Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2024 – 02:04 PM EDT

PDB ID	:	9C3S
Title	:	Crystal structure of DNA N6-Adenine Methyltransferase M.BceJIV from Burkholderia cenocepacia in complex with duplex DNA substrate containing GTATAC as recognition sequence
Authors	:	Kottur, J.; Quintana-Feliciano, R.; Aggarwal, A.K.
Deposited on	:	2024-06-02
Resolution	:	2.16 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

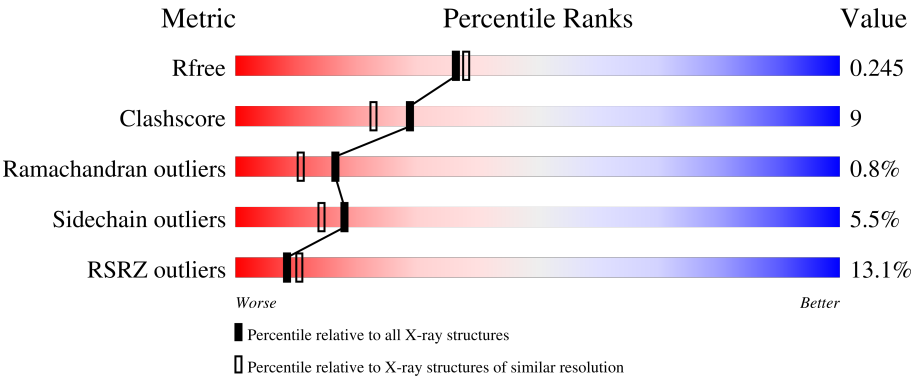
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 2.16 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}	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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	283	2% 74% 13% • 12%
1	B	283	% 73% 15% 12%
1	C	283	28% 67% 16% • 14%
1	D	283	19% 65% 19% • 15%

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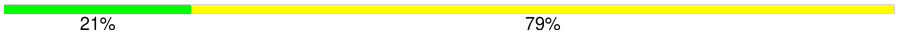
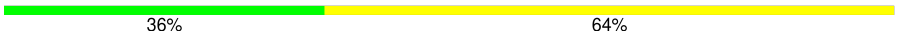
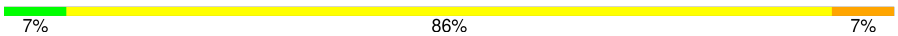
Mol	Chain	Length	Quality of chain
2	E	14	
2	G	14	
2	I	14	
2	K	14	
3	F	14	
3	H	14	
3	J	14	
3	L	14	
4	M	2	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10295 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 Methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	1	0
			1976	1257	346	363	10			
1	B	249	Total	C	N	O	S	0	0	0
			1983	1263	347	363	10			
1	C	244	Total	C	N	O	S	0	1	0
			1806	1137	323	337	9			
1	D	241	Total	C	N	O	S	0	0	0
			1814	1151	317	336	10			

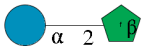
- Molecule 2 is a DNA chain called DNA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	P	0	0	0
			282	137	49	83	13			
2	G	14	Total	C	N	O	P	0	0	0
			281	137	49	82	13			
2	I	14	Total	C	N	O	P	0	0	0
			282	137	49	83	13			
2	K	14	Total	C	N	O	P	0	0	0
			281	137	49	82	13			

- Molecule 3 is a DNA chain called DNA2.

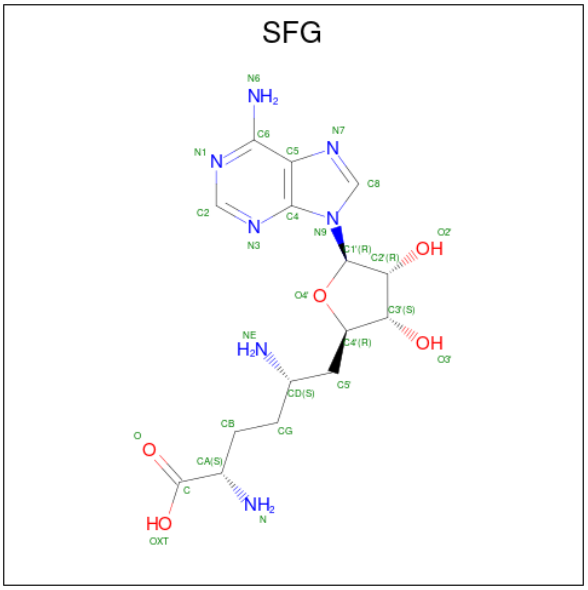
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	14	Total	C	N	O	P	0	0	0
			286	138	54	81	13			
3	H	14	Total	C	N	O	P	0	0	0
			285	138	54	80	13			
3	J	14	Total	C	N	O	P	0	0	0
			286	138	54	81	13			
3	L	14	Total	C	N	O	P	0	0	0
			286	138	54	81	13			

- Molecule 4 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	M	2	Total C O 23 12 11	0	0	0

- Molecule 5 is SINEFUNGIN (three-letter code: SFG) (formula: $C_{15}H_{23}N_7O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 27 15 7 5	0	0
5	B	1	Total C N O 27 15 7 5	0	0
5	C	1	Total C N O 27 15 7 5	0	0
5	D	1	Total C N O 27 15 7 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	66	Total O 66 66	0	0

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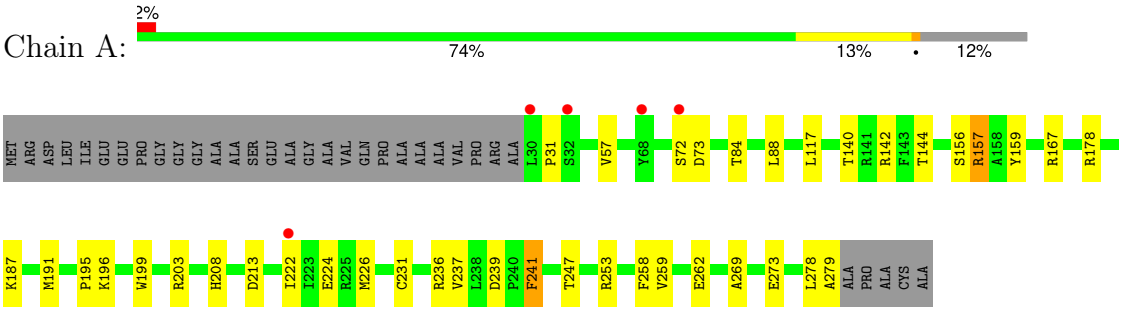
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	77	Total O 77 77	0	0
6	C	35	Total O 35 35	0	0
6	D	33	Total O 33 33	0	0
6	E	16	Total O 16 16	0	0
6	F	11	Total O 11 11	0	0
6	G	19	Total O 19 19	0	0
6	H	22	Total O 22 22	0	0
6	I	6	Total O 6 6	0	0
6	J	15	Total O 15 15	0	0
6	K	5	Total O 5 5	0	0
6	L	11	Total O 11 11	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.

