Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 07:38 PM EDT

PDB ID	:	2B5T
Title	:	2.1 Angstrom structure of a nonproductive complex between antithrombin, synthetic heparin mimetic SR123781 and two S195A thrombin molecules
Authors	:	Johnson, D.J.; Li, W.; Luis, S.A.; Carrell, R.W.; Huntington, J.A.
Deposited on	:	2005-09-29
Resolution	:	2.10 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

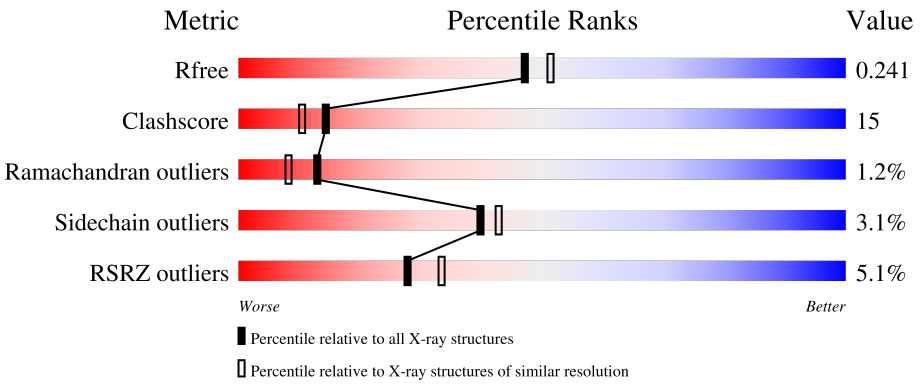
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	A	49	2%, 65%, 31%, •
1	C	49	6%, 80%, 14%, 6%
2	B	259	2%, 75%, 20%, • •
2	D	259	4%, 78%, 19%, •
3	I	432	8%, 60%, 33%, • •

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Mol	Chain	Length	Quality of chain
4	E	2	50% 50%
4	F	2	50% 50%
5	G	16	38% 62%
6	H	7	57% 14% 29%
7	J	2	50% 50%

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	E	1	-	-	X	-
4	FUC	E	2	-	-	X	X
4	NAG	F	1	X	-	-	-
4	FUC	F	2	-	-	-	X
5	GU8	G	10	-	-	-	X
5	GU8	G	12	-	-	X	-
5	GU6	G	15	X	-	-	-
6	NAG	H	1	X	-	-	-
6	NAG	H	2	-	-	-	X
6	MAN	H	6	-	-	-	X
7	NAG	J	2	-	-	-	X
8	GOL	A	1102	-	-	X	-
8	GOL	B	1103	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 9026 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
			Total	C	N	O	S			
1	A	47	394	245	65	83	1	0	1	0
1	C	46	372	233	60	78	1	0	0	0

- Molecule 2 is a protein called Thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	252	2065	1317	368	366	14	0	3	0
2	D	252	2022	1290	353	365	14	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	415	3233	2065	540	609	19	0	0	0

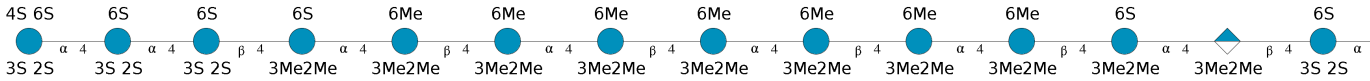
There are 3 discrepancies between the modelled and reference sequences:

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 alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

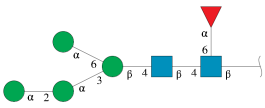
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	2	24	14	1	9	0	0	0
4	F	2	24	14	1	9	0	0	0

- 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	G	16	278	127	134	17	0	0	0

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

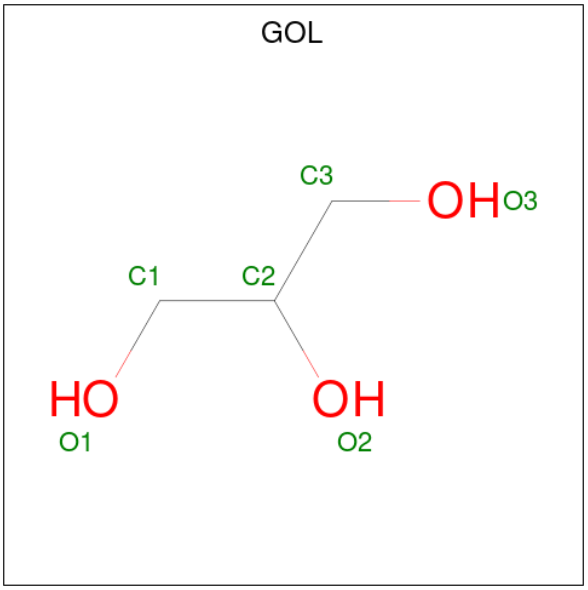


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	H	7	81	46	2	33	0	0	0

- Molecule 7 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
			Total	C	N	O			
7	J	2	28	16	2	10	0	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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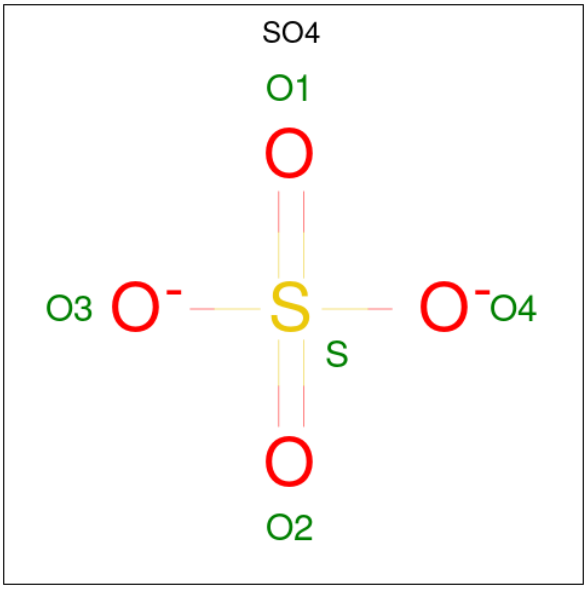
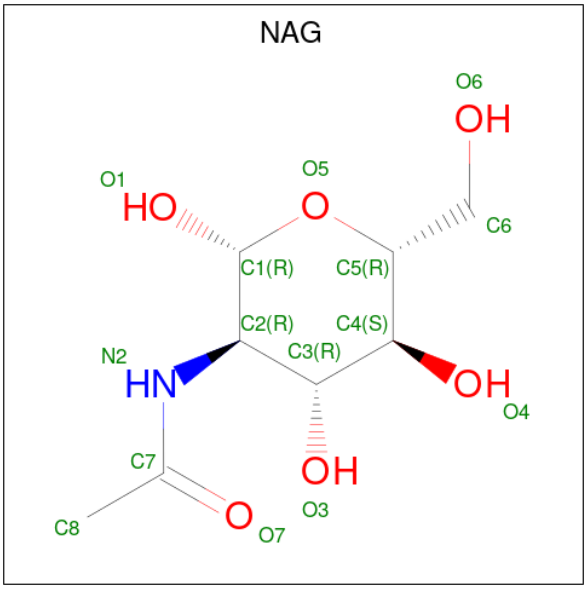
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	D	1	6	3	3	0	0
			Total	C	O		
8	D	1	6	3	3	0	0
			Total	C	O		
8	D	1	6	3	3	0	0
			Total	C	O		
8	D	1	6	3	3	0	0
			Total	C	O		
8	I	1	6	3	3	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
9	B	1	5	4	1	0	0
			Total	O	S		
9	B	1	5	4	1	0	0
			Total	O	S		
9	B	1	5	4	1	0	0
			Total	O	S		
9	B	1	5	4	1	0	0
			Total	O	S		
9	D	1	5	4	1	0	0
			Total	O	S		
9	I	1	5	4	1	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 11 is water.

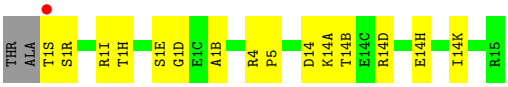
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	29	29	29	0	0
11	B	132	132	132	0	0
11	C	24	24	24	0	0
11	D	117	117	117	0	0
11	I	87	87	87	0	0

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.

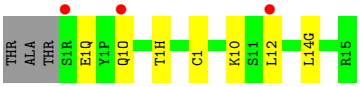
- Molecule 1: Thrombin

Chain A:



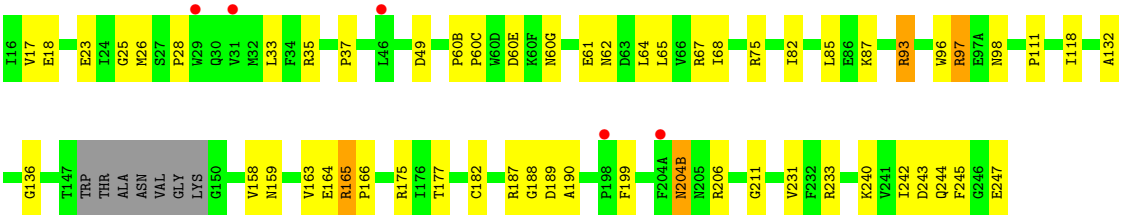
- Molecule 1: Thrombin

Chain C:



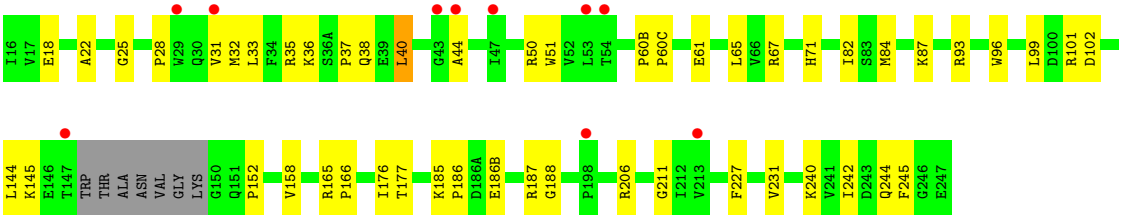
- Molecule 2: Thrombin

Chain B:



