Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 07:30 PM BST

PDB ID	:	4A2M
Title	:	Structure of the periplasmic domain of the heparin and heparan sulphate sensing hybrid two component system BT4663 in apo and ligand bound forms
Authors	:	Lowe, E.C.; Basle, A.; Czjzek, M.; Firbank, S.J.; Bolam, D.N.
Deposited on	:	2011-09-27
Resolution	:	3.40 Å(reported)

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

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

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

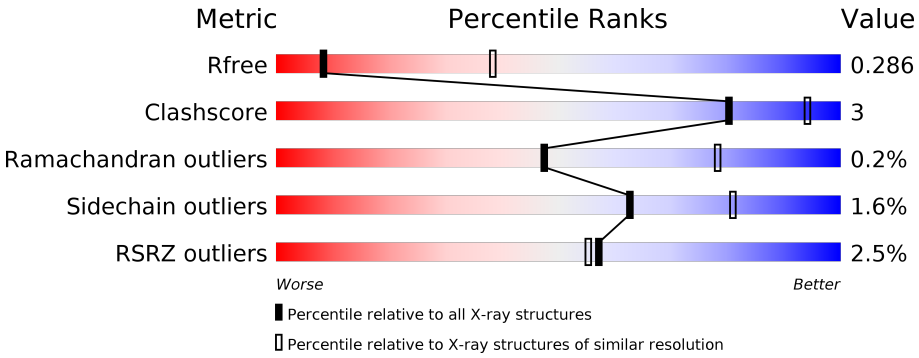
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	795	2% 85% 8% 7%
1	B	795	2% 85% 9% 6%
1	C	795	3% 85% 8% 7%
1	D	795	3% 85% 9% 6%
2	E	2	100%
2	F	2	100%

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Mol	Chain	Length	Quality of chain
2	G	2	100%
2	H	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NGS	F	1	X	-	-	-
2	NGS	G	1	X	-	-	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23370 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 TWO-COMPONENT SYSTEM SENSOR HISTIDINE KINASE/RESPONSE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	741	Total	C	N	O	S	0	0	0
			5791	3684	956	1139	12			
1	B	750	Total	C	N	O	S	0	0	0
			5893	3741	983	1157	12			
1	C	743	Total	C	N	O	S	0	0	0
			5794	3683	960	1139	12			
1	D	745	Total	C	N	O	S	0	0	0
			5772	3671	951	1138	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	788	LEU	-	expression tag	UNP Q89YR8
A	789	GLU	-	expression tag	UNP Q89YR8
A	790	HIS	-	expression tag	UNP Q89YR8
A	791	HIS	-	expression tag	UNP Q89YR8
A	792	HIS	-	expression tag	UNP Q89YR8
A	793	HIS	-	expression tag	UNP Q89YR8
A	794	HIS	-	expression tag	UNP Q89YR8
A	795	HIS	-	expression tag	UNP Q89YR8
B	788	LEU	-	expression tag	UNP Q89YR8
B	789	GLU	-	expression tag	UNP Q89YR8
B	790	HIS	-	expression tag	UNP Q89YR8
B	791	HIS	-	expression tag	UNP Q89YR8
B	792	HIS	-	expression tag	UNP Q89YR8
B	793	HIS	-	expression tag	UNP Q89YR8
B	794	HIS	-	expression tag	UNP Q89YR8
B	795	HIS	-	expression tag	UNP Q89YR8
C	788	LEU	-	expression tag	UNP Q89YR8
C	789	GLU	-	expression tag	UNP Q89YR8
C	790	HIS	-	expression tag	UNP Q89YR8
C	791	HIS	-	expression tag	UNP Q89YR8

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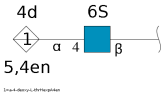
Chain	Residue	Modelled	Actual	Comment	Reference
C	792	HIS	-	expression tag	UNP Q89YR8
C	793	HIS	-	expression tag	UNP Q89YR8
C	794	HIS	-	expression tag	UNP Q89YR8
C	795	HIS	-	expression tag	UNP Q89YR8
D	788	LEU	-	expression tag	UNP Q89YR8
D	789	GLU	-	expression tag	UNP Q89YR8
D	790	HIS	-	expression tag	UNP Q89YR8
D	791	HIS	-	expression tag	UNP Q89YR8
D	792	HIS	-	expression tag	UNP Q89YR8
D	793	HIS	-	expression tag	UNP Q89YR8
D	794	HIS	-	expression tag	UNP Q89YR8
D	795	HIS	-	expression tag	UNP Q89YR8

- Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1 -4)-2-acetamido-2-deoxy-6-O-sulfo-beta-D-glucopyranose.



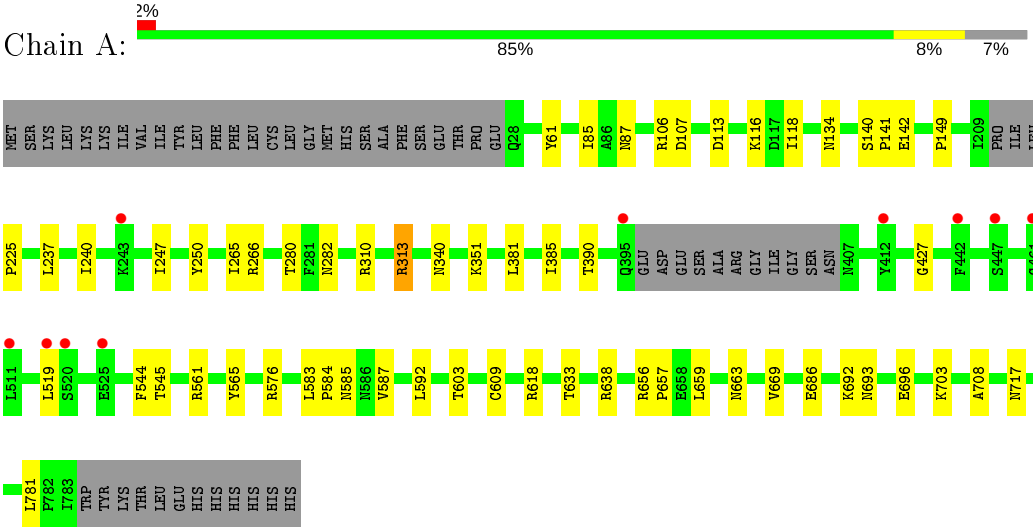
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	S	0	0	0
			30	14	1	14	1			
2	F	2	Total	C	N	O	S	0	0	0
			30	14	1	14	1			
2	G	2	Total	C	N	O	S	0	0	0
			30	14	1	14	1			
2	H	2	Total	C	N	O	S	0	0	0
			30	14	1	14	1			

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.

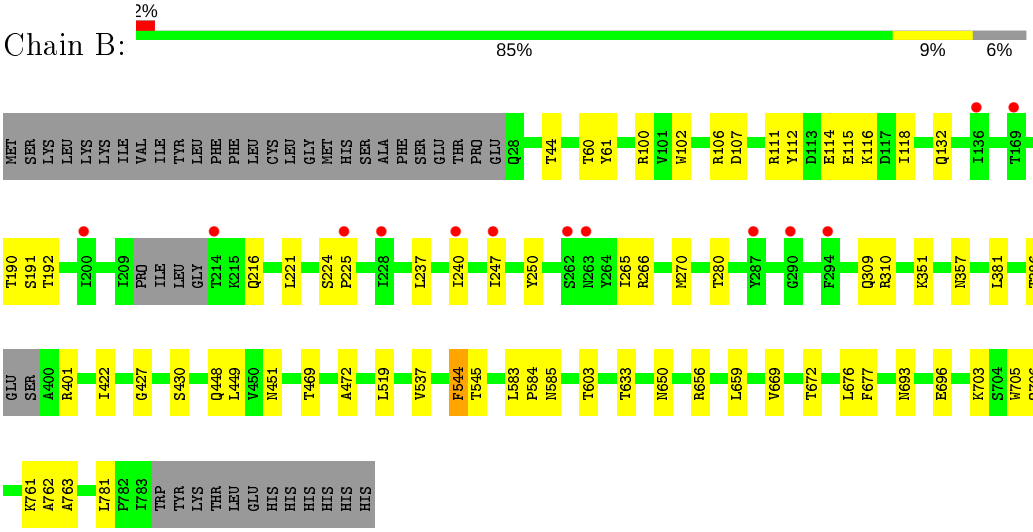
• Molecule 1: TWO-COMPONENT SYSTEM SENSOR HISTIDINE KINASE/RESPONSE