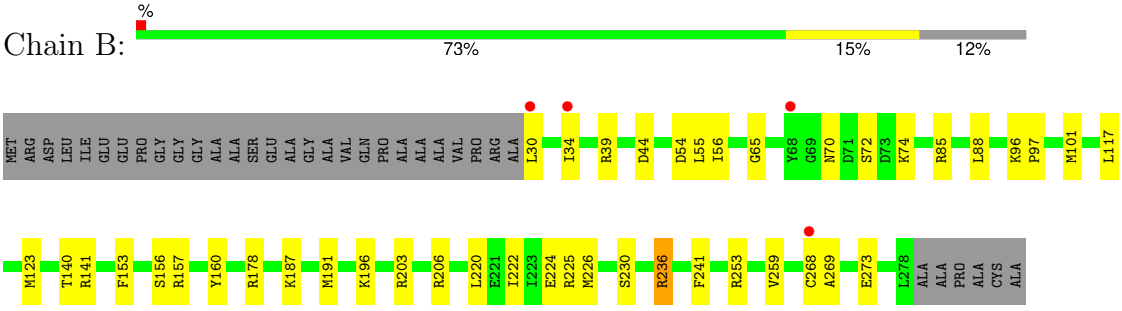
• Molecule 1: Methyltransferase

Chain A:



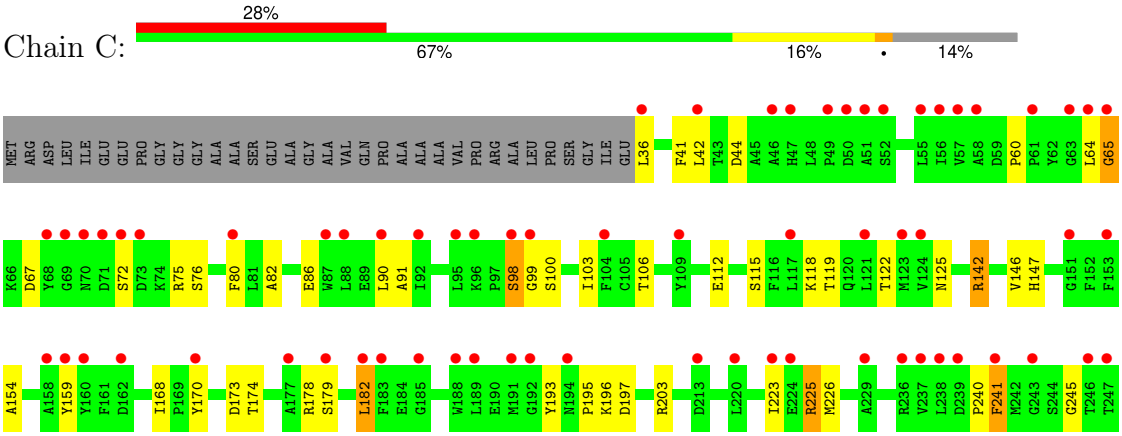
• Molecule 1: Methyltransferase

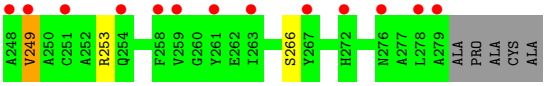
Chain B:



• Molecule 1: Methyltransferase

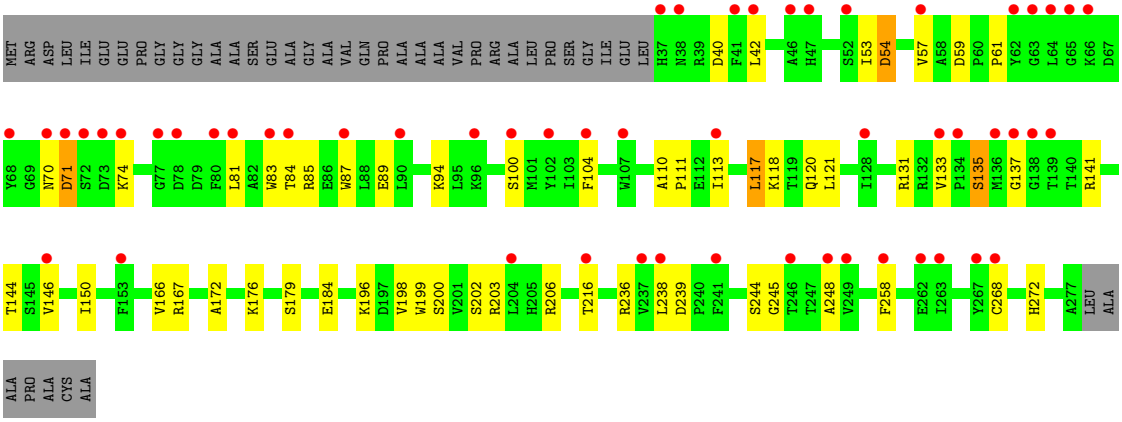
Chain C:





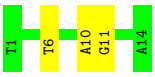
• Molecule 1: Methyltransferase

Chain D:



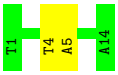
• Molecule 2: DNA1

Chain E:



• Molecule 2: DNA1

Chain G:

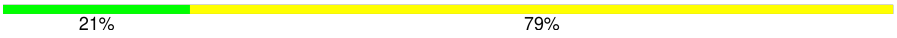


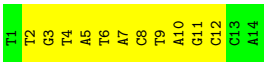
• Molecule 2: DNA1

Chain I:

• Molecule 2: DNA1

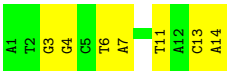
Chain K:





• Molecule 3: DNA2

Chain F:



• Molecule 3: DNA2

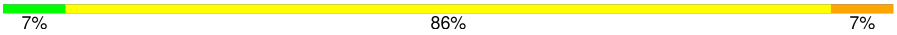
Chain H:

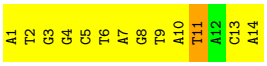
• Molecule 3: DNA2

Chain J:

• Molecule 3: DNA2

Chain L:





• Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain M:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	137.73Å 137.73Å 167.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.76 – 2.16 32.76 – 2.16	Depositor EDS
% Data completeness (in resolution range)	50.6 (32.76-2.16) 50.6 (32.76-2.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.20rc3_4406: ???)	Depositor
R, R_{free}	0.189 , 0.244 0.200 , 0.245	Depositor DCC
R_{free} test set	4159 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.035 for -h,k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10295	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: SFG, GLC, FRU

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	0.37	1/2034 (0.0%)	0.62	0/2764
1	B	0.28	0/2038	0.55	0/2767
1	C	0.44	0/1860	0.67	0/2543
1	D	0.28	0/1866	0.52	0/2545
2	E	0.60	0/315	1.12	1/484 (0.2%)
2	G	0.56	0/314	0.98	0/482
2	I	0.53	0/315	0.98	0/484
2	K	0.60	0/314	0.98	0/482
3	F	0.63	0/321	0.97	0/494
3	H	0.65	0/320	0.94	0/493
3	J	0.58	0/321	0.94	0/494
3	L	0.62	0/321	0.97	2/494 (0.4%)
All	All	0.42	1/10339 (0.0%)	0.72	3/14526 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	SER	CA-CB	-5.19	1.45	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	6	DT	OP2-P-O3'	6.68	119.90	105.20
3	L	11	DT	N3-C4-O4	5.44	123.17	119.90
3	L	11	DT	C5-C4-O4	-5.31	121.18	124.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	225	ARG	Sidechain

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	1976	0	1885	24	0
1	B	1983	0	1918	27	0
1	C	1806	0	1578	31	0
1	D	1814	0	1625	40	0
2	E	282	0	161	2	0
2	G	281	0	159	1	0
2	I	282	0	161	6	0
2	K	281	0	159	10	0
3	F	286	0	160	6	0
3	H	285	0	157	10	0
3	J	286	0	160	3	0
3	L	286	0	160	17	0
4	M	23	0	21	0	0
5	A	27	0	21	2	0
5	B	27	0	21	1	0
5	C	27	0	21	2	0
5	D	27	0	21	4	0
6	A	66	0	0	0	0
6	B	77	0	0	7	0
6	C	35	0	0	5	0
6	D	33	0	0	1	0
6	E	16	0	0	0	0
6	F	11	0	0	0	0
6	G	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	22	0	0	1	0
6	I	6	0	0	0	0
6	J	15	0	0	0	0
6	K	5	0	0	1	0
6	L	11	0	0	1	0
All	All	10295	0	8388	158	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 9.

