	0
3	I	412/432 (95%)	0.06	10 (2%)	59	62	22, 40, 70, 82	0
All	All	714/740 (96%)	0.03	16 (2%)	62	65	22, 42, 70, 90	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	1(R)	SER	7.6
3	I	358	GLY	3.8
3	I	359	ARG	3.7
3	I	387	ALA	3.4
2	H	247	GLU	3.0
2	H	186(A)	ASP	2.7
3	I	131	TYR	2.7
3	I	81	LEU	2.3
2	H	204(A)	PHE	2.3
3	I	247	CYS	2.2
3	I	386	THR	2.2
3	I	80	PRO	2.1
3	I	160	ASP	2.1
1	L	14(K)	ILE	2.1
1	L	1(Q)	GLU	2.0
3	I	360	ASP	2.0

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

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

6.3 Carbohydrates (i)

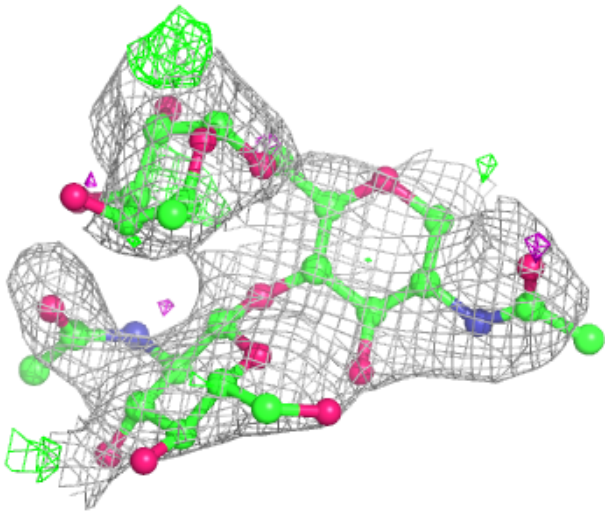
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

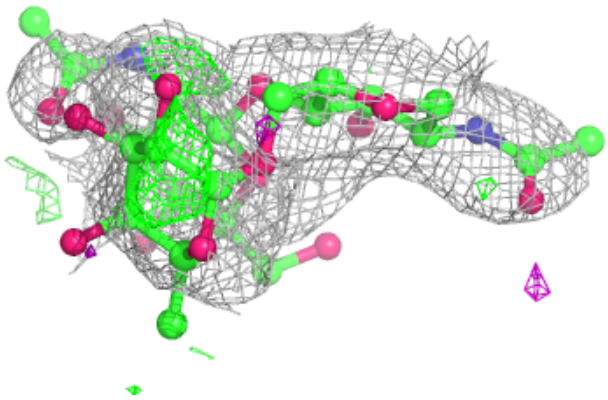
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MAN	C	5	11/12	0.49	0.60	119,122,123,124	0
6	MAN	C	4	11/12	0.53	0.56	118,123,125,125	0
7	NAG	D	2	14/15	0.54	0.56	102,104,106,107	0
7	NAG	D	1	14/15	0.55	0.36	87,92,94,98	0
7	BMA	D	3	11/12	0.58	0.42	106,108,108,109	0
4	FUC	A	3	10/11	0.63	0.39	86,89,91,92	0
6	BMA	C	3	11/12	0.78	0.26	91,103,110,115	0
4	NAG	A	2	14/15	0.78	0.48	89,92,94,94	0
4	NAG	A	1	14/15	0.81	0.29	67,74,84,86	0
5	GU9	B	11	14/15	0.82	0.24	62,74,76,76	0
5	GU8	B	8	14/15	0.88	0.31	74,75,76,77	0
5	GU8	B	6	14/15	0.88	0.23	66,69,71,72	0
5	GU6	B	15	23/24	0.88	0.19	41,52,64,67	0
5	GU8	B	10	14/15	0.90	0.27	76,77,79,79	0
5	GU9	B	9	14/15	0.91	0.32	73,76,77,77	0
5	GU9	B	7	14/15	0.91	0.19	73,74,76,76	0
5	GU2	B	2	14/15	0.92	0.22	65,66,70,70	0
6	NAG	C	2	14/15	0.92	0.17	46,58,66,78	0
5	GU6	B	3	23/24	0.92	0.17	53,65,70,71	0
5	GU1	B	4	14/15	0.92	0.16	57,59,62,63	0
5	GU8	B	12	14/15	0.93	0.15	49,55,59,59	0
5	GU3	B	1	22/22	0.94	0.14	58,64,74,75	0
5	GU4	B	16	27/28	0.95	0.13	43,54,60,61	0
5	GU5	B	13	17/18	0.95	0.12	43,46,51,53	0
5	GU0	B	14	23/24	0.96	0.13	28,43,47,51	0
6	NAG	C	1	14/15	0.96	0.18	42,48,50,51	0
5	GU5	B	5	17/18	0.96	0.11	47,54,57,63	0