Chain A:



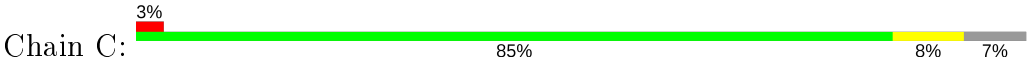
• Molecule 1: TWO-COMPONENT SYSTEM SENSOR HISTIDINE KINASE/RESPONSE

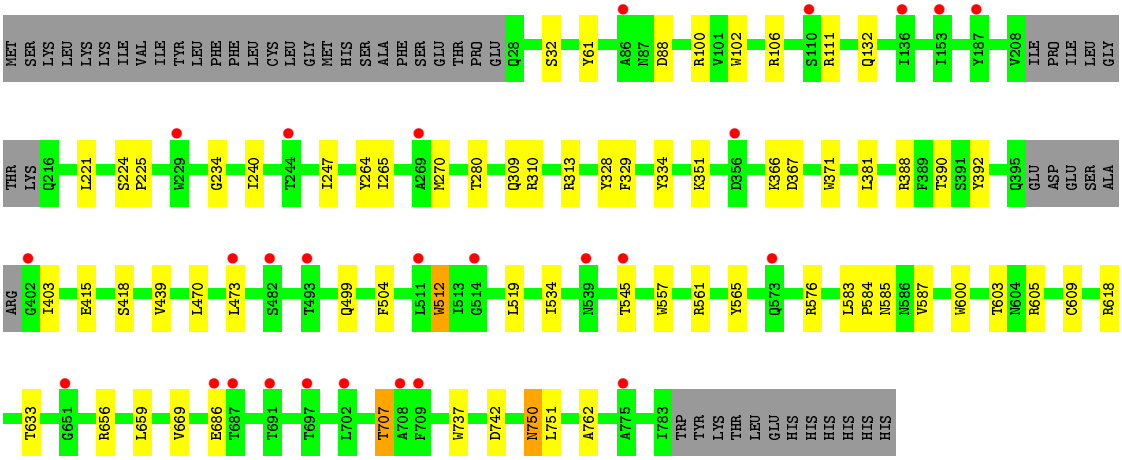
Chain B:



• Molecule 1: TWO-COMPONENT SYSTEM SENSOR HISTIDINE KINASE/RESPONSE

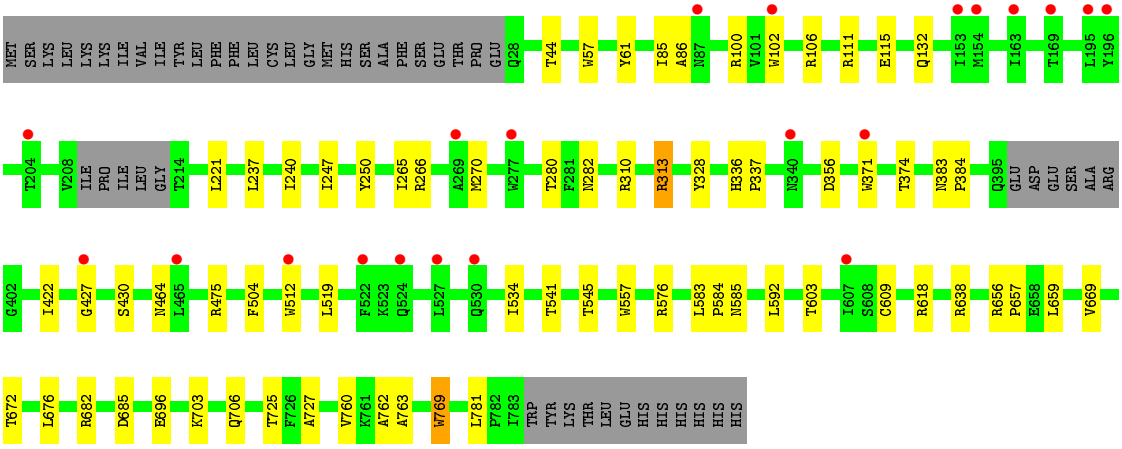
Chain C:





• Molecule 1: TWO-COMPONENT SYSTEM SENSOR HISTIDINE KINASE/RESPONSE

Chain D:



• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-beta-D-glucopyranose

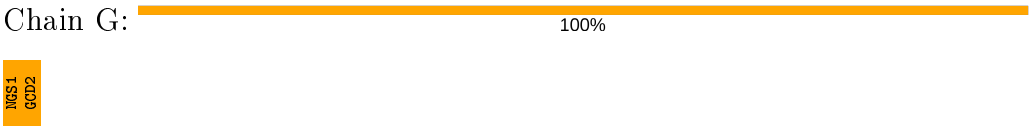
Chain E:

• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-beta-D-glucopyranose

Chain F:

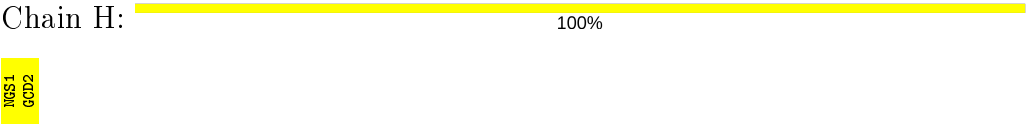
• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-beta-D-glucopyranose

Chain G:



• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-beta-D-glucopyranose

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.12Å 80.83Å 228.94Å 90.00° 93.96° 90.00°	Depositor
Resolution (Å)	55.73 – 3.40 55.73 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (55.73-3.40) 97.6 (55.73-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.268 , 0.286 0.267 , 0.286	Depositor DCC
R_{free} test set	2544 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å^2)	58.9	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	23370	wwPDB-VP
Average B, all atoms (Å^2)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: GCD, NGS

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	0.43	0/5926	0.46	0/8076
1	B	0.43	2/6028 (0.0%)	0.47	0/8205
1	C	0.43	6/5929 (0.1%)	0.46	0/8081
1	D	0.43	5/5907 (0.1%)	0.46	0/8060
All	All	0.43	13/23790 (0.1%)	0.46	0/32422

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	371	TRP	CD2-CE2	5.11	1.47	1.41
1	D	557	TRP	CD2-CE2	5.08	1.47	1.41
1	D	102	TRP	CD2-CE2	5.05	1.47	1.41
1	C	102	TRP	CD2-CE2	5.05	1.47	1.41
1	C	512	TRP	CD2-CE2	5.04	1.47	1.41
1	D	57	TRP	CD2-CE2	5.04	1.47	1.41
1	C	600	TRP	CD2-CE2	5.04	1.47	1.41
1	B	102	TRP	CD2-CE2	5.03	1.47	1.41
1	C	737	TRP	CD2-CE2	5.03	1.47	1.41
1	C	371	TRP	CD2-CE2	5.03	1.47	1.41
1	C	557	TRP	CD2-CE2	5.01	1.47	1.41
1	B	705	TRP	CD2-CE2	5.00	1.47	1.41
1	D	769	TRP	CD2-CE2	5.00	1.47	1.41

There are no bond angle outliers.