All (158) 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:249:VAL:O	6:C:401:HOH:O	1.88	0.91
3:L:1:DA:N3	6:L:101:HOH:O	2.13	0.80
1:C:118:LYS:NZ	6:C:402:HOH:O	2.13	0.80
1:A:167:ARG:NH2	3:H:9:DT:OP1	2.17	0.78
1:C:36:LEU:N	6:C:403:HOH:O	2.17	0.78
1:B:70:ASN:OD1	1:B:72:SER:OG	2.00	0.77
3:H:14:DA:N3	6:H:101:HOH:O	2.15	0.77
1:A:187:LYS:HG2	1:A:191:MET:SD	2.26	0.76
1:D:133:VAL:HG11	1:D:203:ARG:HH21	1.52	0.75
1:A:159:TYR:O	1:B:141:ARG:NH2	2.20	0.74
1:D:268:CYS:O	1:D:272:HIS:ND1	2.21	0.74
1:B:30:LEU:N	6:B:402:HOH:O	2.22	0.72
2:E:10:DA:H2"	2:E:11:DG:C8	2.24	0.72
1:C:170:TYR:OH	3:L:11:DT:OP2	2.08	0.69
1:C:159:TYR:O	1:D:141:ARG:NH2	2.26	0.67
1:D:40:ASP:OD1	1:D:42:LEU:N	2.29	0.65
1:D:59:ASP:OD2	5:D:301:SFG:N	2.30	0.65
1:C:122:THR:HG22	1:C:154:ALA:O	1.97	0.64
1:D:167:ARG:NH2	3:J:9:DT:OP1	2.29	0.63
1:C:178:ARG:HD2	3:L:11:DT:H72	1.80	0.63
1:A:88:LEU:HD22	1:A:117:LEU:HD21	1.81	0.62
1:B:54:ASP:OD1	1:B:96:LYS:HD2	2.00	0.62
1:D:53:ILE:HG21	1:D:238:LEU:HB3	1.81	0.61
1:D:133:VAL:HG11	1:D:203:ARG:NH2	2.14	0.61
1:B:236:ARG:NH1	1:B:259:VAL:HG21	2.15	0.61
1:A:157:ARG:N	1:A:157:ARG:HD3	2.16	0.60
1:A:84:THR:HG22	1:A:88:LEU:HD12	1.85	0.58
2:K:5:DA:OP2	6:K:101:HOH:O	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2:DT:H2"	2:K:3:DG:C8	2.40	0.57
1:A:57:VAL:O	1:A:239:ASP:OD1	2.23	0.56
1:D:57:VAL:O	1:D:239:ASP:OD1	2.23	0.56
1:D:244:SER:OG	5:D:301:SFG:O	2.19	0.56
3:H:6:DT:H2'	3:H:7:DA:C8	2.41	0.56
2:G:4:DT:H2"	2:G:5:DA:C8	2.41	0.55
1:B:123:MET:HG3	1:B:153:PHE:CE2	2.41	0.55
1:D:135:SER:OG	2:K:8:DC:OP2	2.20	0.55
3:F:6:DT:H2'	3:F:7:DA:C8	2.41	0.54
1:D:74:LYS:O	6:D:401:HOH:O	2.18	0.54
1:D:131:ARG:O	1:D:133:VAL:N	2.41	0.54
1:D:176:LYS:N	1:D:176:LYS:HD3	2.22	0.53
1:B:88:LEU:HD22	1:B:117:LEU:HD21	1.90	0.53
1:A:241:PHE:HB3	5:A:301:SFG:O4'	2.09	0.53
3:L:5:DC:H2'	3:L:6:DT:C6	2.44	0.53
3:L:6:DT:H2'	3:L:7:DA:C8	2.44	0.53
1:C:64:LEU:HD21	1:C:106:THR:HG21	1.92	0.52
1:C:42:LEU:HA	1:C:90:LEU:HD23	1.91	0.52
1:C:75:ARG:HB3	1:C:80:PHE:HB2	1.92	0.51
1:C:241:PHE:HB3	5:C:301:SFG:O4'	2.10	0.51
3:F:13:DC:H2'	3:F:14:DA:C8	2.44	0.51
3:L:3:DG:H2"	3:L:4:DG:C8	2.44	0.51
2:K:5:DA:H2"	2:K:6:DT:C5	2.45	0.51
1:D:59:ASP:HB3	5:D:301:SFG:HN2	1.75	0.51
3:H:4:DG:H2"	3:H:5:DC:OP2	2.11	0.51
3:H:5:DC:H2'	3:H:6:DT:H71	1.93	0.51
1:C:82:ALA:O	1:C:86:GLU:HG3	2.10	0.50
1:B:269:ALA:O	1:B:273:GLU:HG3	2.12	0.50
1:A:269:ALA:O	1:A:273:GLU:HG3	2.11	0.50
3:L:5:DC:H2"	3:L:6:DT:O5'	2.10	0.50
1:B:253:ARG:NH2	6:B:403:HOH:O	2.35	0.50
2:K:9:DT:H2"	2:K:10:DA:C8	2.46	0.50
1:B:222:ILE:O	1:B:226:MET:HG3	2.12	0.50
3:L:2:DT:H2'	3:L:3:DG:C8	2.47	0.50
1:B:196:LYS:NZ	6:B:406:HOH:O	2.42	0.50
1:C:178:ARG:HD2	3:L:11:DT:C7	2.40	0.50
1:D:94:LYS:HD2	1:D:94:LYS:N	2.26	0.50
1:D:84:THR:HA	1:D:87:TRP:CD1	2.47	0.50
1:A:224:GLU:OE2	1:A:253:ARG:HD2	2.12	0.49
1:B:187:LYS:HG2	1:B:191:MET:SD	2.52	0.49
1:C:174:THR:O	1:C:178:ARG:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:ALA:HB2	1:D:258:PHE:CE2	2.47	0.49
1:B:56:ILE:HB	1:B:101:MET:HG3	1.94	0.49
3:L:6:DT:H4'	3:L:7:DA:OP1	2.13	0.49
3:F:3:DG:H2"	3:F:4:DG:C8	2.48	0.48
3:F:6:DT:H4'	3:F:7:DA:OP1	2.13	0.48
3:J:5:DC:H2"	3:J:6:DT:O5'	2.13	0.48
1:B:39:ARG:HD3	1:B:44:ASP:OD2	2.13	0.48
1:D:40:ASP:OD1	1:D:40:ASP:C	2.51	0.48
1:D:54:ASP:OD1	1:D:236:ARG:N	2.41	0.48
1:B:156:SER:OG	1:B:157:ARG:N	2.47	0.48
1:B:178:ARG:HD3	3:F:11:DT:H71	1.95	0.48
1:C:41:PHE:CZ	1:C:91:ALA:HB2	2.49	0.48
1:D:85:ARG:O	1:D:89:GLU:HG3	2.13	0.48
1:C:253:ARG:HB2	6:C:401:HOH:O	2.13	0.47
1:A:222:ILE:O	1:A:226:MET:HG3	2.14	0.47
3:L:13:DC:H2'	3:L:14:DA:C8	2.49	0.47
1:A:84:THR:HG22	1:A:88:LEU:CD1	2.43	0.47
1:B:236:ARG:NH1	1:B:259:VAL:CG2	2.78	0.47