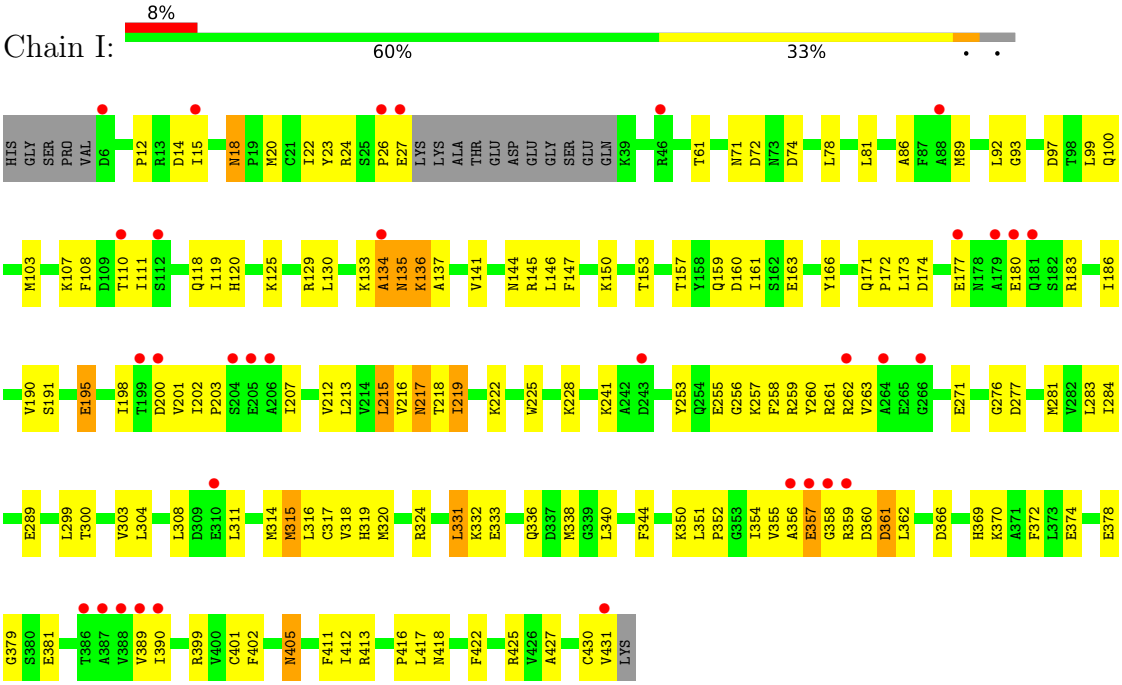
- Molecule 2: Thrombin

Chain D:



- Molecule 3: Antithrombin-III

Chain I:



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

Chain E:

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

Chain F:

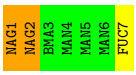
• Molecule 5: 2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-sulfonato-beta-D-glucopyranose-(1-4)-2,3-di-O-methyl-6-O-sulfonato-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3,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