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	5791	0	5420	30	0
1	B	5893	0	5554	31	0
1	C	5794	0	5419	29	0
1	D	5772	0	5349	33	0
2	E	30	0	14	0	0
2	F	30	0	14	0	0
2	G	30	0	14	2	0
2	H	30	0	14	0	0
All	All	23370	0	21798	123	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 3.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:707:THR:HG22	1:C:750:ASN:HA	1.72	0.72
1:C:470:LEU:HD22	1:C:499:GLN:HE21	1.62	0.62
1:A:265:ILE:HG12	1:A:280:THR:HG22	1.84	0.59
1:C:609:CYS:HB3	1:C:618:ARG:HB3	1.84	0.59
1:D:609:CYS:HB3	1:D:618:ARG:HB3	1.85	0.59
1:A:609:CYS:HB3	1:A:618:ARG:HB3	1.85	0.59
1:B:448:GLN:HA	1:B:448:GLN:HE21	1.68	0.58
1:D:100:ARG:HG2	1:D:111:ARG:HH21	1.69	0.56
1:B:583:LEU:HD12	1:B:584:PRO:HD2	1.87	0.55
1:C:240:ILE:HG12	1:C:247:ILE:HG22	1.88	0.55
1:B:265:ILE:HG12	1:B:280:THR:HG22	1.89	0.55
1:B:585:ASN:HB3	1:B:603:THR:HB	1.87	0.54
1:D:669:VAL:HG22	1:D:762:ALA:HB2	1.89	0.54
1:B:237:LEU:HB3	1:B:250:TYR:HB2	1.90	0.54
1:D:237:LEU:HB3	1:D:250:TYR:HB2	1.90	0.54
1:D:240:ILE:HG12	1:D:247:ILE:HG22	1.90	0.54
1:C:585:ASN:HB3	1:C:603:THR:HB	1.89	0.53
1:C:403:ILE:HG22	1:C:439:VAL:HG21	1.90	0.53
1:D:583:LEU:HD12	1:D:584:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:725:THR:HB	1:D:763:ALA:HB3	1.90	0.53
1:A:87:ASN:HD22	1:A:106:ARG:HB3	1.73	0.53
1:B:422:ILE:HB	1:B:430:SER:HB2	1.91	0.52
1:D:585:ASN:HB3	1:D:603:THR:HB	1.91	0.52
1:C:100:ARG:HG2	1:C:111:ARG:HH21	1.75	0.52
1:B:240:ILE:HG12	1:B:247:ILE:HG22	1.91	0.51
1:D:265:ILE:HG12	1:D:280:THR:HG22	1.92	0.51
1:B:656:ARG:HG2	1:B:659:LEU:HD13	1.93	0.51
1:B:656:ARG:HB3	1:B:659:LEU:HB2	1.92	0.51
1:A:140:SER:C	1:A:142:GLU:H	2.12	0.51
1:B:221:LEU:HD21	1:B:270:MET:HG2	1.93	0.51
1:B:725:THR:HB	1:B:763:ALA:HB3	1.93	0.50
1:C:265:ILE:HG12	1:C:280:THR:HG22	1.92	0.50
1:C:669:VAL:HG22	1:C:762:ALA:HB2	1.92	0.50
1:C:221:LEU:HD21	1:C:270:MET:HG2	1.92	0.50
1:C:313:ARG:HD2	1:C:328:TYR:HD2	1.76	0.50
1:A:282:ASN:HA	1:A:310:ARG:HG2	1.93	0.50
1:A:703:LYS:HA	1:A:781:LEU:HD12	1.94	0.50
1:C:584:PRO:HB2	1:C:605:ARG:HB3	1.94	0.50
1:C:392:TYR:HB3	1:C:403:ILE:HG21	1.94	0.49
1:A:266:ARG:HD3	1:A:313:ARG:HE	1.77	0.49
1:A:585:ASN:HB3	1:A:603:THR:HB	1.93	0.49
1:C:656:ARG:HG2	1:C:659:LEU:HD13	1.94	0.49
1:D:519:LEU:HD13	1:D:545:THR:HG21	1.94	0.49
1:A:134:ASN:HD21	1:A:149:PRO:HG3	1.78	0.49
2:G:1:NGS:C8	2:G:1:NGS:H1	2.43	0.49
1:B:703:LYS:HA	1:B:781:LEU:HD12	1.94	0.48
2:G:1:NGS:O3	2:G:2:GCD:C1	2.61	0.48
1:C:656:ARG:HB3	1:C:659:LEU:HB2	1.93	0.48
1:C:565:TYR:HB3	1:C:576:ARG:HG2	1.96	0.48
1:B:381:LEU:HB3	1:B:390:THR:HB	1.96	0.48
1:C:519:LEU:HD13	1:C:545:THR:HG21	1.96	0.48
1:A:224:SER:HB2	1:A:225:PRO:HD2	1.96	0.47
1:A:240:ILE:HG12	1:A:247:ILE:HG22	1.96	0.47
1:B:676:LEU:HD21	1:B:706:GLN:HG2	1.96	0.47
1:A:583:LEU:HD12	1:A:584:PRO:HD2	1.97	0.47
1:B:100:ARG:HG2	1:B:111:ARG:HH21	1.80	0.47
1:D:763:ALA:HB2	1:D:769:TRP:CD2	2.50	0.47
1:A:519:LEU:HD13	1:A:545:THR:HG21	1.97	0.46
1:C:366:LYS:HD2	1:C:415:GLU:HG2	1.97	0.46
1:C:583:LEU:HD12	1:C:584:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:656:ARG:HG2	1:D:659:LEU:HD13	1.97	0.46
1:A:656:ARG:HB3	1:A:659:LEU:HB2	1.96	0.46
1:C:561:ARG:HA	1:C:587:VAL:HA	1.98	0.46
1:A:116:LYS:HB2	1:A:118:ILE:HG12	1.97	0.46
1:A:656:ARG:HG2	1:A:659:LEU:HD13	1.97	0.46
1:A:669:VAL:HG22	1:A:762:ALA:HB2	1.97	0.46
1:C:381:LEU:HB3	1:C:390:THR:HB	1.97	0.46
1:D:115:GLU:HA	1:D:696:GLU:HG3	1.96	0.46
1:A:561:ARG:HA	1:A:587:VAL:HA	1.99	0.45
1:D:266:ARG:HG2	1:D:313:ARG:HE	1.80	0.45
1:B:191:SER:HA	1:B:216:GLN:HG3	1.99	0.45
1:B:727:ALA:HB3	1:B:761:LYS:HB2	1.99	0.45
1:D:106:ARG:HA	1:D:132:GLN:HG3	1.99	0.45
1:D:356:ASP:HB3	1:D:374:THR:HB	1.99	0.45
1:A:565:TYR:HB3	1:A:576:ARG:HG2	1.98	0.44
1:A:692:LYS:HB3	1:A:696:GLU:HB2	2.00	0.44
1:B:401:ARG:HH21	1:C:418:SER:HB3	1.82	0.44
1:B:693:ASN:HB3	1:B:696:GLU:HG2	1.99	0.44
1:D:422:ILE:HB	1:D:430:SER:HB2	1.99	0.44
1:D:656:ARG:HB3	1:D:659:LEU:HB2	2.00	0.44
1:C:309:GLN:HG3	1:C:329:PHE:HB2	1.98	0.43
1:B:106:ARG:HA	1:B:132:GLN:HG3	2.00	0.43
1:A:725:THR:HB	1:A:763:ALA:HB3	2.01	0.43
1:A:113:ASP:HB3	1:A:118:ILE:HG13	2.00	0.43
1:A:656:ARG:HA	1:A:657:PRO:HD2	1.91	0.43
1:B:115:GLU:HA	1:B:696:GLU:HG3	2.01	0.43
1:C:224:SER:HB2	1:C:225:PRO:HD2	2.01	0.43
1:C:234:GLY:H	1:C:264:TYR:HA	1.84	0.43
1:D:592:LEU:HD22	1:D:638:ARG:HB2	2.01	0.43
1:A:381:LEU:HB3	1:A:390:THR:HB	2.00	0.43
1:D:221:LEU:HD21	1:D:270:MET:HG2	2.01	0.43
1:D:534:ILE:H	1:D:534:ILE:HG13	1.68	0.43
1:D:676:LEU:HD21	1:D:706:GLN:HG2	2.01	0.43
1:D:703:LYS:HA	1:D:781:LEU:HD12	2.01	0.42
1:C:32:SER:HB2	1:C:334:TYR:HB3	2.00	0.42
1:C:504:PHE:HB3	1:C:512:TRP:HB2	2.00	0.42
1:B:112:TYR:CE2	1:B:114:GLU:HG2	2.54	0.42
1:D:282:ASN:HA	1:D:310:ARG:HG2	2.00	0.42
1:B:116:LYS:HB2	1:B:118:ILE:HG12	2.02	0.42
1:A:266:ARG:HD3	1:A:313:ARG:NE	2.35	0.42
1:D:682:ARG:HB2	1:D:685:ASP:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:THR:OG1	1:B:472:ALA:O	2.37	0.41
1:C:106:ARG:HA	1:C:132:GLN:HG3	2.01	0.41
1:D:727:ALA:O	1:D:760:VAL:HA	2.20	0.41
1:A:663:ASN:HD21	1:A:717:ASN:HD21	1.69	0.41
1:B:669:VAL:HG22	1:B:762:ALA:HB2	2.02	0.41
1:A:237:LEU:HB3	1:A:250:TYR:HB2	2.01	0.41
1:B:357:ASN:HB3	1:B:650:ASN:HA	2.03	0.41
1:B:519:LEU:HD13	1:B:545:THR:HG21	2.02	0.41
1:A:708:ALA:HB2	1:B:677:PHE:CD1	2.55	0.41
1:C:534:ILE:H	1:C:534:ILE:HG13	1.69	0.41
1:D:383:ASN:HA	1:D:384:PRO:HD3	1.90	0.41
1:D:504:PHE:HB3	1:D:512:TRP:HB2	2.01	0.41
1:B:224:SER:HB2	1:B:225:PRO:HD2	2.01	0.41
1:B:44:THR:O	1:B:60:THR:HA	2.21	0.41
1:A:693:ASN:HB3	1:A:696:GLU:HG2	2.03	0.41
1:B:451:ASN:HB3	1:B:469:THR:HB	2.01	0.41
1:D:464:ASN:HD22	1:D:475:ARG:HD3	1.86	0.41
1:A:592:LEU:HD22	1:A:638:ARG:HB2	2.03	0.40
1:D:85:ILE:HG13	1:D:86:ALA:N	2.37	0.40
1:D:44:THR:HG23	1:D:328:TYR:HA	2.04	0.40
1:D:336:HIS:HA	1:D:337:PRO:HD2	1.90	0.40
1:D:656:ARG:HA	1:D:657:PRO:HD2	1.96	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	735/795 (92%)	703 (96%)	30 (4%)	2 (0%)	41	72
1	B	744/795 (94%)	707 (95%)	35 (5%)	2 (0%)	41	72
1	C	737/795 (93%)	701 (95%)	34 (5%)	2 (0%)	41	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	739/795 (93%)	707 (96%)	31 (4%)	1 (0%)	51 82
All	All	2955/3180 (93%)	2818 (95%)	130 (4%)	7 (0%)	47 78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	427	GLY
1	B	427	GLY
1	D	427	GLY
1	C	750	ASN
1	C	751	LEU
1	B	544	PHE
1	A	141	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	620/712 (87%)	610 (98%)	10 (2%)	62 81
1	B	635/712 (89%)	621 (98%)	14 (2%)	52 75
1	C	620/712 (87%)	609 (98%)	11 (2%)	59 79
1	D	611/712 (86%)	606 (99%)	5 (1%)	81 91
All	All	2486/2848 (87%)	2446 (98%)	40 (2%)	62 81