1:D:166:VAL:O	1:D:166:VAL:CG1	2.62	0.47
3:J:6:DT:H2'	3:J:7:DA:C8	2.50	0.47
3:L:2:DT:H4'	3:L:3:DG:OP1	2.14	0.47
1:A:278:LEU:O	1:A:279:ALA:HB3	2.14	0.46
1:D:239:ASP:HB2	1:D:258:PHE:HE1	1.79	0.46
1:B:241:PHE:HB3	5:B:301:SFG:O4'	2.16	0.46
3:L:8:DG:H2'	3:L:9:DT:C6	2.51	0.46
1:D:59:ASP:CB	5:D:301:SFG:HN2	2.28	0.46
1:D:216:THR:HG21	2:K:7:DA:C4	2.51	0.46
2:K:5:DA:H2"	2:K:6:DT:C7	2.45	0.46
3:L:10:DA:H2"	3:L:11:DT:H71	1.98	0.45
1:C:60:PRO:HG3	1:C:103:ILE:HD11	1.99	0.45
1:D:196:LYS:O	1:D:199:TRP:NE1	2.47	0.45
1:B:225:ARG:NH2	6:B:409:HOH:O	2.49	0.45
1:D:71:ASP:N	1:D:71:ASP:OD1	2.49	0.45
1:B:34:ILE:N	1:B:34:ILE:HD13	2.32	0.45
1:B:206:ARG:NE	6:B:410:HOH:O	2.49	0.45
1:D:245:GLY:O	1:D:248:ALA:HB3	2.18	0.44
2:I:5:DA:H2"	2:I:6:DT:C6	2.53	0.44
3:H:13:DC:H2'	3:H:14:DA:C8	2.52	0.44
1:C:60:PRO:O	2:I:7:DA:N6	2.50	0.44
3:L:2:DT:H2"	3:L:3:DG:O5'	2.17	0.44
1:C:112:GLU:OE2	1:D:118:LYS:HE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:ARG:CB	6:C:401:HOH:O	2.66	0.44
1:D:81:LEU:O	1:D:84:THR:OG1	2.26	0.44
1:B:160:TYR:OH	6:B:401:HOH:O	2.20	0.43
1:C:195:PRO:HB3	1:C:225:ARG:HH11	1.82	0.43
2:I:9:DT:H2"	2:I:10:DA:C8	2.53	0.43
3:H:5:DC:C2'	3:H:6:DT:H71	2.49	0.43
1:A:196:LYS:NZ	3:H:11:DT:OP1	2.45	0.43
1:D:172:ALA:O	1:D:176:LYS:HD3	2.18	0.43
1:A:178:ARG:HD2	3:H:11:DT:H71	2.00	0.43
1:C:223:ILE:HA	1:C:226:MET:HE2	2.00	0.43
1:A:140:THR:O	1:A:140:THR:CG2	2.66	0.43
1:D:61:PRO:HD2	1:D:83:TRP:HH2	1.84	0.43
1:B:220:LEU:HG	1:B:224:GLU:HG3	2.01	0.43
1:D:206:ARG:CB	2:K:5:DA:H4'	2.49	0.43
1:D:104:PHE:CE1	1:D:150:ILE:HD11	2.53	0.43
1:B:96:LYS:HB2	1:B:97:PRO:HD2	2.01	0.43
1:C:72:SER:CB	5:C:301:SFG:H8	2.49	0.42
3:L:6:DT:H2"	3:L:7:DA:O5'	2.19	0.42
1:A:231:CYS:SG	1:A:237:VAL:HG12	2.60	0.42
1:B:55:LEU:HD13	1:B:230:SER:HB2	2.01	0.42
1:C:64:LEU:O	1:C:65:GLY:C	2.56	0.42
1:D:54:ASP:OD1	1:D:54:ASP:N	2.50	0.42
3:H:3:DG:C2'	3:H:4:DG:C8	3.03	0.42
3:L:3:DG:H2"	3:L:4:DG:H8	1.84	0.42
1:D:146:VAL:HG22	1:D:146:VAL:O	2.19	0.42
1:C:170:TYR:CE1	1:C:193:TYR:CD1	3.08	0.42
1:B:225:ARG:NH1	6:B:407:HOH:O	2.44	0.42
1:A:199:TRP:CE3	1:A:222:ILE:HG23	2.55	0.42
2:K:11:DG:H2'	2:K:12:DC:C6	2.55	0.42
1:C:142:ARG:NH1	2:I:10:DA:OP1	2.53	0.41
1:A:195:PRO:C	1:A:196:LYS:HG3	2.41	0.41
1:A:236:ARG:HE	1:A:259:VAL:CG2	2.34	0.41
1:C:245:GLY:O	1:C:249:VAL:HG13	2.20	0.41
1:D:110:ALA:N	1:D:111:PRO:HD2	2.36	0.41
1:A:142:ARG:HD2	2:E:10:DA:OP1	2.19	0.41
1:A:239:ASP:HB2	1:A:258:PHE:HE1	1.86	0.41
1:B:65:GLY:HA2	1:B:74:LYS:HD3	2.03	0.41
1:C:115:SER:O	1:C:119:THR:HG23	2.21	0.41
1:A:208:HIS:CD2	3:F:13:DC:H5"	2.55	0.41
1:C:147:HIS:HB3	1:D:198:VAL:CG2	2.50	0.41
1:A:262:GLU:OE2	5:A:301:SFG:O2'	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5:DA:C2'	2:I:6:DT:H72	2.50	0.41
2:K:3:DG:H1'	2:K:4:DT:H5'	2.02	0.41
1:C:182:LEU:HD13	1:C:182:LEU:C	2.42	0.40
1:D:113:ILE:O	1:D:117:LEU:HD22	2.20	0.40
1:C:41:PHE:CG	1:C:240:PRO:HB3	2.56	0.40
2:I:5:DA:H2"	2:I:6:DT:C7	2.52	0.40
1:D:53:ILE:HG21	1:D:238:LEU:CB	2.51	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	249/283 (88%)	231 (93%)	17 (7%)	1 (0%)	30 27
1	B	247/283 (87%)	236 (96%)	11 (4%)	0	100 100
1	C	243/283 (86%)	221 (91%)	17 (7%)	5 (2%)	5 2
1	D	239/283 (84%)	218 (91%)	19 (8%)	2 (1%)	16 11
All	All	978/1132 (86%)	906 (93%)	64 (6%)	8 (1%)	16 11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	PRO
1	C	65	GLY
1	C	99	GLY
1	D	71	ASP
1	D	137	GLY
1	C	67	ASP
1	C	98	SER
1	C	146	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	204/231 (88%)	196 (96%)	8 (4%)	27 26
1	B	209/231 (90%)	204 (98%)	5 (2%)	44 47
1	C	164/231 (71%)	148 (90%)	16 (10%)	6 3
1	D	170/231 (74%)	158 (93%)	12 (7%)	12 8
All	All	747/924 (81%)	706 (94%)	41 (6%)	18 14