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

fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.28Å 59.53Å 108.41Å 77.55° 78.94° 68.08°	Depositor
Resolution (Å)	35.70 – 2.10 35.72 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.4 (35.70-2.10) 92.5 (35.72-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.247 0.199 , 0.241	Depositor DCC
R_{free} test set	2937 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 61.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9026	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GU2, SO4, GU8, BMA, GU1, GU9, GU6, NAG, GU5, GU0, GU4, MAN, FUC, GOL, 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	A	0.40	0/401	0.66	0/535
1	C	0.42	0/379	0.66	0/506
2	B	0.36	0/2118	0.66	0/2859
2	D	0.35	0/2074	0.64	0/2805
3	I	0.39	0/3299	0.65	2/4470 (0.0%)
All	All	0.38	0/8271	0.65	2/11175 (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	402	PHE	N-CA-C	-5.51	96.14	111.00
3	I	360	ASP	N-CA-C	-5.47	96.24	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	394	0	369	15	0
1	C	372	0	346	5	0
2	B	2065	0	2030	52	0
2	D	2022	0	1965	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	3233	0	3143	122	0
4	E	24	0	22	8	0
4	F	24	0	22	4	0
5	G	278	0	192	26	0
6	H	81	0	68	6	0
7	J	28	0	25	1	0
8	A	12	0	16	5	0
8	B	30	0	40	4	0
8	D	24	0	32	4	0
8	I	6	0	8	2	0
9	B	20	0	0	2	0
9	D	5	0	0	0	0
9	I	5	0	0	0	0
10	I	14	0	13	0	0
11	A	29	0	0	0	0
11	B	132	0	0	0	0
11	C	24	0	0	0	0
11	D	117	0	0	1	0
11	I	87	0	0	4	0
All	All	9026	0	8291	262	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (262) 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)
2:B:93[A]:ARG:HH11	2:B:93[A]:ARG:HB3	1.09	1.14
3:I:129:ARG:HD3	3:I:417:LEU:HD11	1.35	1.03
3:I:358:GLY:HA2	3:I:361:ASP:OD1	1.66	0.94
2:D:18:GLU:HG3	2:D:187:ARG:HG3	1.50	0.94
3:I:361:ASP:HB3	11:I:2052:HOH:O	1.68	0.92
3:I:319:HIS:HE1	3:I:399:ARG:HE	1.19	0.90
5:G:7:GU9:H4	5:G:7:GU9:H92	1.54	0.89
3:I:283:LEU:HD11	3:I:320:MET:HE1	1.52	0.88
6:H:1:NAG:H61	6:H:7:FUC:H5	1.59	0.82
1:A:1(B):ALA:HB3	8:A:1102:GOL:H32	1.63	0.80
3:I:107:LYS:O	3:I:110:THR:HG22	1.80	0.80
2:B:93[A]:ARG:HB3	2:B:93[A]:ARG:NH1	1.94	0.80
3:I:26:PRO:O	3:I:27:GLU:HB2	1.80	0.80
4:F:1:NAG:H62	4:F:2:FUC:H3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93[A]:ARG:HH11	2:B:93[A]:ARG:CB	1.94	0.78
4:E:1:NAG:H62	4:E:2:FUC:H3	1.66	0.77
2:D:35:ARG:HD2	2:D:37:PRO:O	1.85	0.76
3:I:355:VAL:HG12	3:I:362:LEU:HD22	1.68	0.75
3:I:129:ARG:CD	3:I:417:LEU:HD11	2.15	0.74
3:I:405:ASN:H	3:I:405:ASN:HD22	1.35	0.74
1:A:1(D):GLY:H	8:A:1102:GOL:H2	1.53	0.74
3:I:134:ALA:C	3:I:136:LYS:H	1.91	0.73
3:I:281:MET:HE3	3:I:283:LEU:HD21	1.70	0.73
3:I:217:ASN:H	3:I:217:ASN:HD22	1.35	0.72
2:D:240:LYS:HE2	8:D:1106:GOL:O1	1.90	0.71
2:D:61:GLU:HG2	2:D:87:LYS:HA	1.71	0.71
3:I:135:ASN:O	3:I:137:ALA:N	2.24	0.70
2:B:159:ASN:H	8:B:1103:GOL:H31	1.58	0.69
3:I:324:ARG:HH22	8:I:1112:GOL:H11	1.58	0.68
2:D:61:GLU:CD	2:D:61:GLU:H	1.97	0.68
3:I:283:LEU:HD11	3:I:320:MET:CE	2.23	0.66
2:D:240:LYS:HD2	5:G:16:GU4:O25	1.94	0.66
2:D:61:GLU:CG	2:D:87:LYS:HA	2.25	0.66
4:E:1:NAG:H62	4:E:2:FUC:H5	1.77	0.65
3:I:257:LYS:HA	3:I:314:MET:O	1.98	0.64
3:I:356:ALA:O	3:I:357:GLU:HB2	1.96	0.64
3:I:222:LYS:HG2	3:I:381:GLU:HB3	1.79	0.63
2:D:158:VAL:HA	8:D:1110:GOL:H2	1.79	0.63
2:B:60(G):ASN:HD22	4:E:1:NAG:H61	1.64	0.63
2:B:65:LEU:HD21	2:B:82:ILE:HD13	1.80	0.62
7:J:1:NAG:H62	7:J:2:NAG:O7	1.99	0.62
2:B:97:ARG:HG3	2:B:97:ARG:HH11	1.64	0.62
1:A:14(A):LYS:HG3	1:A:14(B):THR:HG23	1.80	0.62
3:I:125:LYS:HE2	11:I:2033:HOH:O	2.00	0.62
3:I:284:ILE:N	3:I:284:ILE:HD12	2.15	0.62
3:I:300:THR:OG1	3:I:303:VAL:HG23	1.98	0.62
3:I:12:PRO:HG2	5:G:3:GU6:O17	1.98	0.62
2:B:158:VAL:HA	8:B:1103:GOL:H31	1.82	0.61
5:G:12:GU8:H62	5:G:13:GU5:H5	1.82	0.61
3:I:198:ILE:HD11	3:I:372:PHE:HE2	1.66	0.61
3:I:157:THR:O	3:I:161:ILE:HG13	1.99	0.61
4:E:1:NAG:H62	4:E:2:FUC:C3	2.30	0.61
2:D:177:THR:HA	8:D:1111:GOL:H2	1.83	0.61
3:I:135:ASN:C	3:I:137:ALA:H	2.03	0.61
3:I:174:ASP:OD2	3:I:177:GLU:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:GLU:CD	2:B:61:GLU:H	2.04	0.60
2:D:36:LYS:HE2	2:D:65:LEU:HD13	1.83	0.60
2:B:132:ALA:CB	2:B:164:GLU:HG3	2.31	0.60
1:A:1(D):GLY:H	8:A:1102:GOL:C2	2.15	0.59
3:I:258:PHE:HB2	3:I:316:LEU:HD21	1.85	0.59
6:H:1:NAG:C6	6:H:7:FUC:H5	2.32	0.58
2:B:35:ARG:HD2	2:B:37:PRO:O	2.04	0.58
3:I:389:VAL:HG12	3:I:390:ILE:N	2.19	0.58
3:I:217:ASN:HD22	3:I:217:ASN:N	2.00	0.57
6:H:1:NAG:H62	6:H:7:FUC:H3	1.86	0.57
4:F:1:NAG:H62	4:F:2:FUC:C3	2.34	0.57
2:B:165:ARG:HD2	9:B:2002:SO4:O1	2.04	0.57
2:B:17:VAL:HG12	2:B:18:GLU:HG2	1.87	0.57
3:I:22:ILE:HD12	3:I:24:ARG:NH2	2.19	0.57
2:D:18:GLU:HB2	2:D:188:GLY:HA2	1.87	0.56
5:G:12:GU8:C8	5:G:12:GU8:H72	2.36	0.56
2:B:165:ARG:NH1	2:B:177:THR:O	2.39	0.56
5:G:1:GU3:O2	5:G:1:GU3:H8A	2.04	0.56
2:B:25:GLY:O	2:B:28:PRO:HD3	2.05	0.56
2:D:65:LEU:HD11	2:D:84:MET:SD	2.45	0.56
5:G:11:GU9:H62	5:G:12:GU8:O2	2.06	0.56
2:D:65:LEU:HD11	2:D:84:MET:CE	2.36	0.56
5:G:12:GU8:O4	5:G:13:GU5:H72	2.06	0.55
3:I:119:ILE:CG2	3:I:120:HIS:N	2.70	0.55
2:B:61:GLU:CG	2:B:87:LYS:HA	2.38	0.54
3:I:153:THR:O	3:I:355:VAL:HG23	2.07	0.54
1:A:1(S):THR:HG22	1:A:1(R):SER:N	2.21	0.54
3:I:222:LYS:HG2	3:I:381:GLU:CB	2.38	0.54
5:G:4:GU1:O2	5:G:4:GU1:H82	2.08	0.54
1:A:14(H):GLU:O	1:A:14(K):ILE:HG13	2.07	0.54
2:B:189:ASP:OD1	2:B:190:ALA:N	2.41	0.54
3:I:354:ILE:N	3:I:354:ILE:HD12	2.22	0.54
3:I:89:MET:HA	3:I:166:TYR:OH	2.07	0.54
2:D:144:LEU:HD21	2:D:152:PRO:HB3	1.90	0.53
2:B:60(G):ASN:ND2	4:E:1:NAG:H61	2.23	0.53
2:B:240:LYS:NZ	5:G:14:GU0:O3	2.41	0.53
3:I:324:ARG:NH2	8:I:1112:GOL:H11	2.24	0.53
3:I:350:LYS:C	3:I:352:PRO:HD3	2.29	0.53
3:I:405:ASN:H	3:I:405:ASN:ND2	2.05	0.53
2:D:176:ILE:HD12	2:D:227:PHE:CE2	2.42	0.53
6:H:1:NAG:H61	6:H:7:FUC:C5	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:183:ARG:HE	3:I:203:PRO:C	2.13	0.52
3:I:412:ILE:HB	3:I:422:PHE:HB2	1.90	0.52
5:G:9:GU9:H83	5:G:9:GU9:O4	2.09	0.52
2:B:204(B):ASN:ND2	2:B:206:ARG:H	2.07	0.52
3:I:99:LEU:O	3:I:103:MET:HG2	2.10	0.52
5:G:6:GU8:O4	5:G:7:GU9:H72	2.09	0.52
3:I:89:MET:HE3	3:I:166:TYR:HB3	1.92	0.51
3:I:425:ARG:HD3	3:I:427:ALA:HB2	1.92	0.51
3:I:133:LYS:O	3:I:135:ASN:N	2.43	0.51
2:B:211:GLY:HA2	2:B:231:VAL:HG23	1.92	0.51
3:I:201:VAL:HG23	11:I:2040:HOH:O	2.09	0.51
3:I:319:HIS:CE1	3:I:399:ARG:HE	2.11	0.51
3:I:332:LYS:HG3	3:I:344:PHE:CE1	2.45	0.51
4:F:1:NAG:C6	4:F:2:FUC:H5	2.40	0.51
3:I:417:LEU:O	3:I:418:ASN:HB2	2.10	0.51
3:I:81:LEU:HD21	3:I:130:LEU:CD1	2.41	0.51
3:I:261:ARG:HD3	3:I:262:ARG:N	2.27	0.50
3:I:405:ASN:HD22	3:I:405:ASN:N	1.99	0.50
2:B:204(B):ASN:C	2:B:204(B):ASN:HD22	2.15	0.50
2:B:64:LEU:HB2	2:B:85:LEU:HD12	1.93	0.50
3:I:23:TYR:O	3:I:24:ARG:HD3	2.12	0.50
4:E:1:NAG:H62	4:E:2:FUC:C5	2.40	0.50
3:I:351:LEU:N	3:I:352:PRO:HD3	2.27	0.50
3:I:190:VAL:HG21	3:I:201:VAL:HG21	1.94	0.50
3:I:430:CYS:O	3:I:431:VAL:HB	2.12	0.50
2:D:60(B):PRO:HD2	2:D:96:TRP:CD2	2.46	0.49
3:I:93:GLY:HA3	3:I:354:ILE:CD1	2.42	0.49
2:B:68:ILE:HG22	2:B:118:ILE:HG12	1.93	0.49
5:G:3:GU6:O4	5:G:4:GU1:H73	2.12	0.49
2:D:31:VAL:HB	2:D:44:ALA:HB3	1.94	0.49
4:E:1:NAG:C6	4:E:2:FUC:H5	2.40	0.49
2:B:165:ARG:HB3	2:B:166:PRO:HD3	1.93	0.49
3:I:253:TYR:HA	3:I:318:VAL:O	2.12	0.49
3:I:271:GLU:OE2	3:I:413:ARG:NH1	2.39	0.49
2:B:98:ASN:HD21	2:B:175:ARG:NH2	2.10	0.49
3:I:89:MET:HG2	3:I:166:TYR:CZ	2.48	0.49
3:I:186:ILE:HD12	3:I:207:ILE:HD11	1.93	0.49
3:I:186:ILE:HG21	3:I:202:ILE:CD1	2.43	0.49
2:B:247:GLU:OE1	3:I:228:LYS:NZ	2.46	0.48
2:D:67:ARG:HG2	2:D:82:ILE:HG12	1.94	0.48
3:I:20:MET:SD	3:I:352:PRO:HB2	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:99:LEU:O	2:D:102:ASP:HB2	2.13	0.48
3:I:198:ILE:HD11	3:I:372:PHE:CE2	2.48	0.48
2:D:144:LEU:O	2:D:145:LYS:HG3	2.13	0.48
3:I:134:ALA:C	3:I:136:LYS:N	2.62	0.48
3:I:228:LYS:NZ	3:I:378:GLU:OE1	2.43	0.48
1:A:1(S):THR:HG22	1:A:1(R):SER:H	1.78	0.48
3:I:355:VAL:CG1	3:I:362:LEU:HB2	2.44	0.48
2:D:65:LEU:CD1	2:D:84:MET:SD	3.01	0.48
3:I:332:LYS:HG3	3:I:344:PHE:CD1	2.48	0.48
3:I:134:ALA:O	3:I:136:LYS:N	2.43	0.48
3:I:108:PHE:O	3:I:111:ILE:HG12	2.14	0.48
1:A:14:ASP:HB2	2:B:23:GLU:OE2	2.14	0.47
1:C:1:CYS:O	2:D:206:ARG:HD3	2.14	0.47
5:G:7:GU9:H92	5:G:7:GU9:C4	2.34	0.47
2:D:35:ARG:O	2:D:38:GLN:HA	2.15	0.47
3:I:191:SER:O	3:I:195:GLU:HA	2.14	0.47
2:D:25:GLY:O	2:D:28:PRO:HD3	2.14	0.47
3:I:319:HIS:HE1	3:I:399:ARG:NE	2.01	0.47
3:I:276:GLY:O	3:I:277:ASP:HB2	2.15	0.47
1:A:1(E):SER:HB2	8:A:1102:GOL:O2	2.14	0.47
2:D:185:LYS:HB2	2:D:186(B):GLU:HG3	1.96	0.47
3:I:146:LEU:HD12	3:I:146:LEU:N	2.30	0.47
3:I:218:THR:HG22	3:I:370:LYS:HB3	1.97	0.47
3:I:283:LEU:C	3:I:284:ILE:HD12	2.35	0.47
3:I:259:ARG:HH12	3:I:311:LEU:HB2	1.79	0.46
3:I:260:TYR:CG	3:I:261:ARG:N	2.83	0.46
1:A:1(R):SER:OG	2:B:206:ARG:NE	2.44	0.46
2:B:65:LEU:HD11	2:B:82:ILE:CG2	2.45	0.46
3:I:146:LEU:HG	3:I:215:LEU:HD22	1.98	0.46
3:I:186:ILE:HG21	3:I:202:ILE:HD11	1.96	0.46
3:I:225:TRP:NE1	3:I:379:GLY:HA2	2.31	0.46
3:I:261:ARG:HG3	3:I:263:VAL:HG13	1.96	0.46
4:E:1:NAG:H4	4:E:2:FUC:H3	1.98	0.46
3:I:336:GLN:HA	3:I:340:LEU:O	2.15	0.46
3:I:86:ALA:O	3:I:89:MET:HB2	2.15	0.46
2:B:61:GLU:HG2	2:B:87:LYS:HA	1.98	0.45
3:I:23:TYR:CE2	3:I:100:GLN:HG3	2.51	0.45
3:I:331:LEU:HB2	3:I:369:HIS:CD2	2.52	0.45
5:G:11:GU9:H72	5:G:11:GU9:O3	2.15	0.45
1:A:1(H):THR:HB	2:B:242:ILE:O	2.16	0.45
2:B:60(B):PRO:HB2	2:B:96:TRP:CZ3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:93:GLY:HA3	3:I:354:ILE:HD12	1.98	0.45
1:A:1(D):GLY:N	8:A:1102:GOL:H2	2.27	0.45
2:B:132:ALA:HB2	2:B:164:GLU:HG3	1.97	0.45
3:I:190:VAL:HG11	3:I:201:VAL:CG2	2.47	0.45
3:I:357:GLU:HB3	3:I:358:GLY:H	1.47	0.45
5:G:12:GU8:H72	5:G:12:GU8:H83	1.99	0.45
6:H:1:NAG:C6	6:H:7:FUC:C5	2.95	0.45
2:D:22:ALA:O	2:D:71:HIS:HE1	2.00	0.45
5:G:10:GU8:C8	5:G:10:GU8:H72	2.48	0.45
3:I:389:VAL:CG1	3:I:390:ILE:N	2.80	0.44
2:B:60(C):PRO:HD3	2:B:96:TRP:CZ3	2.51	0.44
1:C:10:LYS:O	1:C:12:LEU:HG	2.17	0.44
3:I:18:ASN:HD22	3:I:118:GLN:HE22	1.66	0.44
4:F:1:NAG:H62	4:F:2:FUC:H5	1.99	0.44
6:H:1:NAG:O4	6:H:2:NAG:H82	2.18	0.44
1:C:14(G):LEU:H	1:C:14(G):LEU:HD22	1.82	0.44
3:I:355:VAL:HG11	3:I:362:LEU:HB2	2.00	0.44
2:D:211:GLY:HA2	2:D:231:VAL:HG23	1.99	0.43
5:G:7:GU9:O4	5:G:8:GU8:H73	2.17	0.43
3:I:160:ASP:O	3:I:163:GLU:HB3	2.18	0.43
3:I:218:THR:O	3:I:219:ILE:HB	2.18	0.43
5:G:12:GU8:H83	5:G:12:GU8:C7	2.48	0.43
2:D:165:ARG:HB3	2:D:166:PRO:HD3	1.99	0.43
2:B:67:ARG:HG2	2:B:82:ILE:HG12	2.01	0.43
2:D:87:LYS:HD2	11:D:2095:HOH:O	2.17	0.43
3:I:119:ILE:HG23	3:I:120:HIS:N	2.32	0.43
3:I:256:GLY:HA2	3:I:315:MET:CE	2.49	0.43
5:G:5:GU5:O2	5:G:5:GU5:H82	2.18	0.43
1:A:1(I):ARG:HH12	3:I:228:LYS:HZ3	1.66	0.43
2:D:165:ARG:NH1	8:D:1107:GOL:H12	2.33	0.43
5:G:12:GU8:H72	5:G:12:GU8:O3	2.19	0.43
2:B:244:GLN:HG3	2:B:245:PHE:CE2	2.54	0.43
3:I:14:ASP:C	3:I:15:ILE:HG13	2.39	0.43
3:I:61:THR:HG22	3:I:338:MET:HE3	1.99	0.43
3:I:171:GLN:HA	3:I:172:PRO:HD3	1.85	0.43
1:A:14(D):ARG:O	1:A:14(H):GLU:HG2	2.19	0.43
2:B:18:GLU:HB2	2:B:188:GLY:HA2	2.00	0.43
2:B:75:ARG:CZ	9:B:2006:SO4:O3	2.66	0.43
1:C:1(Q):GLU:H	1:C:1(Q):GLU:HG2	1.68	0.43
5:G:8:GU8:H62	5:G:9:GU9:H5	2.00	0.43
3:I:26:PRO:O	3:I:27:GLU:CB	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:180:GLU:O	3:I:183:ARG:HB3	2.18	0.43
2:B:18:GLU:HG3	2:B:187:ARG:HG3	2.01	0.42
2:B:60(B):PRO:O	2:B:60(E):ASP:N	2.37	0.42
3:I:299:LEU:HD21	3:I:411:PHE:HZ	1.83	0.42
2:B:93[B]:ARG:NH2	5:G:16:GU4:O4	2.52	0.42
2:D:32:MET:CG	2:D:40:LEU:HD22	2.50	0.42
3:I:71:ASN:HB3	3:I:74:ASP:OD2	2.20	0.42
5:G:1:GU3:O2	5:G:1:GU3:H7A	2.19	0.42
3:I:281:MET:HE3	3:I:320:MET:HE1	2.02	0.42
2:B:204(B):ASN:HD22	2:B:206:ARG:H	1.67	0.42
2:B:49:ASP:O	2:B:111:PRO:HA	2.20	0.42
3:I:399:ARG:HD2	3:I:401:CYS:SG	2.59	0.42
5:G:2:GU2:H82	5:G:2:GU2:H4	1.90	0.42
2:B:159:ASN:H	8:B:1103:GOL:C3	2.28	0.41
3:I:89:MET:HG2	3:I:166:TYR:CE1	2.56	0.41
3:I:304:LEU:O	3:I:308:LEU:HG	2.21	0.41
2:D:60(C):PRO:HD3	2:D:96:TRP:CE3	2.56	0.41
3:I:120:HIS:CD2	3:I:120:HIS:H	2.38	0.41
3:I:144:ASN:O	3:I:145:ARG:HB2	2.19	0.41
3:I:255:GLU:CG	3:I:317:CYS:HB3	2.50	0.41
2:B:98:ASN:ND2	2:B:175:ARG:NH2	2.68	0.41
3:I:150:LYS:N	3:I:173:LEU:O	2.53	0.41
5:G:4:GU1:C6	5:G:5:GU5:H5	2.50	0.41
2:B:97:ARG:HG3	2:B:97:ARG:NH1	2.34	0.41
2:B:136:GLY:HA3	2:B:199:PHE:CE1	2.56	0.41
3:I:144:ASN:HA	3:I:216:VAL:O	2.21	0.41
1:C:1(H):THR:HB	2:D:242:ILE:O	2.20	0.41
3:I:147:PHE:O	3:I:213:LEU:HD12	2.21	0.41
3:I:159:GLN:HA	3:I:159:GLN:OE1	2.21	0.41
3:I:405:ASN:ND2	3:I:405:ASN:N	2.67	0.41
2:B:23:GLU:OE2	2:B:26:MET:HE3	2.20	0.41
2:D:185:LYS:HB3	2:D:186:PRO:HD2	2.03	0.41
2:B:60(B):PRO:HB2	2:B:60(C):PRO:HD3	2.01	0.41
1:A:4:ARG:HA	1:A:5:PRO:HD3	1.92	0.41
3:I:61:THR:HG22	3:I:338:MET:CE	2.51	0.41
2:D:244:GLN:HG3	2:D:245:PHE:CD2	2.56	0.40
3:I:157:THR:HG22	3:I:161:ILE:HD11	2.02	0.40
2:D:50:ARG:HG3	2:D:51:TRP:CD1	2.57	0.40
3:I:319:HIS:HD2	11:I:2019:HOH:O	2.02	0.40
2:B:159:ASN:N	8:B:1103:GOL:H31	2.32	0.40
2:B:163:VAL:HB	2:B:182:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:317:CYS:O	3:I:401:CYS:HB3	2.21	0.40
3:I:324:ARG:HH11	3:I:374:GLU:HB2	1.87	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	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
1	C	44/49 (90%)	42 (96%)	2 (4%)	0	100	100
2	B	251/259 (97%)	244 (97%)	7 (3%)	0	100	100
2	D	248/259 (96%)	239 (96%)	9 (4%)	0	100	100
3	I	411/432 (95%)	378 (92%)	21 (5%)	12 (3%)	4	1
All	All	1000/1048 (95%)	948 (95%)	40 (4%)	12 (1%)	13	8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	134	ALA
3	I	136	LYS
3	I	195	GLU
3	I	241	LYS
3	I	357	GLU
3	I	359	ARG
3	I	18	ASN
3	I	72	ASP
3	I	289	GLU
3	I	92	LEU
3	I	135	ASN
3	I	219	ILE