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	TYR
1	A	85	ILE
1	A	107	ASP
1	A	313	ARG
1	A	340	ASN
1	A	351	LYS
1	A	385	ILE

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Mol	Chain	Res	Type
1	A	544	PHE
1	A	633	THR
1	A	686	GLU
1	B	61	TYR
1	B	107	ASP
1	B	190	THR
1	B	192	THR
1	B	266	ARG
1	B	309	GLN
1	B	310	ARG
1	B	351	LYS
1	B	386	THR
1	B	449	LEU
1	B	537	VAL
1	B	544	PHE
1	B	633	THR
1	B	672	THR
1	C	61	TYR
1	C	88	ASP
1	C	310	ARG
1	C	351	LYS
1	C	367	ASP
1	C	388	ARG
1	C	473	LEU
1	C	633	THR
1	C	686	GLU
1	C	707	THR
1	C	742	ASP
1	D	61	TYR
1	D	313	ARG
1	D	541	THR
1	D	576	ARG
1	D	672	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	134	ASN
1	A	395	GLN
1	A	663	ASN
1	B	87	ASN

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Mol	Chain	Res	Type
1	B	132	GLN
1	B	241	ASN
1	B	448	GLN
1	B	663	ASN
1	C	134	ASN
1	C	340	ASN
1	C	499	GLN
1	C	678	ASN
1	D	87	ASN
1	D	132	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NGS	E	1	2	19,19,19	0.55	0	26,28,28	1.61	7 (26%)
2	GCD	E	2	2	7,11,12	2.68	2 (28%)	8,15,17	1.58	1 (12%)
2	NGS	F	1	2	19,19,19	0.66	0	26,28,28	1.44	5 (19%)
2	GCD	F	2	2	7,11,12	2.68	2 (28%)	8,15,17	2.05	2 (25%)
2	NGS	G	1	2	19,19,19	0.81	0	26,28,28	1.69	6 (23%)
2	GCD	G	2	2	7,11,12	2.58	1 (14%)	8,15,17	2.08	2 (25%)
2	NGS	H	1	2	19,19,19	0.57	0	26,28,28	1.51	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GCD	H	2	2	7,11,12	2.59	1 (14%)	8,15,17	1.60	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NGS	E	1	2	-	5/10/30/30	0/1/1/1
2	GCD	E	2	2	-	0/0/17/20	0/1/1/1
2	NGS	F	1	2	1/1/7/8	7/10/30/30	0/1/1/1
2	GCD	F	2	2	-	0/0/17/20	0/1/1/1
2	NGS	G	1	2	1/1/7/8	6/10/30/30	0/1/1/1
2	GCD	G	2	2	-	0/0/17/20	0/1/1/1
2	NGS	H	1	2	-	2/10/30/30	0/1/1/1
2	GCD	H	2	2	-	0/0/17/20	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	GCD	O5-C5	6.53	1.46	1.37
2	E	2	GCD	O5-C5	6.52	1.46	1.37
2	F	2	GCD	O5-C5	6.36	1.46	1.37
2	G	2	GCD	O5-C5	6.27	1.46	1.37
2	F	2	GCD	C4-C5	2.22	1.35	1.32
2	E	2	GCD	C4-C5	2.18	1.35	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2	GCD	O5-C5-C4	-4.93	120.65	124.81
2	G	2	GCD	O5-C5-C4	-4.57	120.95	124.81
2	F	1	NGS	C1-C2-N2	-4.39	105.64	110.73
2	E	2	GCD	O5-C5-C4	-3.97	121.46	124.81
2	G	1	NGS	C2-N2-C7	3.91	132.69	123.18
2	H	1	NGS	C1-C2-N2	-3.83	106.29	110.73
2	G	2	GCD	C1-C2-C3	3.57	114.06	109.67
2	G	1	NGS	O4-C4-C3	3.48	118.40	110.35
2	E	1	NGS	C1-C2-N2	-3.47	106.70	110.73
2	E	1	NGS	O5-C1-C2	-3.22	106.28	109.52
2	H	1	NGS	O5-C1-C2	-3.15	106.35	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	NGS	C8-C7-N2	3.03	121.23	116.10
2	F	1	NGS	O4-C4-C3	2.95	117.18	110.35
2	H	2	GCD	C1-C2-C3	2.93	113.26	109.67
2	E	1	NGS	O4-C4-C5	-2.89	102.12	109.30
2	H	1	NGS	C3-C2-N2	-2.80	105.33	110.62
2	F	2	GCD	C1-C2-C3	2.73	113.02	109.67
2	H	2	GCD	O5-C5-C4	-2.70	122.53	124.81
2	E	1	NGS	C3-C2-N2	-2.63	105.64	110.62
2	H	1	NGS	C4-C3-C2	2.55	114.08	110.34
2	E	1	NGS	C4-C3-C2	2.51	114.02	110.34
2	F	1	NGS	O6-C6-C5	2.50	112.28	107.62
2	G	1	NGS	C1-O5-C5	2.46	118.30	113.66
2	G	1	NGS	O5-C1-C2	2.27	111.80	109.52
2	E	1	NGS	C3-C4-C5	2.21	114.18	110.24
2	F	1	NGS	C3-C2-N2	-2.21	106.45	110.62
2	G	1	NGS	C3-C4-C5	2.19	114.15	110.24
2	E	1	NGS	O5-C5-C4	2.19	113.66	109.69
2	F	1	NGS	O5-C5-C6	2.05	110.80	106.67
2	H	1	NGS	O6-C6-C5	2.03	111.40	107.62
2	H	1	NGS	O5-C5-C4	2.00	113.33	109.69