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ASP
1	A	144	THR
1	A	156	SER
1	A	157	ARG
1	A	203	ARG
1	A	213	ASP
1	A	241	PHE
1	A	247	THR
1	B	85	ARG
1	B	140	THR
1	B	203	ARG
1	B	236	ARG
1	B	268	CYS
1	C	44	ASP
1	C	76	SER
1	C	98	SER
1	C	100	SER
1	C	125	ASN
1	C	142	ARG
1	C	168	ILE
1	C	173	ASP
1	C	179	SER
1	C	182	LEU
1	C	196	LYS

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Mol	Chain	Res	Type
1	C	197	ASP
1	C	203	ARG
1	C	241	PHE
1	C	249	VAL
1	C	266	SER
1	D	54	ASP
1	D	70	ASN
1	D	100	SER
1	D	117	LEU
1	D	120	GLN
1	D	121	LEU
1	D	135	SER
1	D	144	THR
1	D	179	SER
1	D	184	GLU
1	D	200	SER
1	D	202	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	70	ASN
1	D	120	GLN

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)

2 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	GLC	M	1	4	11,11,12	0.59	0	15,15,17	0.77	0
4	FRU	M	2	4	11,12,12	0.46	0	10,18,18	0.91	1 (10%)

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	GLC	M	1	4	-	2/2/19/22	0/1/1/1
4	FRU	M	2	4	-	3/5/24/24	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	2	FRU	C6-C5-C4	-2.14	110.05	115.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