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	43/43 (100%)	43 (100%)	0	100	100
1	C	40/43 (93%)	39 (98%)	1 (2%)	47	52
2	B	220/224 (98%)	210 (96%)	10 (4%)	27	27
2	D	214/224 (96%)	210 (98%)	4 (2%)	57	63
3	I	345/382 (90%)	331 (96%)	14 (4%)	30	31
All	All	862/916 (94%)	833 (97%)	29 (3%)	40	39

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	33	LEU
2	B	62	ASN
2	B	93[A]	ARG
2	B	93[B]	ARG
2	B	97	ARG
2	B	165	ARG
2	B	204(B)	ASN
2	B	233[A]	ARG
2	B	233[B]	ARG
2	B	243	ASP
1	C	1(O)	GLN
2	D	33	LEU
2	D	40	LEU
2	D	93	ARG
2	D	101	ARG
3	I	78	LEU
3	I	97	ASP
3	I	141	VAL
3	I	200	ASP
3	I	212	VAL
3	I	215	LEU
3	I	217	ASN
3	I	315	MET

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Mol	Chain	Res	Type
3	I	331	LEU
3	I	333	GLU
3	I	361	ASP
3	I	366	ASP
3	I	405	ASN
3	I	416	PRO

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

Mol	Chain	Res	Type
1	A	1(O)	GLN
2	B	156	GLN
2	B	204(B)	ASN
2	B	205	ASN
2	B	239	GLN
1	C	1(O)	GLN
2	D	71	HIS
2	D	156	GLN
2	D	205	ASN
2	D	239	GLN
2	D	244	GLN
3	I	18	ASN
3	I	120	HIS
3	I	181	GLN
3	I	217	ASN
3	I	268	GLN
3	I	319	HIS
3	I	405	ASN

5.3.3 RNA (i)

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)

29 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	E	1	4,2	14,14,15	0.66	0	17,19,21	0.95	1 (5%)
4	FUC	E	2	4	10,10,11	0.61	0	14,14,16	0.71	0
4	NAG	F	1	4,2	14,14,15	0.71	0	17,19,21	0.86	1 (5%)
4	FUC	F	2	4	10,10,11	0.58	0	14,14,16	0.74	0
5	GU3	G	1	5	22,22,22	1.68	3 (13%)	28,33,33	1.11	1 (3%)
5	GU8	G	10	5	14,14,15	0.40	0	18,18,20	0.63	0
5	GU9	G	11	5	14,14,15	0.49	0	18,18,20	1.74	2 (11%)
5	GU8	G	12	5	14,14,15	0.39	0	18,18,20	0.88	1 (5%)
5	GU5	G	13	5	17,17,18	1.33	1 (5%)	22,24,26	0.76	0
5	GU0	G	14	5	23,23,24	1.91	4 (17%)	25,36,38	0.97	2 (8%)
5	GU6	G	15	5	23,23,24	3.31	10 (43%)	25,36,38	4.05	9 (36%)
5	GU4	G	16	5	27,27,28	2.00	5 (18%)	29,43,45	1.09	2 (6%)
5	GU2	G	2	5	14,14,15	0.70	1 (7%)	15,19,21	0.87	0
5	GU6	G	3	5	23,23,24	1.93	4 (17%)	25,36,38	1.36	3 (12%)
5	GU1	G	4	5	14,14,15	0.71	1 (7%)	15,19,21	0.89	0
5	GU5	G	5	5	17,17,18	1.33	1 (5%)	22,24,26	1.24	2 (9%)
5	GU8	G	6	5	14,14,15	0.40	0	18,18,20	0.62	0
5	GU9	G	7	5	14,14,15	0.42	0	18,18,20	0.68	0
5	GU8	G	8	5	14,14,15	0.42	0	18,18,20	0.62	0
5	GU9	G	9	5	14,14,15	0.39	0	18,18,20	0.69	0
6	NAG	H	1	3,6	14,14,15	0.67	0	17,19,21	0.84	1 (5%)
6	NAG	H	2	6	14,14,15	0.58	0	17,19,21	0.80	1 (5%)
6	BMA	H	3	6	11,11,12	0.61	0	15,15,17	0.47	0
6	MAN	H	4	6	11,11,12	0.69	0	15,15,17	0.68	0
6	MAN	H	5	6	10,10,12	0.54	0	13,13,17	0.58	0
6	MAN	H	6	6	11,11,12	0.58	0	15,15,17	0.73	0
6	FUC	H	7	6	10,10,11	0.56	0	14,14,16	0.73	0
7	NAG	J	1	3,7	14,14,15	0.64	0	17,19,21	0.91	1 (5%)
7	NAG	J	2	7	14,14,15	0.55	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
4	NAG	E	1	4,2	-	4/6/23/26	0/1/1/1
4	FUC	E	2	4	-	-	0/1/1/1
4	NAG	F	1	4,2	1/1/5/7	4/6/23/26	0/1/1/1
4	FUC	F	2	4	-	-	0/1/1/1
5	GU3	G	1	5	-	2/15/35/35	0/1/1/1
5	GU8	G	10	5	-	2/7/24/27	0/1/1/1
5	GU9	G	11	5	-	2/7/24/27	0/1/1/1
5	GU8	G	12	5	-	2/7/24/27	0/1/1/1
5	GU5	G	13	5	-	3/10/27/30	0/1/1/1
5	GU0	G	14	5	-	3/16/33/36	0/1/1/1
5	GU6	G	15	5	1/1/7/8	6/16/33/36	0/1/1/1
5	GU4	G	16	5	-	0/21/38/41	0/1/1/1
5	GU2	G	2	5	-	2/8/25/28	0/1/1/1
5	GU6	G	3	5	-	0/16/33/36	0/1/1/1
5	GU1	G	4	5	-	0/8/25/28	0/1/1/1
5	GU5	G	5	5	-	0/10/27/30	0/1/1/1
5	GU8	G	6	5	-	2/7/24/27	0/1/1/1
5	GU9	G	7	5	-	1/7/24/27	0/1/1/1
5	GU8	G	8	5	-	2/7/24/27	0/1/1/1
5	GU9	G	9	5	-	0/7/24/27	0/1/1/1
6	NAG	H	1	3,6	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	H	2	6	-	4/6/23/26	0/1/1/1
6	BMA	H	3	6	-	2/2/19/22	0/1/1/1
6	MAN	H	4	6	-	0/2/19/22	0/1/1/1
6	MAN	H	5	6	-	0/2/16/22	0/1/1/1
6	MAN	H	6	6	-	2/2/19/22	0/1/1/1
6	FUC	H	7	6	-	-	0/1/1/1
7	NAG	J	1	3,7	-	4/6/23/26	0/1/1/1
7	NAG	J	2	7	-	5/6/23/26	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	15	GU6	O2-C2	-6.72	1.36	1.47
5	G	15	GU6	C4-C5	-6.41	1.39	1.53
5	G	15	GU6	O6-S6	-5.13	1.43	1.56
5	G	13	GU5	O6-S6	-4.97	1.43	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1	GU3	O6-S6	-4.97	1.43	1.56
5	G	15	GU6	C3-C2	-4.97	1.39	1.52
5	G	5	GU5	O6-S6	-4.96	1.43	1.56
5	G	3	GU6	O6-S6	-4.93	1.43	1.56
5	G	16	GU4	O6-S6	-4.91	1.43	1.56
5	G	14	GU0	O6-S6	-4.88	1.43	1.56
5	G	15	GU6	C4-C3	-4.75	1.39	1.52
5	G	15	GU6	O3-C3	-4.68	1.36	1.46
5	G	15	GU6	O3-S3	-4.64	1.43	1.57
5	G	15	GU6	O2-S2	-4.60	1.43	1.57
5	G	3	GU6	O3-S3	-4.59	1.43	1.57
5	G	1	GU3	O2-S2	-4.59	1.43	1.57
5	G	3	GU6	O2-S2	-4.58	1.43	1.57
5	G	14	GU0	O2-S2	-4.53	1.43	1.57
5	G	14	GU0	O3-S3	-4.52	1.43	1.57
5	G	16	GU4	O2-S2	-4.48	1.44	1.57
5	G	16	GU4	O3-S3	-4.46	1.44	1.57
5	G	16	GU4	O4-S4	-4.45	1.44	1.57
5	G	15	GU6	O5-C5	-3.07	1.37	1.43
5	G	15	GU6	O4-C4	-2.58	1.36	1.43
5	G	3	GU6	O2-C2	-2.40	1.43	1.47
5	G	14	GU0	O2-C2	-2.39	1.43	1.47
5	G	16	GU4	O2-C2	-2.33	1.43	1.47
5	G	1	GU3	O1-C1	2.25	1.44	1.40
5	G	4	GU1	O6B-C6	-2.19	1.23	1.30
5	G	2	GU2	O6-C6	-2.14	1.23	1.30