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	1	NGS	C4
2	F	1	NGS	C4

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NGS	C6-O6-S-O8
2	G	1	NGS	C1-C2-N2-C7
2	G	1	NGS	C4-C5-C6-O6
2	F	1	NGS	C4-C5-C6-O6
2	F	1	NGS	O5-C5-C6-O6
2	F	1	NGS	C6-O6-S-O8
2	E	1	NGS	O7-C7-N2-C2
2	E	1	NGS	C8-C7-N2-C2
2	G	1	NGS	O7-C7-N2-C2
2	G	1	NGS	C8-C7-N2-C2
2	F	1	NGS	O7-C7-N2-C2
2	F	1	NGS	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	H	1	NGS	O7-C7-N2-C2
2	H	1	NGS	C8-C7-N2-C2
2	E	1	NGS	C6-O6-S-O7A
2	F	1	NGS	C6-O6-S-O7A
2	F	1	NGS	C6-O6-S-O9
2	E	1	NGS	C6-O6-S-O9
2	G	1	NGS	O5-C5-C6-O6
2	G	1	NGS	C3-C2-N2-C7

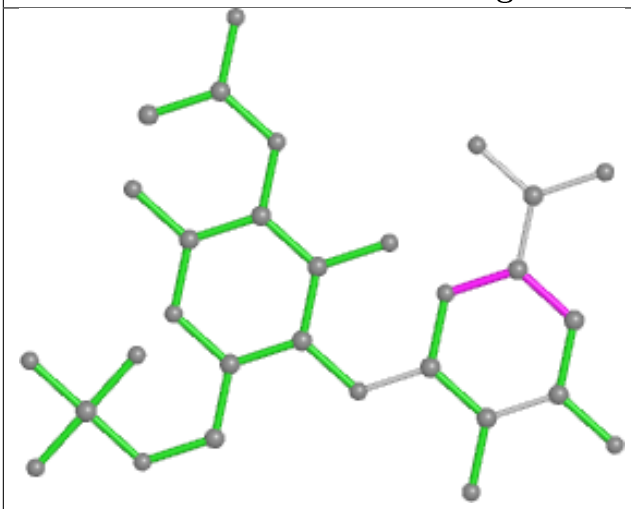
There are no ring outliers.

2 monomers are involved in 2 short contacts:

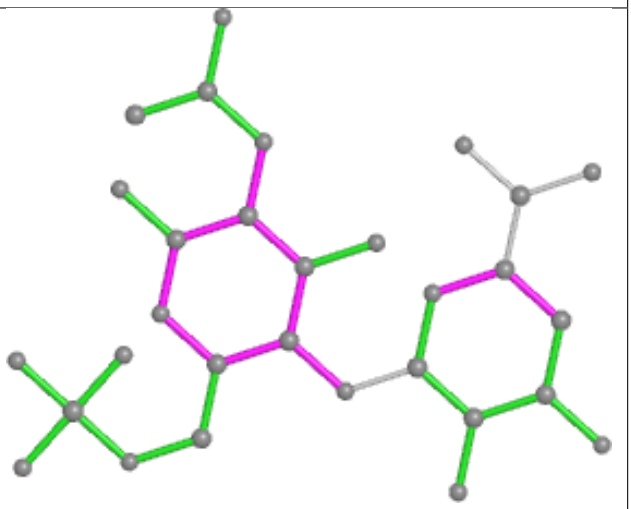
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NGS	2	0
2	G	2	GCD	1	0