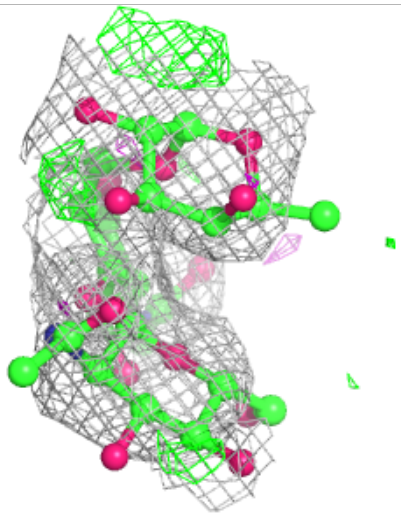
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain A:

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

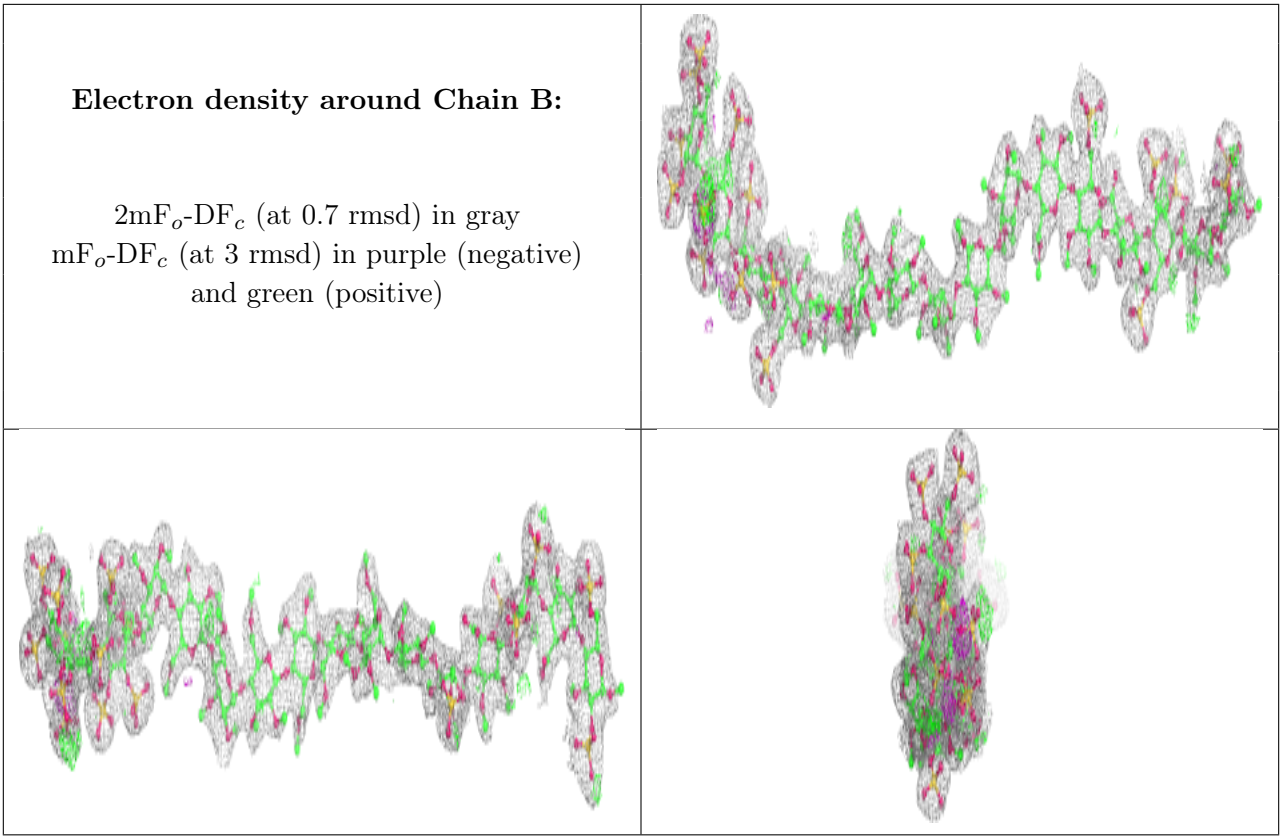






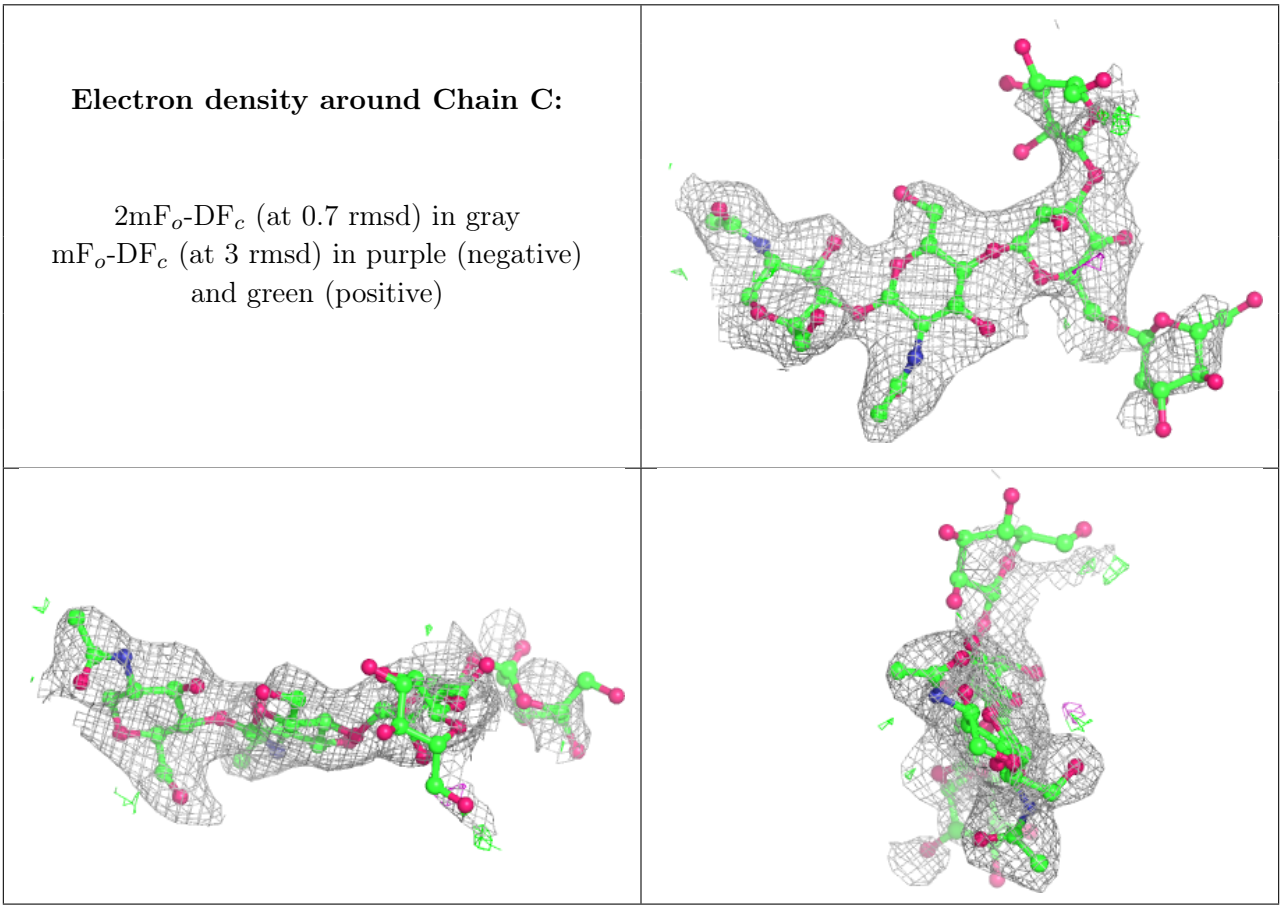
Electron density around Chain B:

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



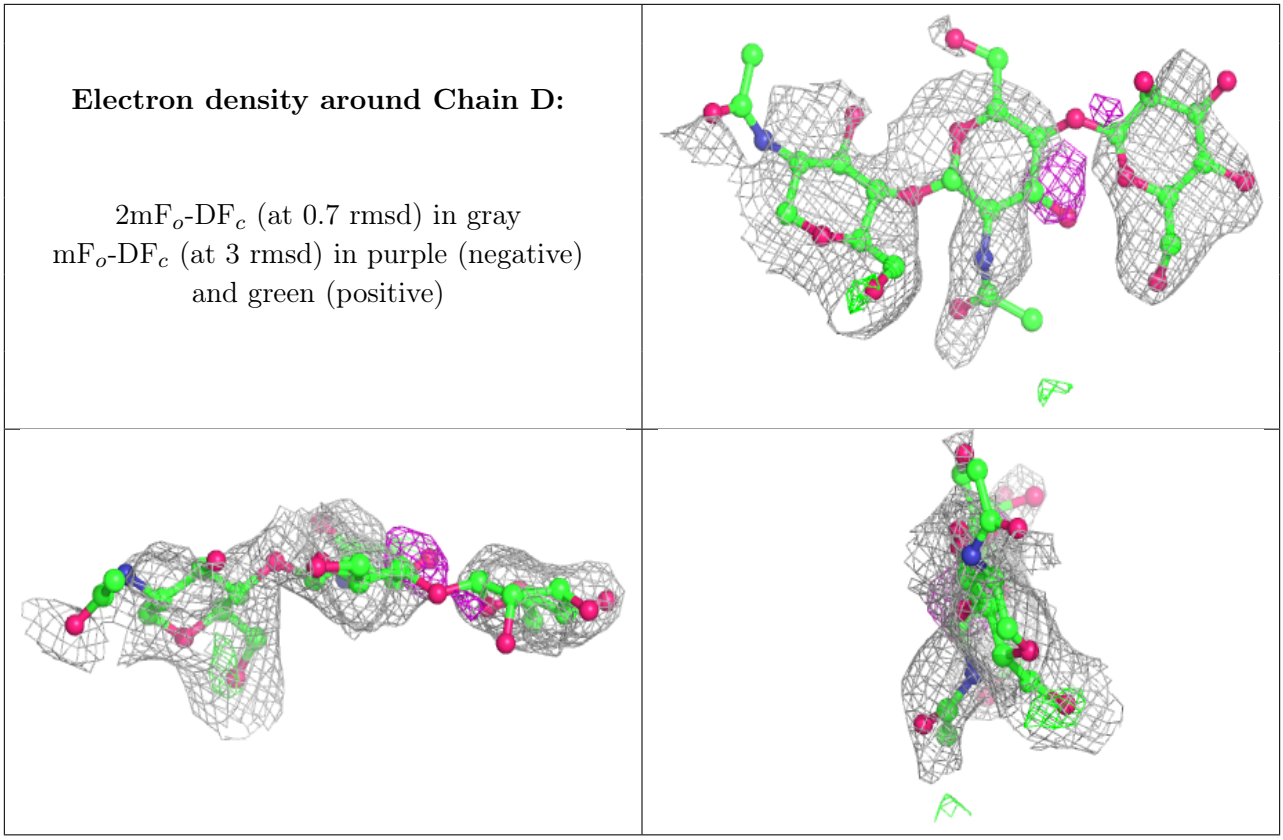
Electron density around Chain C:

$2mF_o$-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
8	MPD	H	782	8/8	0.64	0.52	97,99,100,100	0
9	NAG	I	801	14/15	0.72	0.41	78,82,84,85	0
8	MPD	I	867	8/8	0.79	0.29	98,98,99,99	0
8	MPD	H	784	8/8	0.85	0.31	77,77,78,78	0
8	MPD	H	783	8/8	0.87	0.23	68,69,73,74	0
8	MPD	I	864	8/8	0.87	0.34	83,84,86,87	0
8	MPD	H	781	8/8	0.88	0.30	76,76,77,78	0
8	MPD	I	865	8/8	0.90	0.25	72,73,74,75	0
8	MPD	I	866	8/8	0.92	0.23	89,90,91,91	0

6.5 Other polymers

There are no such residues in this entry.