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	15	GU6	O2-C2-C3	16.09	124.46	106.65
5	G	11	GU9	O4-C4-C3	-6.54	92.60	109.94
5	G	15	GU6	O4-C4-C3	6.49	127.14	109.94
5	G	15	GU6	C6-C5-C4	5.53	123.63	112.09
5	G	15	GU6	O5-C5-C6	4.83	118.31	107.61
5	G	5	GU5	O4-C4-C5	-4.06	99.23	109.30
5	G	15	GU6	O4-C4-C5	3.93	119.07	109.30
5	G	3	GU6	C2-O2-S2	-3.77	112.99	117.91
5	G	1	GU3	C2-O2-S2	-3.73	111.67	118.88
5	G	15	GU6	C1-O5-C5	3.37	116.75	112.19
5	G	3	GU6	C3-O3-S3	-3.30	112.49	118.88
5	G	3	GU6	O2-C2-C3	3.03	110.01	106.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	15	GU6	O5-C5-C4	2.95	117.99	110.83
5	G	12	GU8	C1-C2-C3	-2.72	105.33	109.40
5	G	15	GU6	C4-C3-C2	-2.64	104.88	110.93
5	G	16	GU4	C1-O5-C5	2.54	115.64	112.19
5	G	5	GU5	O6-C6-C5	2.29	111.89	107.62
5	G	11	GU9	C6-C5-C4	-2.28	107.33	112.09
5	G	16	GU4	O2-C2-C3	2.28	109.17	106.65
7	J	1	NAG	C2-N2-C7	-2.28	119.66	122.90
6	H	2	NAG	C2-N2-C7	-2.23	119.73	122.90
4	E	1	NAG	C1-O5-C5	2.22	115.20	112.19
5	G	14	GU0	O2-C2-C3	2.21	109.10	106.65
4	F	1	NAG	C2-N2-C7	-2.16	119.82	122.90
5	G	14	GU0	O6-C6-C5	2.12	111.57	107.62
6	H	1	NAG	C2-N2-C7	-2.09	119.92	122.90
5	G	15	GU6	C2-O2-S2	2.00	120.52	117.91

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	1	NAG	C1
5	G	15	GU6	C5
6	H	1	NAG	C1

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1	GU3	O5-C1-O1-C8
5	G	1	GU3	C2-C1-O1-C8
5	G	7	GU9	C3-C2-O2-C7
5	G	13	GU5	C3-C2-O2-C7
5	G	14	GU0	C3-O3-S3-O26
5	G	14	GU0	C3-O3-S3-O27
5	G	15	GU6	C4-C5-C6-O6
6	H	1	NAG	C8-C7-N2-C2
6	H	1	NAG	O7-C7-N2-C2
6	H	2	NAG	C8-C7-N2-C2
6	H	2	NAG	O7-C7-N2-C2
7	J	1	NAG	C8-C7-N2-C2
7	J	1	NAG	O7-C7-N2-C2
7	J	2	NAG	C3-C2-N2-C7
7	J	2	NAG	C8-C7-N2-C2
7	J	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2
6	H	3	BMA	C4-C5-C6-O6
4	E	1	NAG	O7-C7-N2-C2
4	E	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
6	H	6	MAN	O5-C5-C6-O6
7	J	2	NAG	O5-C5-C6-O6
6	H	2	NAG	C4-C5-C6-O6
6	H	3	BMA	O5-C5-C6-O6
4	F	1	NAG	C8-C7-N2-C2
7	J	1	NAG	O5-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O7-C7-N2-C2
4	E	1	NAG	O5-C5-C6-O6
6	H	6	MAN	C4-C5-C6-O6
7	J	2	NAG	C4-C5-C6-O6
5	G	15	GU6	C6-O6-S6-O20
5	G	15	GU6	C6-O6-S6-O21
7	J	1	NAG	C4-C5-C6-O6
5	G	13	GU5	C2-C3-O3-C8
5	G	11	GU9	C4-C3-O3-C8
5	G	8	GU8	C2-C3-O3-C8
5	G	10	GU8	C4-C3-O3-C8
5	G	15	GU6	C6-O6-S6-O19
5	G	2	GU2	C4-C3-O3-C8
5	G	6	GU8	C4-C3-O3-C8
5	G	12	GU8	C2-C3-O3-C8
5	G	2	GU2	C2-C3-O3-C8
5	G	12	GU8	C4-C3-O3-C8
6	H	1	NAG	O5-C5-C6-O6
5	G	6	GU8	C2-C3-O3-C8
5	G	8	GU8	C4-C3-O3-C8
5	G	10	GU8	C2-C3-O3-C8
5	G	11	GU9	C2-C3-O3-C8
5	G	14	GU0	C3-O3-S3-O25
5	G	15	GU6	C3-O3-S3-O18
5	G	13	GU5	C4-C3-O3-C8
5	G	15	GU6	C3-O3-S3-O16

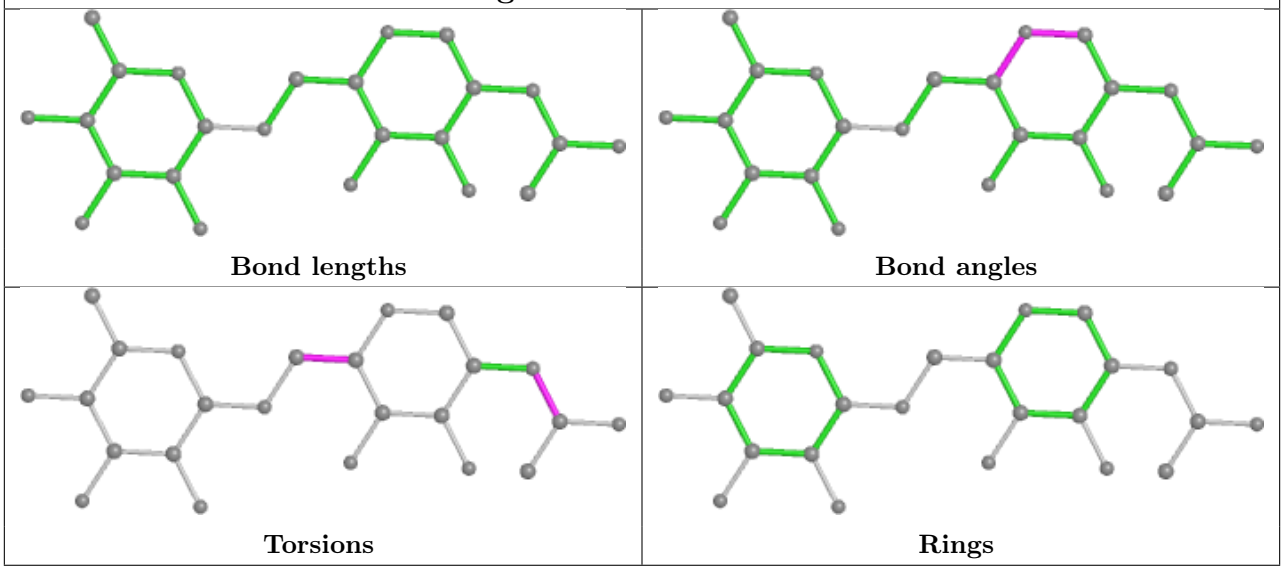
There are no ring outliers.

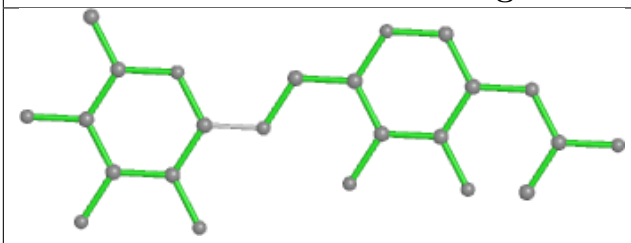
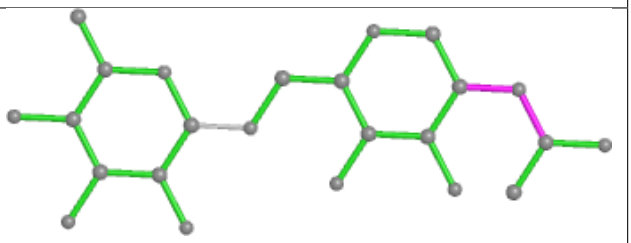
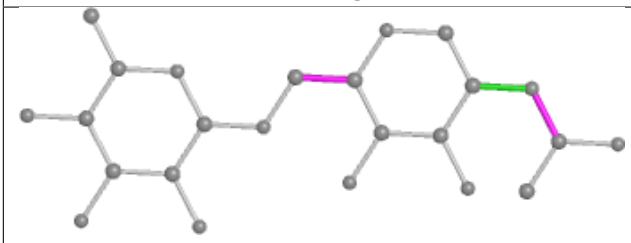
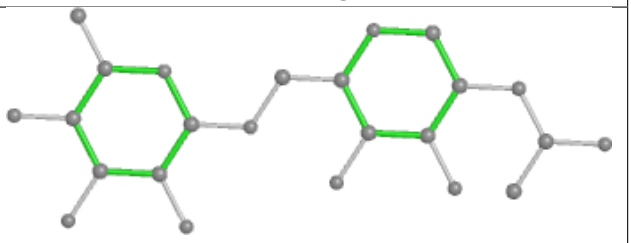
24 monomers are involved in 45 short contacts:

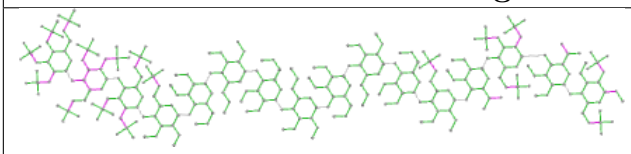
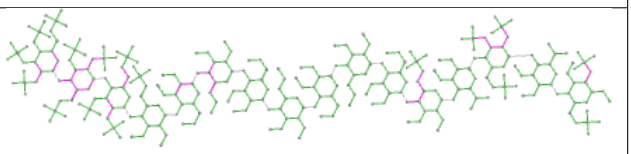
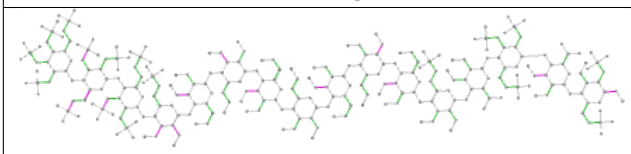
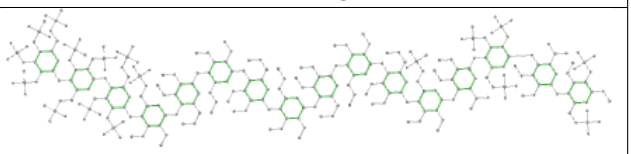
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	16	GU4	2	0
5	G	6	GU8	1	0
5	G	14	GU0	1	0
6	H	2	NAG	1	0
7	J	2	NAG	1	0
4	F	2	FUC	4	0
5	G	2	GU2	1	0
4	E	1	NAG	8	0
5	G	4	GU1	3	0
5	G	13	GU5	2	0
4	F	1	NAG	4	0
5	G	3	GU6	2	0
5	G	7	GU9	4	0
5	G	10	GU8	1	0
5	G	11	GU9	2	0
5	G	9	GU9	2	0
5	G	12	GU8	7	0
5	G	5	GU5	2	0
4	E	2	FUC	6	0
5	G	8	GU8	2	0
6	H	7	FUC	5	0
7	J	1	NAG	1	0
5	G	1	GU3	2	0
6	H	1	NAG	6	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.

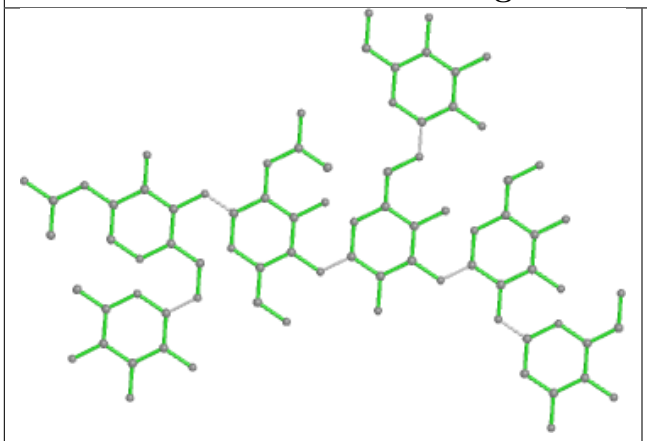
Oligosaccharide Chain E



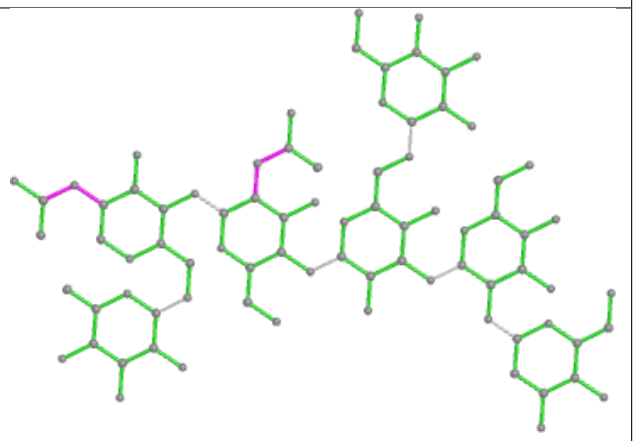
Oligosaccharide Chain F	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