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

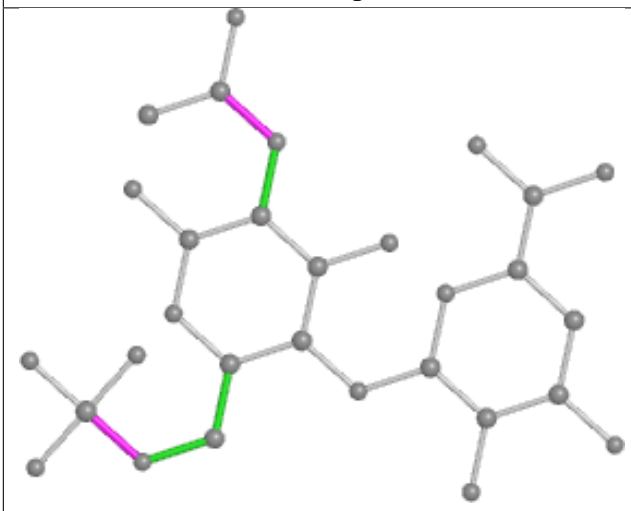
Oligosaccharide Chain E



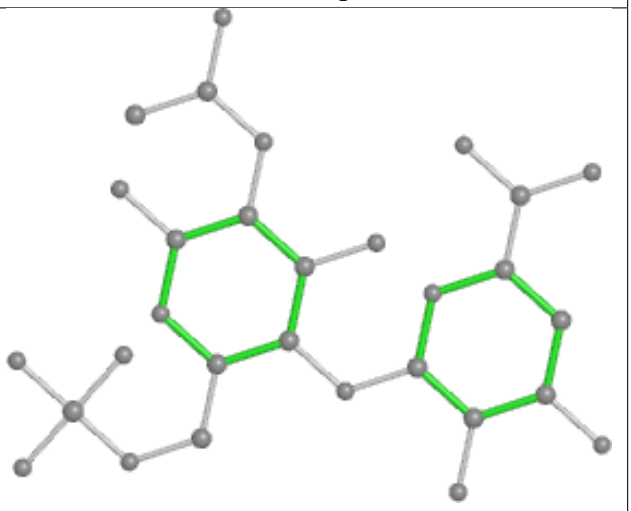
Bond lengths



Bond angles

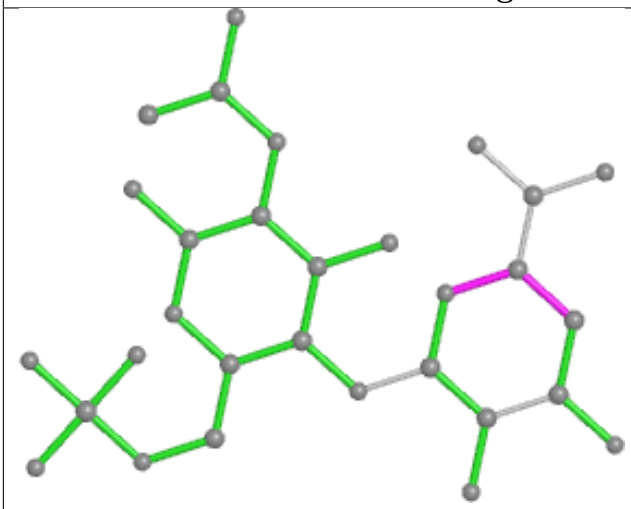


Torsions

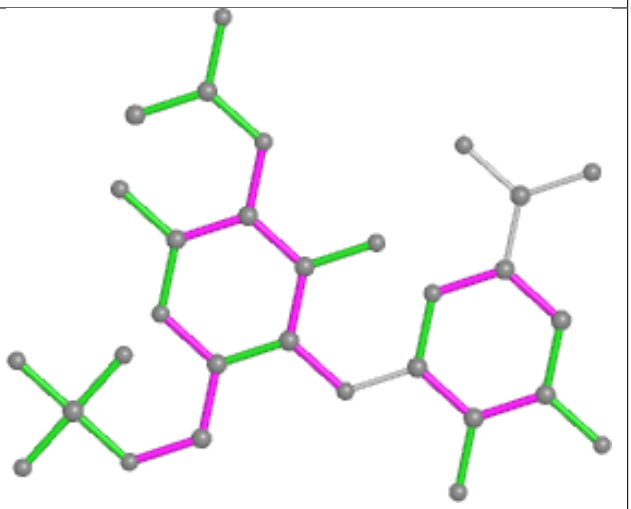


Rings

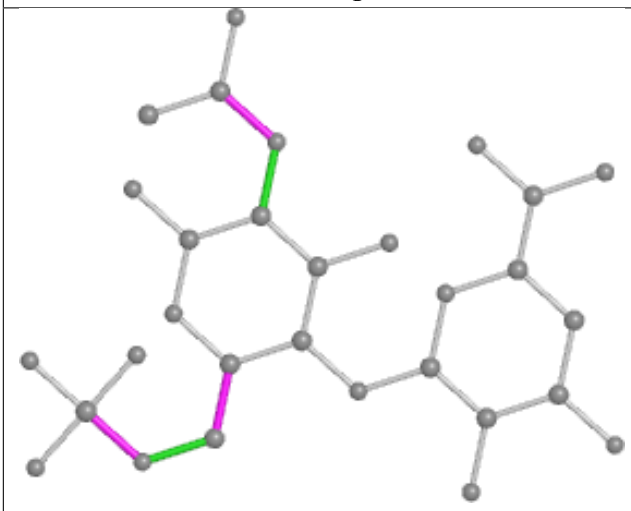
Oligosaccharide Chain F



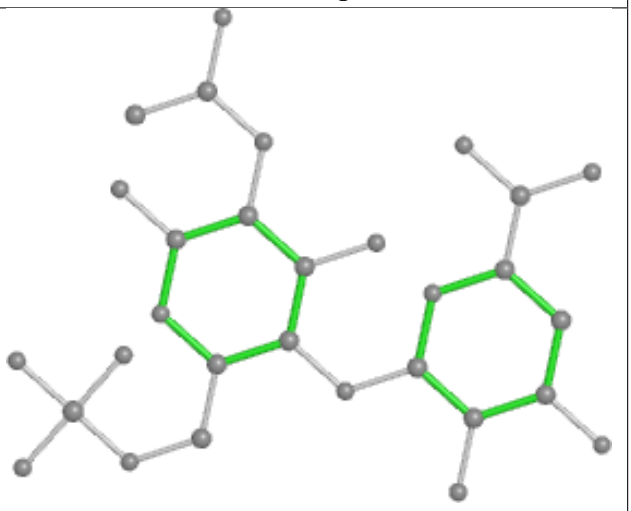
Bond lengths



Bond angles

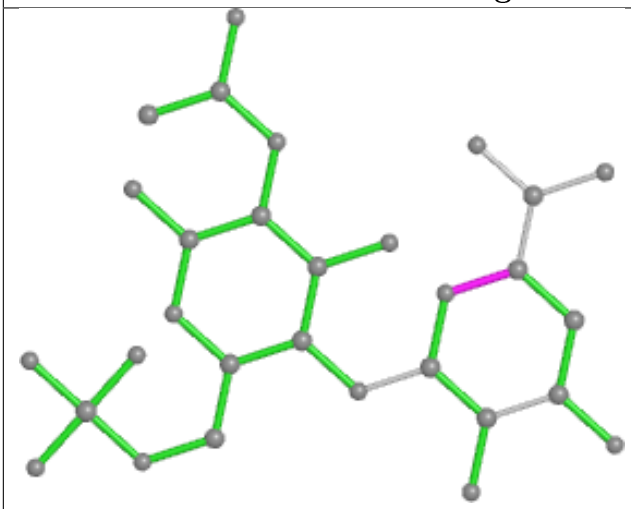


Torsions

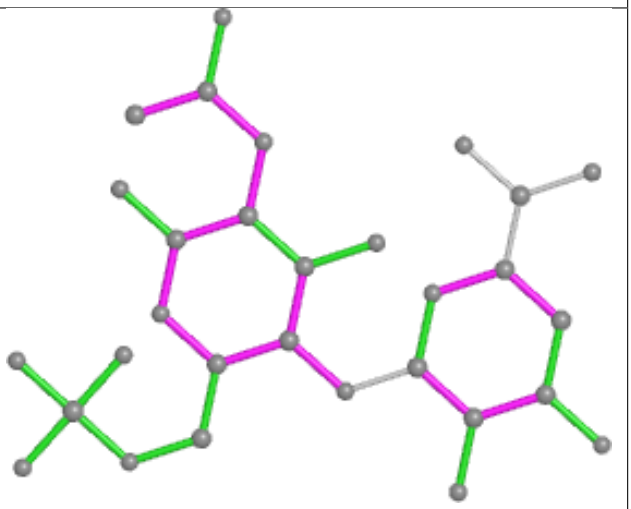


Rings

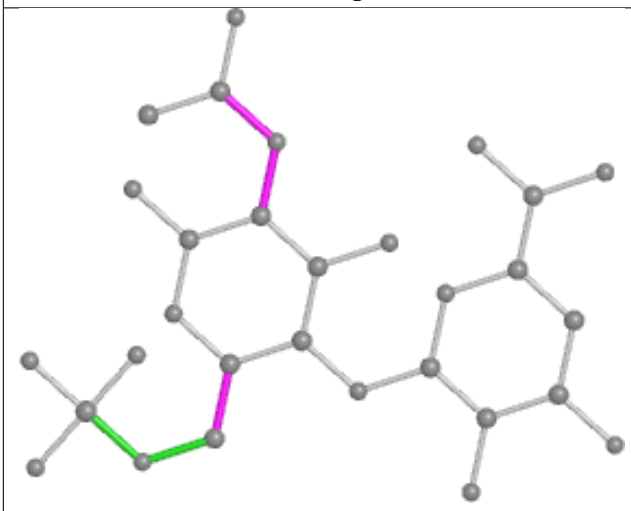
Oligosaccharide Chain G



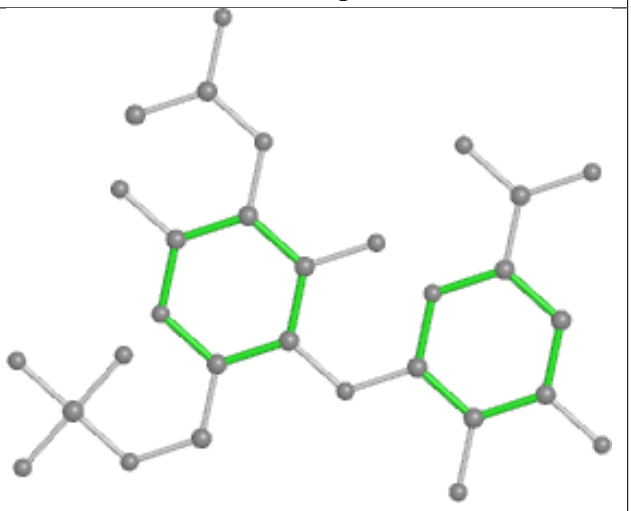
Bond lengths



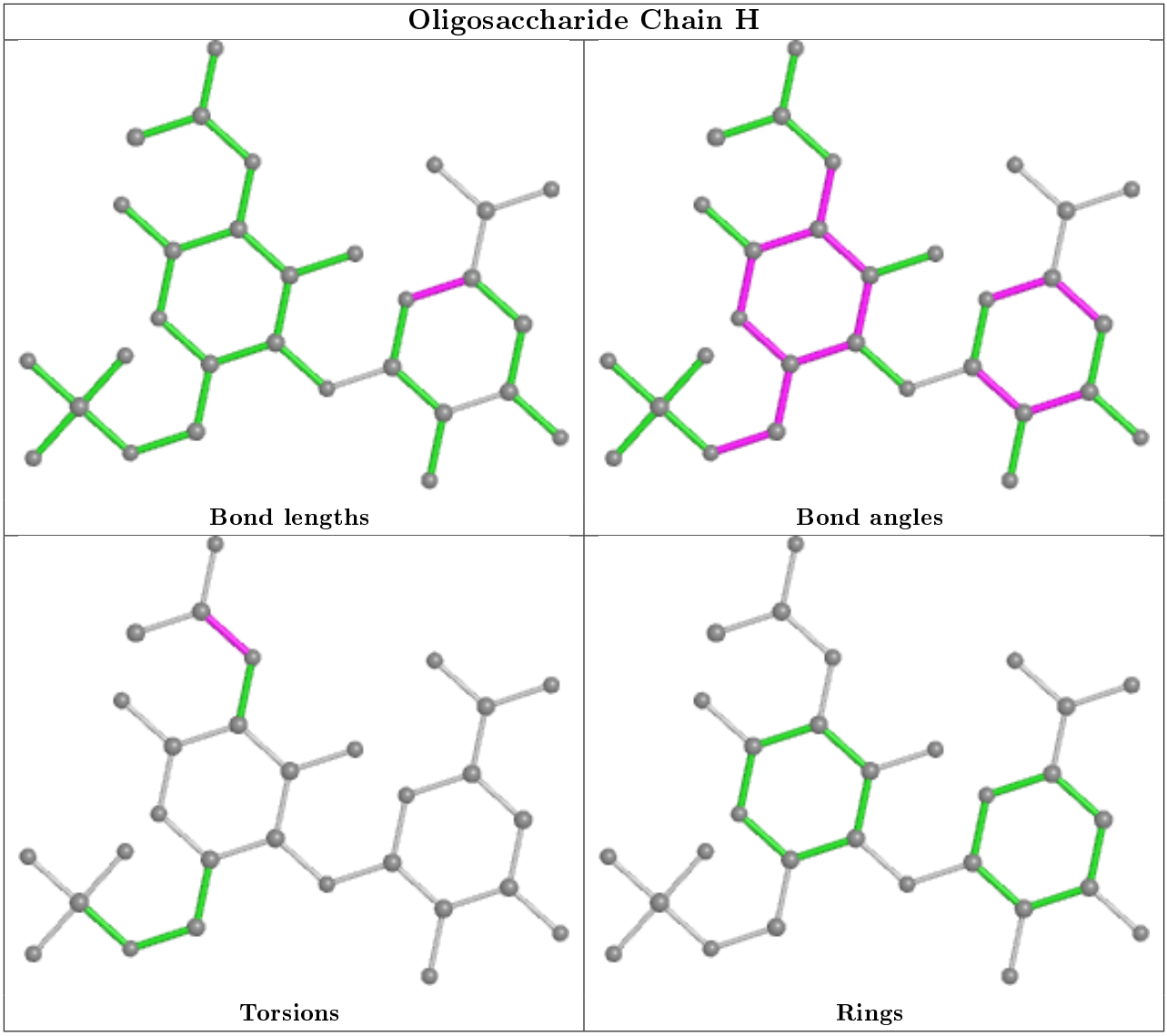
Bond angles



Torsions



Rings



5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	741/795 (93%)	0.21	12 (1%)	72	70	76, 109, 211, 243	0
1	B	750/795 (94%)	0.20	15 (2%)	65	64	72, 105, 208, 257	0
1	C	743/795 (93%)	0.49	27 (3%)	42	42	129, 144, 167, 184	0
1	D	745/795 (93%)	0.43	21 (2%)	53	51	124, 139, 163, 179	0
All	All	2979/3180 (93%)	0.33	75 (2%)	57	55	72, 135, 191, 257	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	102	TRP	5.1
1	D	204	THR	4.5
1	A	520	SER	3.8
1	B	263	ASN	3.7
1	C	709	PHE	3.3
1	D	87	ASN	3.2
1	A	412	TYR	3.2
1	D	154	MET	3.2
1	D	269	ALA	3.2
1	B	176	ALA	3.2
1	C	229	TRP	3.2
1	B	214	THR	3.1
1	B	169	THR	3.1
1	A	519	LEU	3.1
1	A	511	LEU	3.1
1	D	195	LEU	3.0
1	D	524	GLN	3.0
1	C	514	GLY	3.0
1	D	371	TRP	3.0
1	A	461	GLY	3.0
1	C	708	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	187	TYR	2.9
1	D	169	THR	2.9
1	C	511	LEU	2.8
1	C	110	SER	2.8