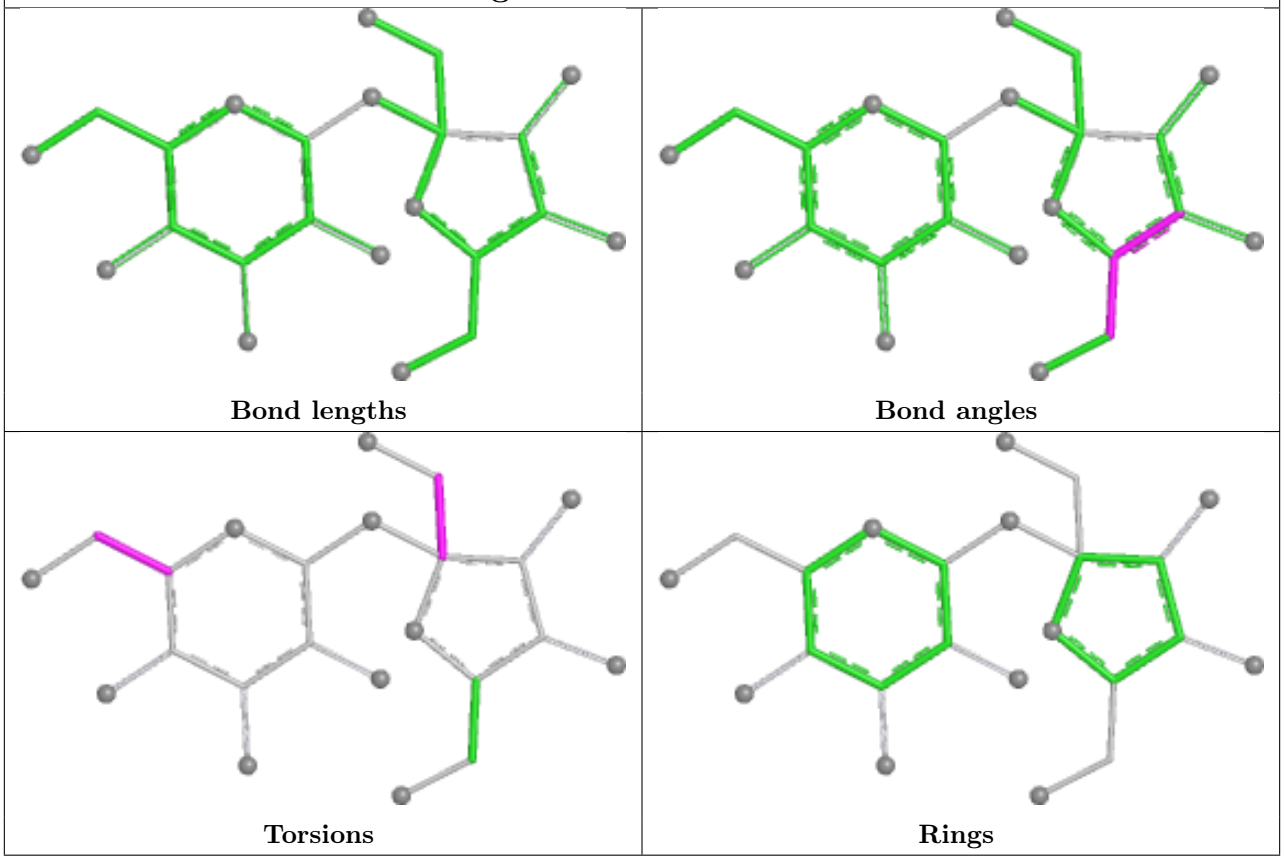
Mol	Chain	Res	Type	Atoms
4	M	2	FRU	O1-C1-C2-C3
4	M	2	FRU	O1-C1-C2-O2
4	M	2	FRU	O1-C1-C2-O5
4	M	1	GLC	O5-C5-C6-O6
4	M	1	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 M



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SFG	C	301	-	24,29,29	3.82	7 (29%)	20,42,42	2.61	4 (20%)
5	SFG	D	301	-	24,29,29	3.85	6 (25%)	20,42,42	2.63	4 (20%)
5	SFG	A	301	-	24,29,29	3.76	6 (25%)	20,42,42	2.81	5 (25%)
5	SFG	B	301	-	24,29,29	3.74	7 (29%)	20,42,42	2.71	5 (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
5	SFG	C	301	-	-	4/13/33/33	0/3/3/3
5	SFG	D	301	-	-	5/13/33/33	0/3/3/3
5	SFG	A	301	-	-	2/13/33/33	0/3/3/3
5	SFG	B	301	-	-	1/13/33/33	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	301	SFG	O4'-C1'	16.33	1.62	1.40
5	C	301	SFG	O4'-C1'	16.12	1.62	1.40
5	A	301	SFG	O4'-C1'	15.65	1.61	1.40
5	B	301	SFG	O4'-C1'	15.61	1.61	1.40
5	A	301	SFG	O4'-C4'	-6.59	1.30	1.45
5	B	301	SFG	O4'-C4'	-6.39	1.30	1.45
5	C	301	SFG	O4'-C4'	-6.37	1.30	1.45
5	D	301	SFG	O4'-C4'	-6.29	1.31	1.45
5	A	301	SFG	C6-N6	3.25	1.45	1.34
5	C	301	SFG	C6-N6	3.24	1.45	1.34
5	B	301	SFG	C6-N6	3.21	1.45	1.34
5	D	301	SFG	C6-N6	3.20	1.45	1.34
5	A	301	SFG	O2'-C2'	2.82	1.49	1.43
5	B	301	SFG	O2'-C2'	2.81	1.49	1.43
5	D	301	SFG	O3'-C3'	-2.78	1.36	1.43
5	C	301	SFG	O2'-C2'	2.77	1.49	1.43
5	C	301	SFG	O3'-C3'	-2.77	1.36	1.43
5	A	301	SFG	O3'-C3'	-2.76	1.36	1.43
5	D	301	SFG	O2'-C2'	2.76	1.49	1.43
5	B	301	SFG	O3'-C3'	-2.75	1.36	1.43
5	B	301	SFG	C2-N3	2.34	1.35	1.32
5	D	301	SFG	C2-N3	2.31	1.35	1.32
5	C	301	SFG	C2-N3	2.30	1.35	1.32
5	A	301	SFG	C2-N3	2.21	1.35	1.32
5	C	301	SFG	C5'-C4'	2.03	1.56	1.52
5	B	301	SFG	C5'-C4'	2.02	1.56	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	301	SFG	C5-C6-N6	7.75	132.12	120.31
5	B	301	SFG	C5-C6-N6	7.58	131.86	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	301	SFG	C5-C6-N6	7.53	131.78	120.31
5	C	301	SFG	C5-C6-N6	7.51	131.75	120.31
5	A	301	SFG	N3-C2-N1	-6.44	119.93	128.67
5	B	301	SFG	N3-C2-N1	-6.43	119.94	128.67
5	C	301	SFG	N3-C2-N1	-6.40	119.98	128.67
5	D	301	SFG	N3-C2-N1	-6.36	120.03	128.67
5	A	301	SFG	N6-C6-N1	-4.83	108.00	118.33
5	D	301	SFG	N6-C6-N1	-4.74	108.20	118.33
5	B	301	SFG	N6-C6-N1	-4.72	108.24	118.33
5	C	301	SFG	N6-C6-N1	-4.67	108.36	118.33
5	A	301	SFG	C4'-O4'-C1'	-3.87	106.38	109.92
5	B	301	SFG	C1'-N9-C4	-2.76	121.80	126.64
5	B	301	SFG	C4'-O4'-C1'	-2.70	107.45	109.92
5	A	301	SFG	C1'-N9-C4	-2.43	122.38	126.64
5	D	301	SFG	C1'-N9-C4	-2.43	122.38	126.64
5	C	301	SFG	C1'-N9-C4	-2.20	122.78	126.64

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	301	SFG	C5'-CD-CG-CB
5	A	301	SFG	C-CA-CB-CG
5	D	301	SFG	OXT-C-CA-CB
5	D	301	SFG	NE-CD-CG-CB
5	D	301	SFG	O-C-CA-CB
5	C	301	SFG	O4'-C4'-C5'-CD
5	A	301	SFG	O-C-CA-N
5	B	301	SFG	O-C-CA-N
5	C	301	SFG	C3'-C4'-C5'-CD
5	C	301	SFG	O-C-CA-CB
5	C	301	SFG	OXT-C-CA-CB
5	D	301	SFG	C4'-C5'-CD-NE