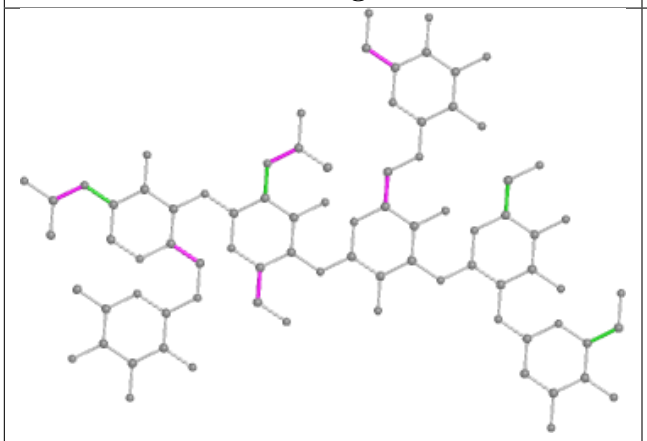
Oligosaccharide Chain H



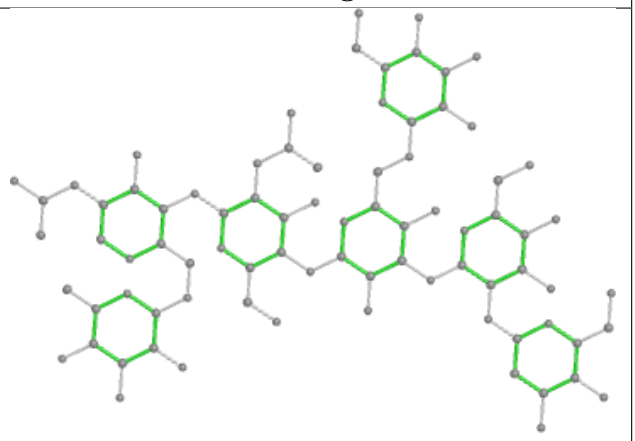
Bond lengths



Bond angles

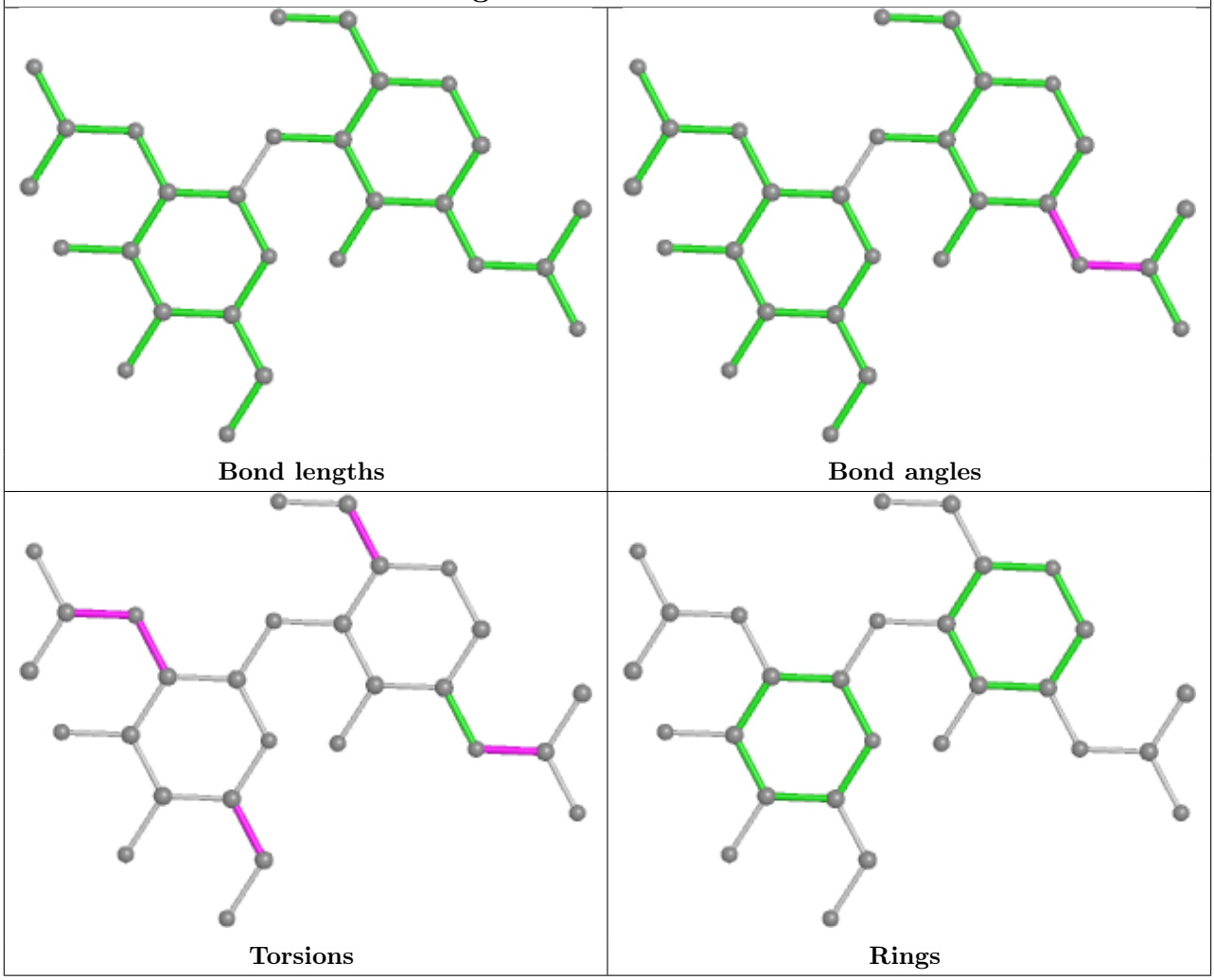


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

19 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	GOL	B	1109	-	5,5,5	0.70	0	5,5,5	0.43	0
9	SO4	I	2005	-	4,4,4	0.30	0	6,6,6	0.11	0
8	GOL	D	1106	-	5,5,5	0.62	0	5,5,5	0.41	0
9	SO4	B	2002	-	4,4,4	0.25	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SO4	B	2006	-	4,4,4	0.30	0	6,6,6	0.08	0
8	GOL	B	1105	-	5,5,5	0.68	0	5,5,5	0.41	0
8	GOL	D	1107	-	5,5,5	0.62	0	5,5,5	0.34	0
9	SO4	D	2004	-	4,4,4	0.24	0	6,6,6	0.09	0
9	SO4	B	2003	-	4,4,4	0.23	0	6,6,6	0.15	0
8	GOL	I	1112	-	5,5,5	0.67	0	5,5,5	0.39	0
8	GOL	B	1103	-	5,5,5	0.76	0	5,5,5	0.43	0
8	GOL	A	1108	-	5,5,5	0.74	0	5,5,5	0.51	0
10	NAG	I	801	3	14,14,15	0.56	0	17,19,21	0.66	0
8	GOL	D	1110	-	5,5,5	0.73	0	5,5,5	0.43	0
8	GOL	B	1101	-	5,5,5	0.81	0	5,5,5	0.43	0
8	GOL	A	1102	-	5,5,5	0.72	0	5,5,5	0.48	0
8	GOL	D	1111	-	5,5,5	0.75	0	5,5,5	0.47	0
9	SO4	B	2001	-	4,4,4	0.24	0	6,6,6	0.10	0
8	GOL	B	1104	-	5,5,5	0.63	0	5,5,5	0.41	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
10	NAG	I	801	3	-	4/6/23/26	0/1/1/1
8	GOL	B	1109	-	-	3/4/4/4	-
8	GOL	D	1111	-	-	2/4/4/4	-
8	GOL	D	1106	-	-	2/4/4/4	-
8	GOL	B	1105	-	-	1/4/4/4	-
8	GOL	D	1107	-	-	4/4/4/4	-
8	GOL	I	1112	-	-	2/4/4/4	-
8	GOL	D	1110	-	-	0/4/4/4	-
8	GOL	B	1103	-	-	0/4/4/4	-
8	GOL	A	1108	-	-	0/4/4/4	-
8	GOL	B	1104	-	-	2/4/4/4	-
8	GOL	B	1101	-	-	4/4/4/4	-
8	GOL	A	1102	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1102	GOL	O1-C1-C2-C3
8	A	1102	GOL	C1-C2-C3-O3
8	A	1102	GOL	O2-C2-C3-O3
8	B	1101	GOL	O1-C1-C2-C3
8	B	1101	GOL	C1-C2-C3-O3
8	B	1109	GOL	C1-C2-C3-O3
8	D	1106	GOL	O1-C1-C2-C3
8	D	1107	GOL	O1-C1-C2-C3
8	D	1107	GOL	O2-C2-C3-O3
10	I	801	NAG	C8-C7-N2-C2
10	I	801	NAG	O7-C7-N2-C2
10	I	801	NAG	O5-C5-C6-O6
10	I	801	NAG	C4-C5-C6-O6
8	A	1102	GOL	O1-C1-C2-O2
8	D	1107	GOL	O1-C1-C2-O2
8	B	1104	GOL	O1-C1-C2-C3
8	D	1107	GOL	C1-C2-C3-O3
8	I	1112	GOL	C1-C2-C3-O3
8	B	1101	GOL	O1-C1-C2-O2
8	B	1101	GOL	O2-C2-C3-O3
8	B	1109	GOL	O2-C2-C3-O3
8	I	1112	GOL	O2-C2-C3-O3
8	D	1111	GOL	O1-C1-C2-O2
8	D	1106	GOL	O1-C1-C2-O2
8	B	1105	GOL	O1-C1-C2-C3
8	B	1109	GOL	O1-C1-C2-C3
8	B	1104	GOL	O1-C1-C2-O2
8	D	1111	GOL	O1-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	1106	GOL	1	0
9	B	2002	SO4	1	0
9	B	2006	SO4	1	0
8	D	1107	GOL	1	0
8	I	1112	GOL	2	0
8	B	1103	GOL	4	0
8	D	1110	GOL	1	0
8	A	1102	GOL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	1111	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	47/49 (95%)	-0.11	1 (2%)	63	68	22, 34, 47, 66	1 (2%)
1	C	46/49 (93%)	0.03	3 (6%)	18	23	28, 38, 51, 58	0
2	B	252/259 (97%)	0.07	5 (1%)	65	69	14, 31, 50, 63	3 (1%)
2	D	252/259 (97%)	0.14	10 (3%)	38	44	18, 33, 47, 64	0
3	I	415/432 (96%)	0.48	33 (7%)	12	16	34, 51, 77, 89	0
All	All	1012/1048 (96%)	0.25	52 (5%)	28	33	14, 41, 68, 89	4 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	388	VAL	7.1
3	I	358	GLY	6.1
3	I	386	THR	5.6
3	I	431	VAL	5.6
3	I	134	ALA	4.4
3	I	199	THR	4.1
3	I	357	GLU	3.9
3	I	179	ALA	3.8
1	A	1(S)	THR	3.7
3	I	389	VAL	3.7
3	I	390	ILE	3.7
3	I	356	ALA	3.7
2	D	29	TRP	3.3
3	I	204	SER	3.2
3	I	15	ILE	3.2
2	D	44	ALA	3.1
1	C	1(R)	SER	2.8
3	I	264	ALA	2.8
3	I	359	ARG	2.8
3	I	266	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	I	387	ALA	2.7
2	D	53	LEU	2.7
2	B	46	LEU	2.6
3	I	243	ASP	2.5
2	B	204(A)[A]	PHE	2.5
1	C	1(O)	GLN	2.5
2	D	198	PRO	2.5
3	I	200	ASP	2.5
3	I	310	GLU	2.5
3	I	27	GLU	2.4
3	I	46	ARG	2.3
2	B	29	TRP	2.3
3	I	206	ALA	2.3
3	I	110	THR	2.3
3	I	205	GLU	2.3
2	D	213	VAL	2.3
2	D	31	VAL	2.2
2	D	47	ILE	2.2
2	B	198	PRO	2.2
3	I	26	PRO	2.2
1	C	12	LEU	2.1
2	B	31	VAL	2.1
3	I	177	GLU	2.1
3	I	6	ASP	2.1
3	I	88	ALA	2.1
3	I	262	ARG	2.1
3	I	180	GLU	2.1
3	I	181	GLN	2.1
2	D	54	THR	2.0
3	I	112	SER	2.0
2	D	147	THR	2.0
2	D	43	GLY	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

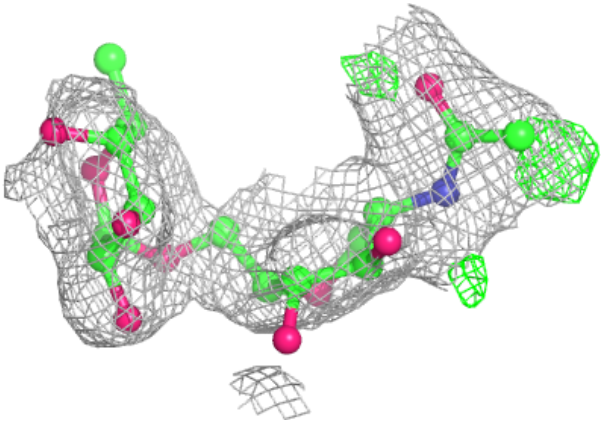
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

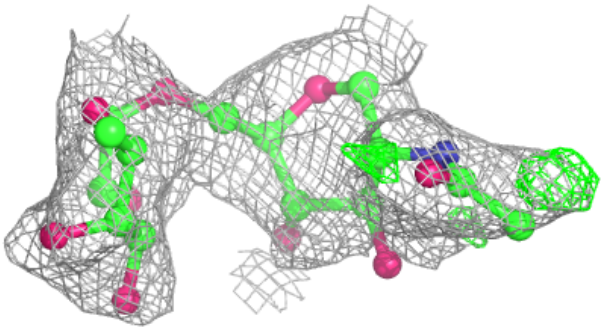
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	E	1	14/15	0.46	0.38	73,77,84,88	0
6	MAN	H	6	11/12	0.51	0.67	115,116,117,118	0
7	NAG	J	2	14/15	0.58	0.45	102,104,105,106	0
6	MAN	H	5	10/12	0.66	0.34	103,104,105,105	0
6	BMA	H	3	11/12	0.70	0.33	103,105,110,113	0
6	MAN	H	4	11/12	0.71	0.32	99,101,102,103	0
4	FUC	F	2	10/11	0.72	0.47	83,84,85,85	0
7	NAG	J	1	14/15	0.74	0.23	92,94,96,99	0
4	NAG	F	1	14/15	0.74	0.32	59,66,74,80	0
5	GU8	G	10	14/15	0.76	0.50	90,92,93,94	0
5	GU9	G	11	14/15	0.77	0.36	70,86,88,89	0
4	FUC	E	2	10/11	0.80	0.43	90,91,91,91	0
6	NAG	H	2	14/15	0.80	0.42	98,100,101,103	0
6	NAG	H	1	14/15	0.82	0.30	83,88,94,98	0
6	FUC	H	7	10/11	0.84	0.47	101,103,104,104	0
5	GU9	G	7	14/15	0.86	0.24	72,75,80,81	0
5	GU9	G	9	14/15	0.89	0.23	84,84,87,88	0
5	GU8	G	8	14/15	0.90	0.27	81,83,84,85	0
5	GU8	G	12	14/15	0.92	0.21	50,59,63,65	0
5	GU2	G	2	14/15	0.92	0.17	61,64,69,70	0
5	GU8	G	6	14/15	0.94	0.12	60,63,69,69	0
5	GU3	G	1	22/22	0.94	0.14	56,61,66,67	0
5	GU6	G	3	23/24	0.95	0.10	47,61,65,67	0
5	GU1	G	4	14/15	0.96	0.08	51,54,57,57	0
5	GU5	G	5	17/18	0.96	0.10	52,58,59,61	0
5	GU6	G	15	23/24	0.97	0.11	25,30,32,37	0
5	GU5	G	13	17/18	0.98	0.09	34,42,47,47	0
5	GU0	G	14	23/24	0.98	0.10	27,33,41,43	0
5	GU4	G	16	27/28	0.99	0.09	22,26,30,33	0

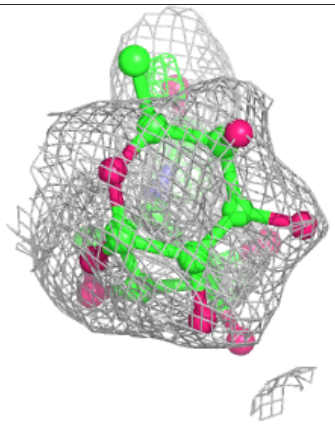
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