1	D	340	ASN	2.8
1	C	687	THR	2.7
1	C	539	ASN	2.7
1	C	691	THR	2.7
1	C	702	LEU	2.6
1	B	287	TYR	2.6
1	C	573	GLN	2.6
1	B	225	PRO	2.6
1	A	447	SER	2.6
1	D	522	PHE	2.5
1	D	427	GLY	2.5
1	C	482	SER	2.5
1	C	244	THR	2.5
1	D	512	TRP	2.5
1	C	651	GLY	2.5
1	B	182	GLN	2.4
1	C	136	ILE	2.4
1	D	530	GLN	2.4
1	A	473	LEU	2.4
1	B	228	ILE	2.4
1	B	247	ILE	2.4
1	B	290	GLY	2.4
1	A	243	LYS	2.4
1	A	462	GLU	2.4
1	C	545	THR	2.4
1	D	465	LEU	2.4
1	C	269	ALA	2.3
1	D	196	TYR	2.3
1	B	262	SER	2.3
1	C	686	GLU	2.3
1	A	395	GLN	2.3
1	C	697	THR	2.2
1	C	86	ALA	2.2
1	C	775	ALA	2.1
1	A	525	GLU	2.1
1	B	240	ILE	2.1
1	B	136	ILE	2.1
1	A	442	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	153	ILE	2.1
1	B	294	PHE	2.1
1	C	356	ASP	2.1
1	C	473	LEU	2.1
1	D	163	ILE	2.0
1	C	402	GLY	2.0
1	D	607	ILE	2.0
1	D	527	LEU	2.0
1	C	493	THR	2.0
1	D	277	TRP	2.0
1	B	200	ILE	2.0
1	D	153	ILE	2.0

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

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

6.3 Carbohydrates (i)

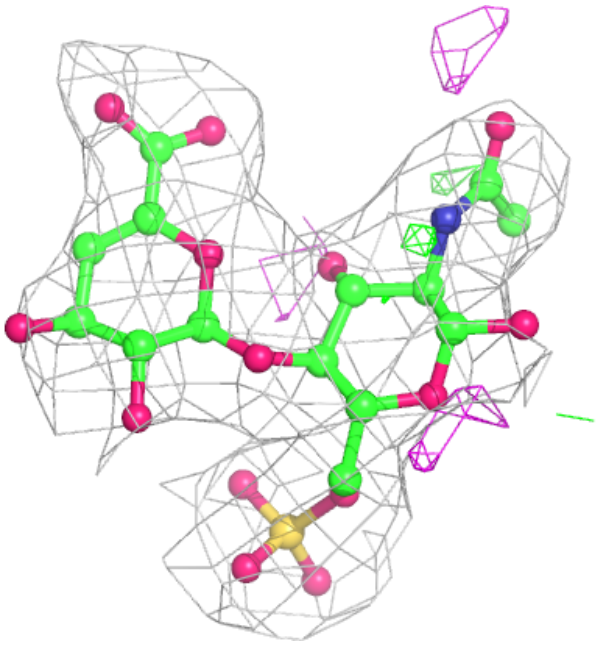
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

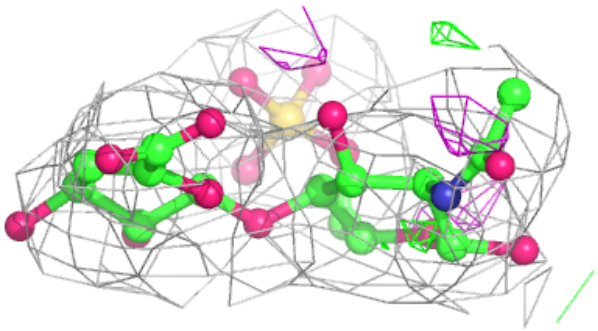
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NGS	F	1	19/19	0.87	0.24	57,57,57,57	0
2	GCD	G	2	11/12	0.87	0.27	57,57,57,57	0
2	GCD	F	2	11/12	0.88	0.32	57,57,57,57	0
2	NGS	H	1	19/19	0.90	0.23	57,57,57,57	0
2	GCD	H	2	11/12	0.91	0.26	57,57,57,57	0
2	NGS	G	1	19/19	0.91	0.20	57,57,57,57	0
2	NGS	E	1	19/19	0.93	0.18	57,57,57,57	0
2	GCD	E	2	11/12	0.95	0.19	57,57,57,57	0

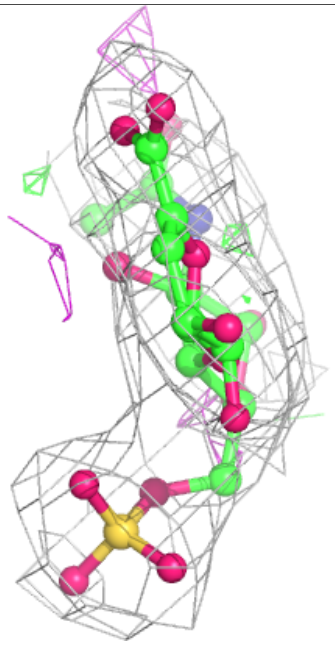
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

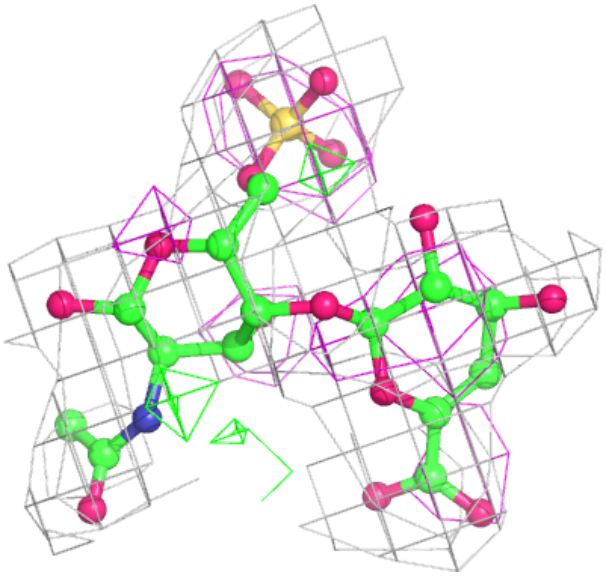


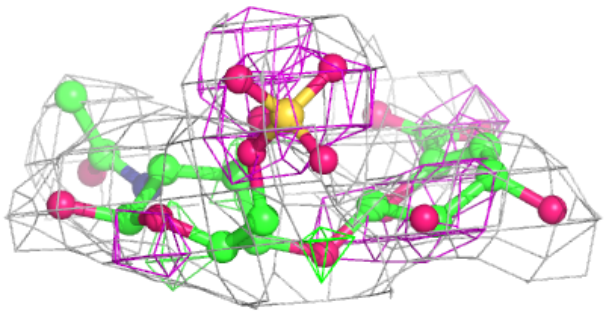


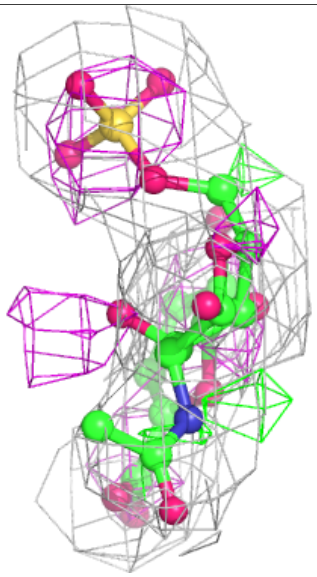


Electron density around Chain F:

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

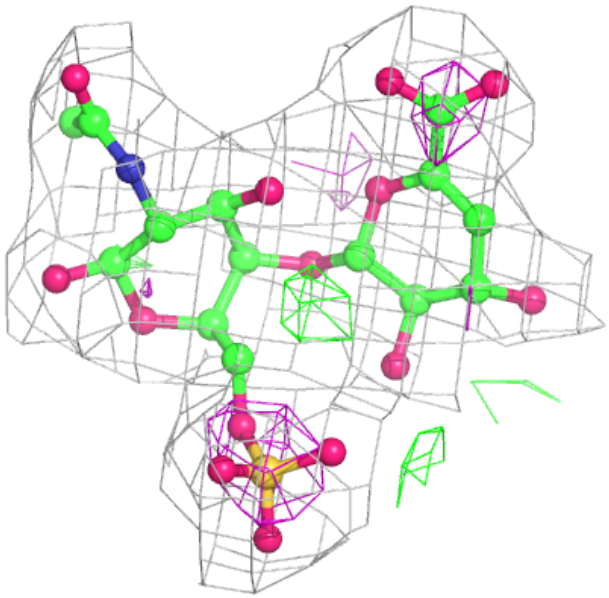


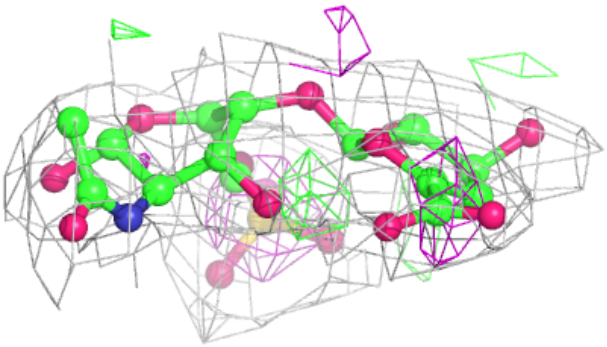




Electron density around Chain G:

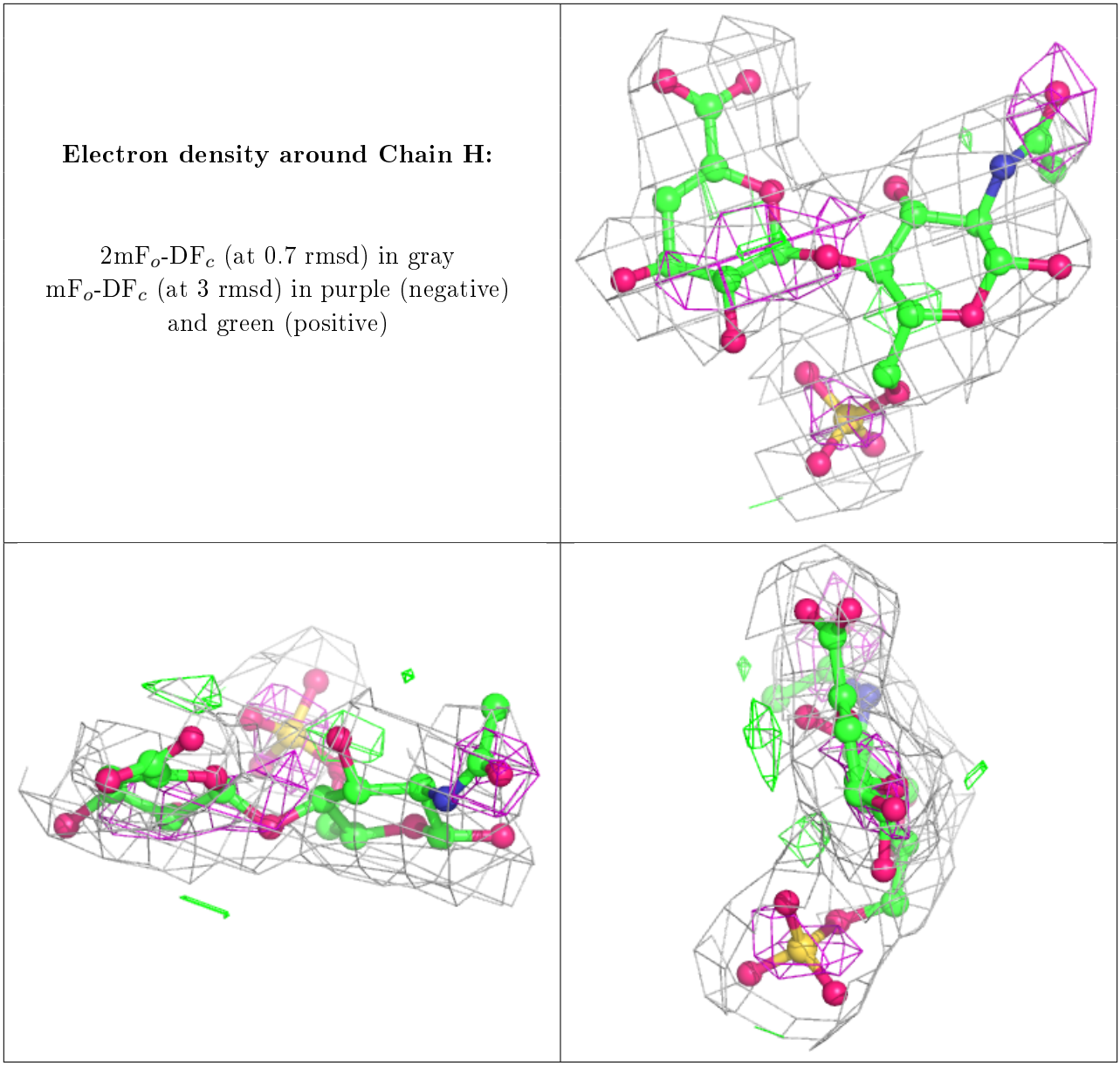
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





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)



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.