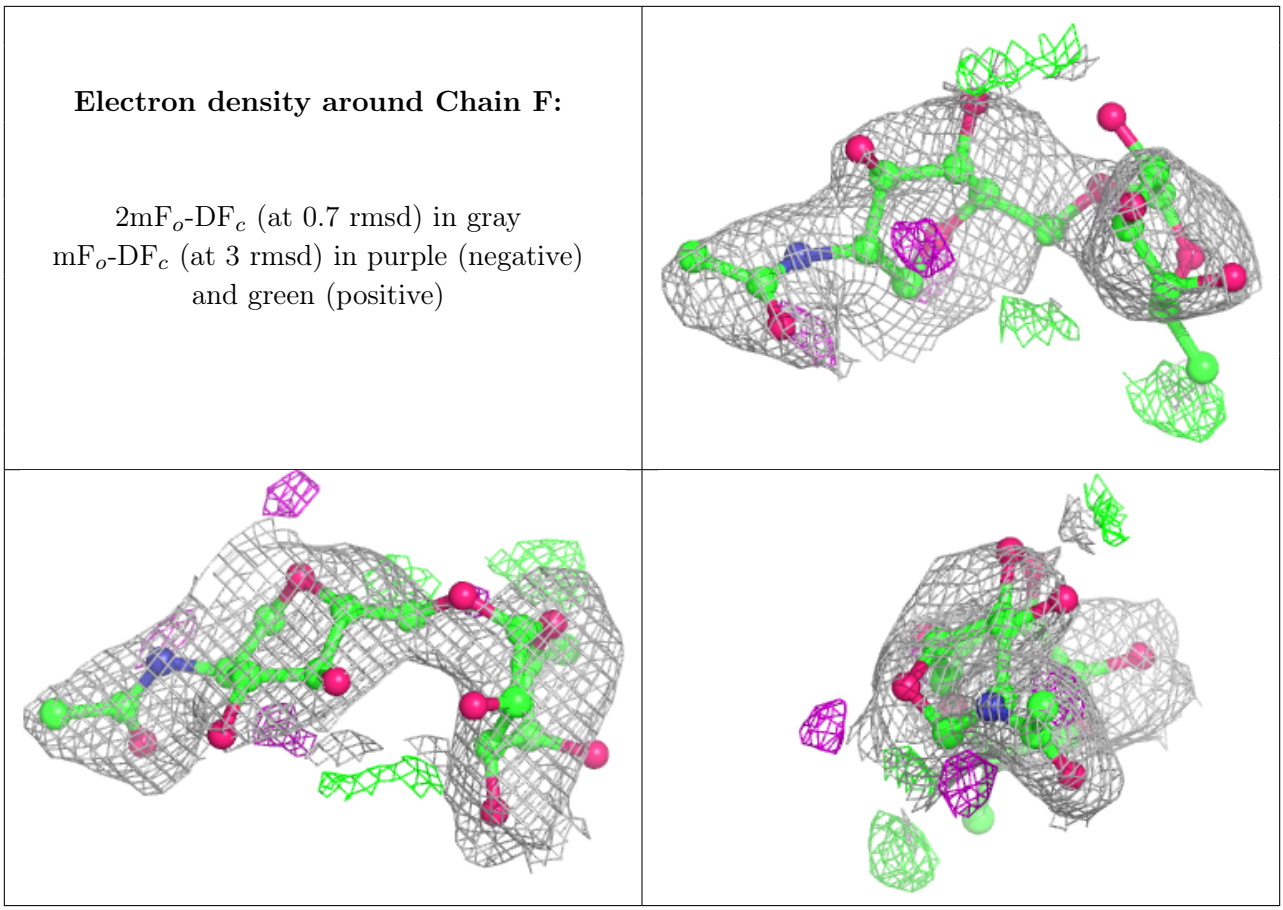






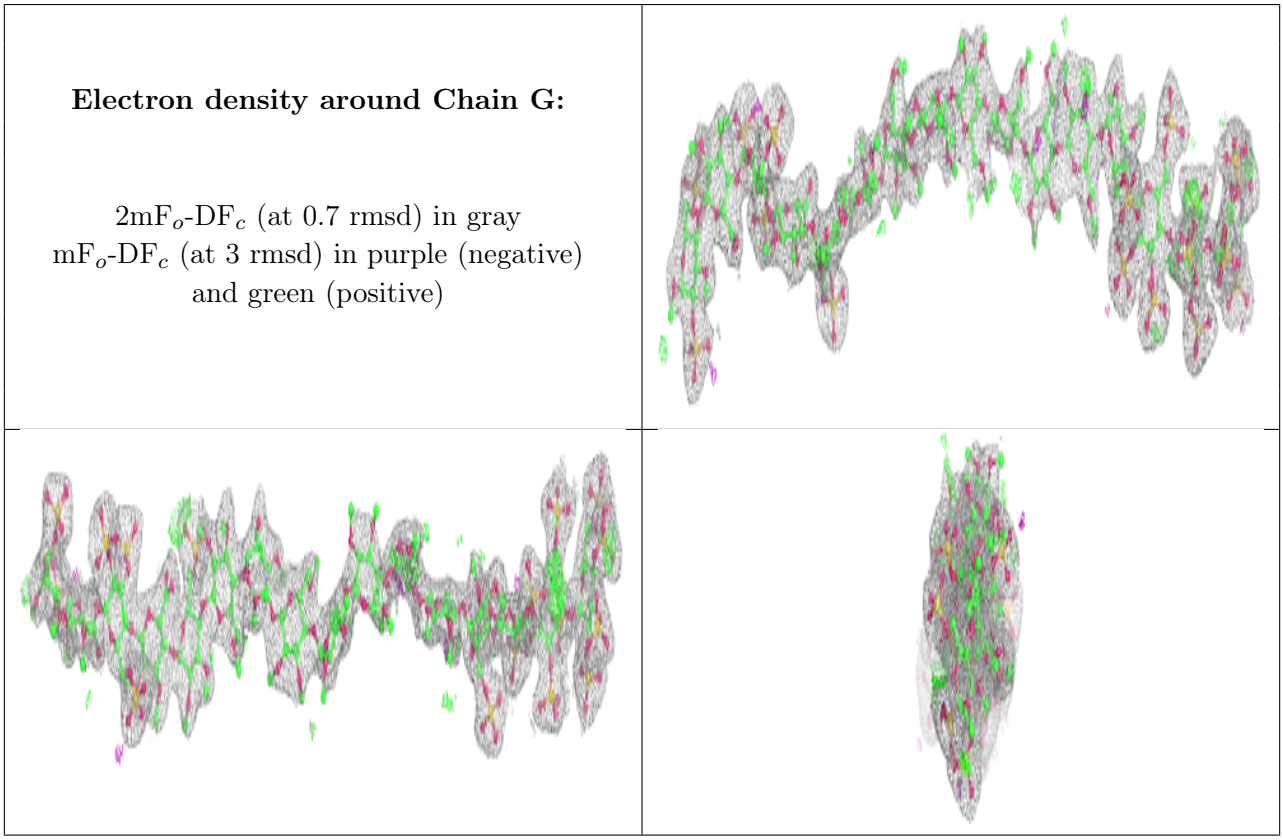
Electron density around Chain F:

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



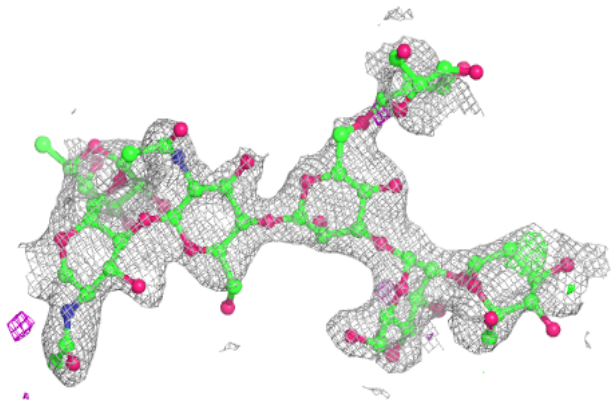
Electron density around Chain G:

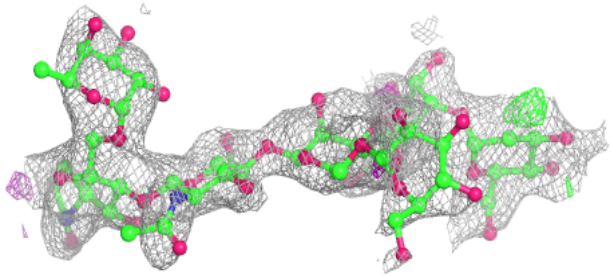
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

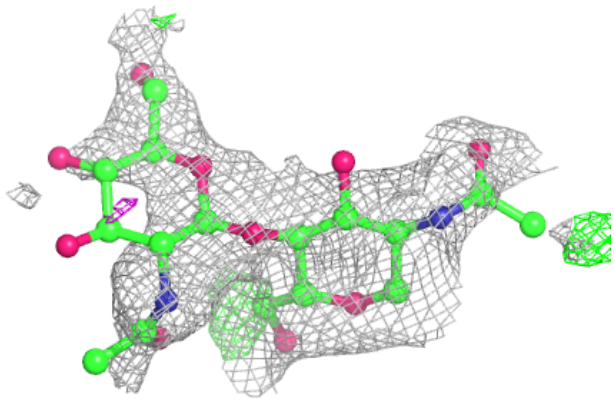
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

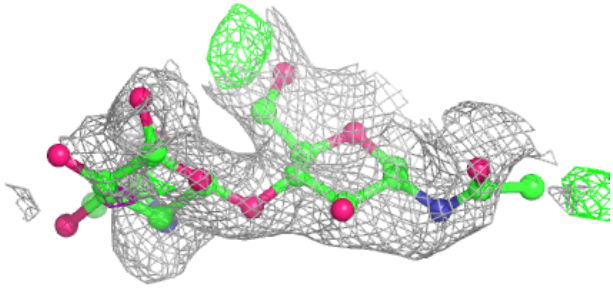


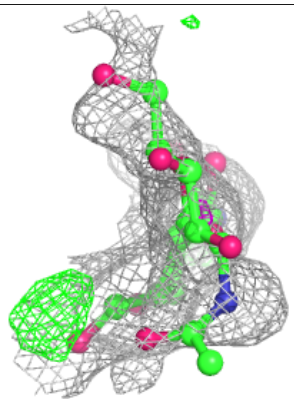


Electron density around Chain J:

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







6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GOL	B	1101	6/6	0.73	0.35	49,55,57,60	0
8	GOL	I	1112	6/6	0.78	0.27	80,81,81,82	0
8	GOL	B	1103	6/6	0.80	0.20	63,65,65,66	0
8	GOL	D	1110	6/6	0.81	0.23	72,75,76,77	0
8	GOL	B	1105	6/6	0.84	0.25	95,95,95,95	0
8	GOL	A	1108	6/6	0.85	0.26	73,76,77,78	0
8	GOL	B	1109	6/6	0.86	0.17	62,62,64,64	0
8	GOL	D	1111	6/6	0.88	0.26	63,64,64,66	0
8	GOL	D	1106	6/6	0.88	0.13	66,67,67,68	0
8	GOL	A	1102	6/6	0.89	0.27	54,57,58,60	0
9	SO4	B	2003	5/5	0.89	0.21	85,86,87,88	0
10	NAG	I	801	14/15	0.89	0.21	66,68,73,74	0
9	SO4	B	2001	5/5	0.94	0.12	85,85,86,87	0
8	GOL	B	1104	6/6	0.95	0.13	30,35,37,46	0
8	GOL	D	1107	6/6	0.95	0.13	32,41,44,45	0
9	SO4	B	2002	5/5	0.96	0.12	89,89,90,91	0
9	SO4	B	2006	5/5	0.97	0.19	56,56,58,59	0
9	SO4	I	2005	5/5	0.98	0.09	63,63,64,64	0
9	SO4	D	2004	5/5	0.98	0.10	61,63,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.