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	301	SFG	2	0
5	D	301	SFG	4	0
5	A	301	SFG	2	0

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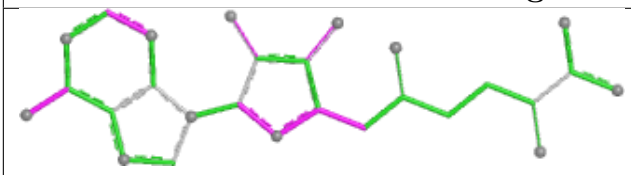
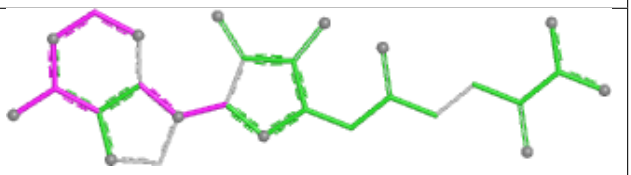
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301	SFG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

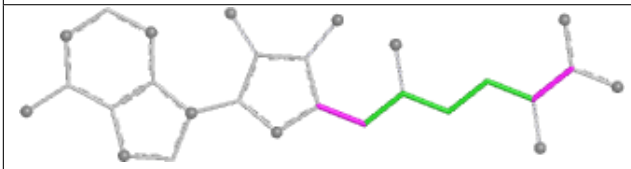
Ligand SFG C 301



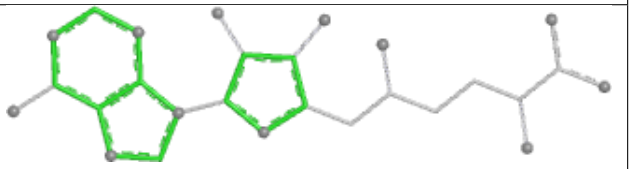
Bond lengths



Bond angles

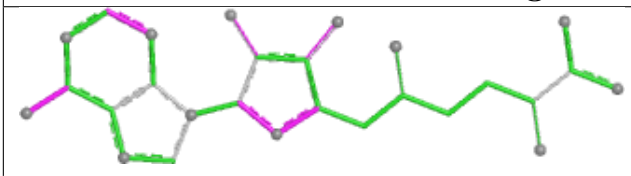


Torsions

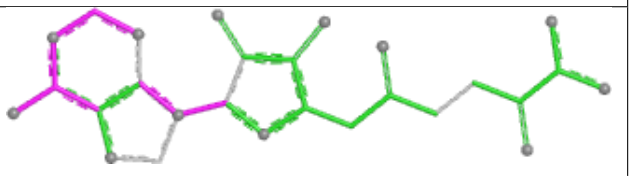


Rings

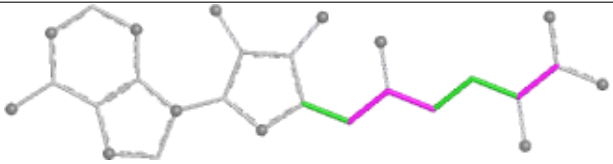
Ligand SFG D 301



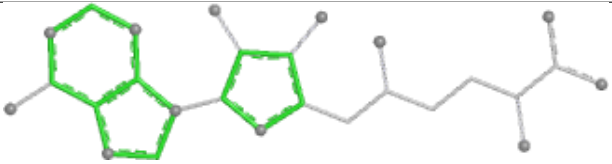
Bond lengths



Bond angles

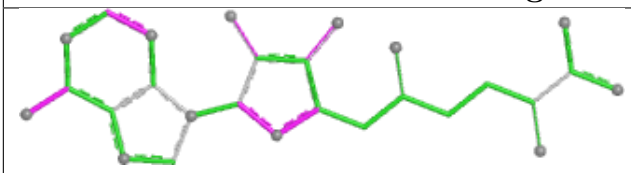


Torsions

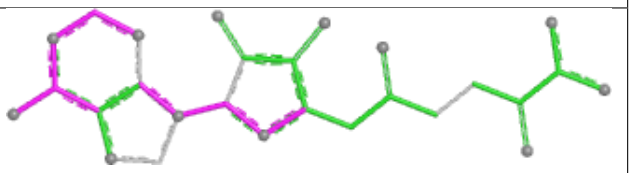


Rings

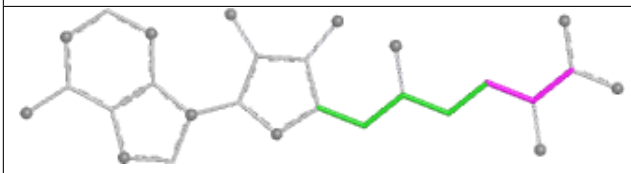
Ligand SFG A 301



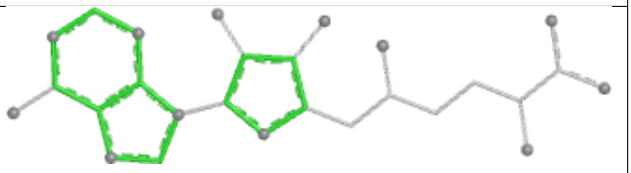
Bond lengths



Bond angles

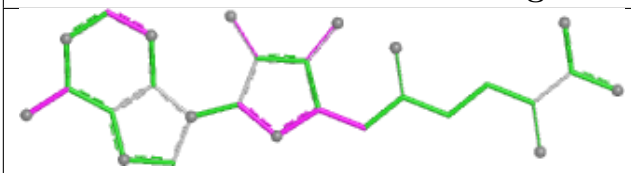


Torsions

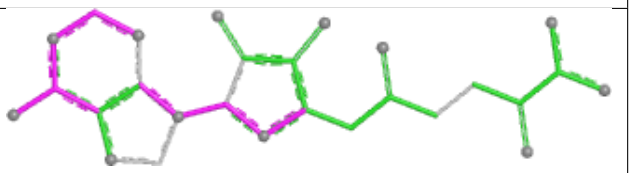


Rings

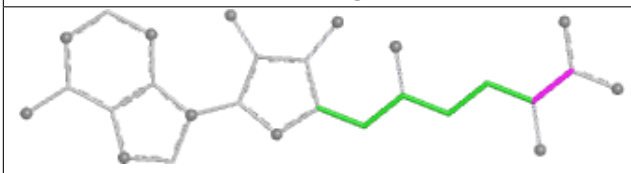
Ligand SFG B 301



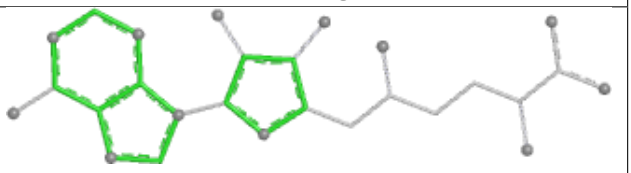
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	250/283 (88%)	0.35	5 (2%) 64 69	12, 38, 64, 80	1 (0%)
1	B	249/283 (87%)	0.19	4 (1%) 70 73	16, 36, 58, 80	0
1	C	244/283 (86%)	1.64	80 (32%) 1 2	25, 68, 85, 100	1 (0%)
1	D	241/283 (85%)	1.39	55 (22%) 2 4	36, 64, 87, 111	0
2	E	14/14 (100%)	-0.21	0 100 100	26, 42, 61, 67	0
2	G	14/14 (100%)	-0.20	0 100 100	29, 38, 66, 67	0
2	I	14/14 (100%)	0.39	0 100 100	52, 55, 69, 71	0
2	K	14/14 (100%)	1.03	0 100 100	61, 76, 85, 88	0
3	F	14/14 (100%)	-0.05	0 100 100	28, 43, 75, 75	0
3	H	14/14 (100%)	0.19	0 100 100	28, 45, 71, 74	0
3	J	14/14 (100%)	0.22	0 100 100	43, 50, 66, 69	0
3	L	14/14 (100%)	0.99	0 100 100	60, 72, 79, 79	0
All	All	1096/1244 (88%)	0.82	144 (13%) 8 10	12, 52, 82, 111	2 (0%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	136	MET	6.3
1	D	68	TYR	5.5
1	D	65	GLY	5.3
1	C	68	TYR	5.3
1	D	72	SER	5.2
1	C	189	LEU	5.1
1	C	223	ILE	4.7
1	D	204	LEU	4.4
1	C	158	ALA	4.3
1	A	68	TYR	4.3
1	D	37	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	38	ASN	4.1
1	D	64	LEU	4.1
1	C	246	THR	4.1
1	D	246	THR	4.0
1	D	42	LEU	4.0
1	C	183	PHE	3.9
1	C	73	ASP	3.8
1	C	151	GLY	3.8
1	C	42	LEU	3.7
1	D	263	ILE	3.7
1	C	160	TYR	3.7
1	C	56	ILE	3.6
1	D	81	LEU	3.6
1	D	268	CYS	3.6
1	C	36	LEU	3.5
1	C	251	CYS	3.5
1	C	64	LEU	3.5
1	D	73	ASP	3.5
1	D	249	VAL	3.4
1	C	238	LEU	3.4
1	C	70	ASN	3.4
1	C	236	ARG	3.4
1	D	90	LEU	3.3
1	D	74	LYS	3.3
1	C	63	GLY	3.3
1	C	57	VAL	3.3
1	D	66	LYS	3.3
1	C	104	PHE	3.3
1	C	52	SER	3.3
1	C	192	GLY	3.2
1	C	263	ILE	3.2
1	C	72	SER	3.1
1	C	162	ASP	3.1
1	C	58	ALA	3.1
1	C	179	SER	3.1
1	D	84	THR	3.1
1	D	258	PHE	3.1
1	A	222	ILE	3.1
1	C	272	HIS	3.0
1	C	65	GLY	3.0
1	D	41	PHE	3.0
1	C	259	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	153	PHE	3.0
1	C	188	TRP	2.9
1	C	95	LEU	2.9
1	C	51	ALA	2.9
1	B	68	TYR	2.9
1	C	88	LEU	2.9
1	D	138	GLY	2.9
1	C	96	LYS	2.8
1	A	30	LEU	2.8
1	C	46	ALA	2.8
1	C	90	LEU	2.8
1	C	220	LEU	2.8
1	A	32	SER	2.8
1	A	72	SER	2.8
1	C	159	TYR	2.7
1	C	121	LEU	2.7
1	D	248	ALA	2.7
1	D	262	GLU	2.7
1	D	87	TRP	2.7
1	C	237	VAL	2.6
1	C	50	ASP	2.6
1	C	177	ALA	2.6
1	B	268	CYS	2.6
1	D	46	ALA	2.5
1	D	78	ASP	2.5
1	D	133	VAL	2.5
1	C	261	TYR	2.5
1	D	241	PHE	2.5
1	C	55	LEU	2.5
1	D	77	GLY	2.5
1	D	57	VAL	2.5
1	D	62	TYR	2.5
1	C	239	ASP	2.5
1	C	254	GLN	2.5
1	C	80	PHE	2.4
1	D	80	PHE	2.4
1	C	98	SER	2.4
1	D	52	SER	2.4
1	C	194	ASN	2.4
1	D	267	TYR	2.4
1	C	258	PHE	2.4
1	C	99	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	137	GLY	2.4
1	C	71	ASP	2.4
1	C	279	ALA	2.4
1	D	107	TRP	2.4
1	C	247	THR	2.4
1	C	87	TRP	2.4
1	D	216	THR	2.3
1	C	182	LEU	2.3
1	D	47	HIS	2.3
1	D	102	TYR	2.3
1	D	134	PRO	2.3
1	C	213	ASP	2.3
1	D	63	GLY	2.2
1	C	241	PHE	2.2
1	C	249	VAL	2.2
1	C	92	ILE	2.2
1	D	128	ILE	2.2
1	B	30	LEU	2.2
1	D	139	THR	2.2
1	C	49	PRO	2.2
1	D	146	VAL	2.2
1	C	117	LEU	2.1
1	C	69	GLY	2.1
1	D	70	ASN	2.1
1	C	191	MET	2.1
1	D	153	PHE	2.1
1	D	113	ILE	2.1
1	C	248	ALA	2.1
1	C	243	GLY	2.1
1	C	276	ASN	2.1
1	C	278	LEU	2.1
1	D	71	ASP	2.1
1	D	100	SER	2.1
1	C	229	ALA	2.1
1	C	123	MET	2.1
1	C	185	GLY	2.1
1	D	237	VAL	2.1
1	C	47	HIS	2.1
1	D	238	LEU	2.1
1	B	34	ILE	2.1
1	D	104	PHE	2.1
1	C	224	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	109	TYR	2.0
1	C	170	TYR	2.0
1	C	267	TYR	2.0
1	C	61	PRO	2.0
1	D	96	LYS	2.0
1	D	83	TRP	2.0
1	C	124	VAL	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)

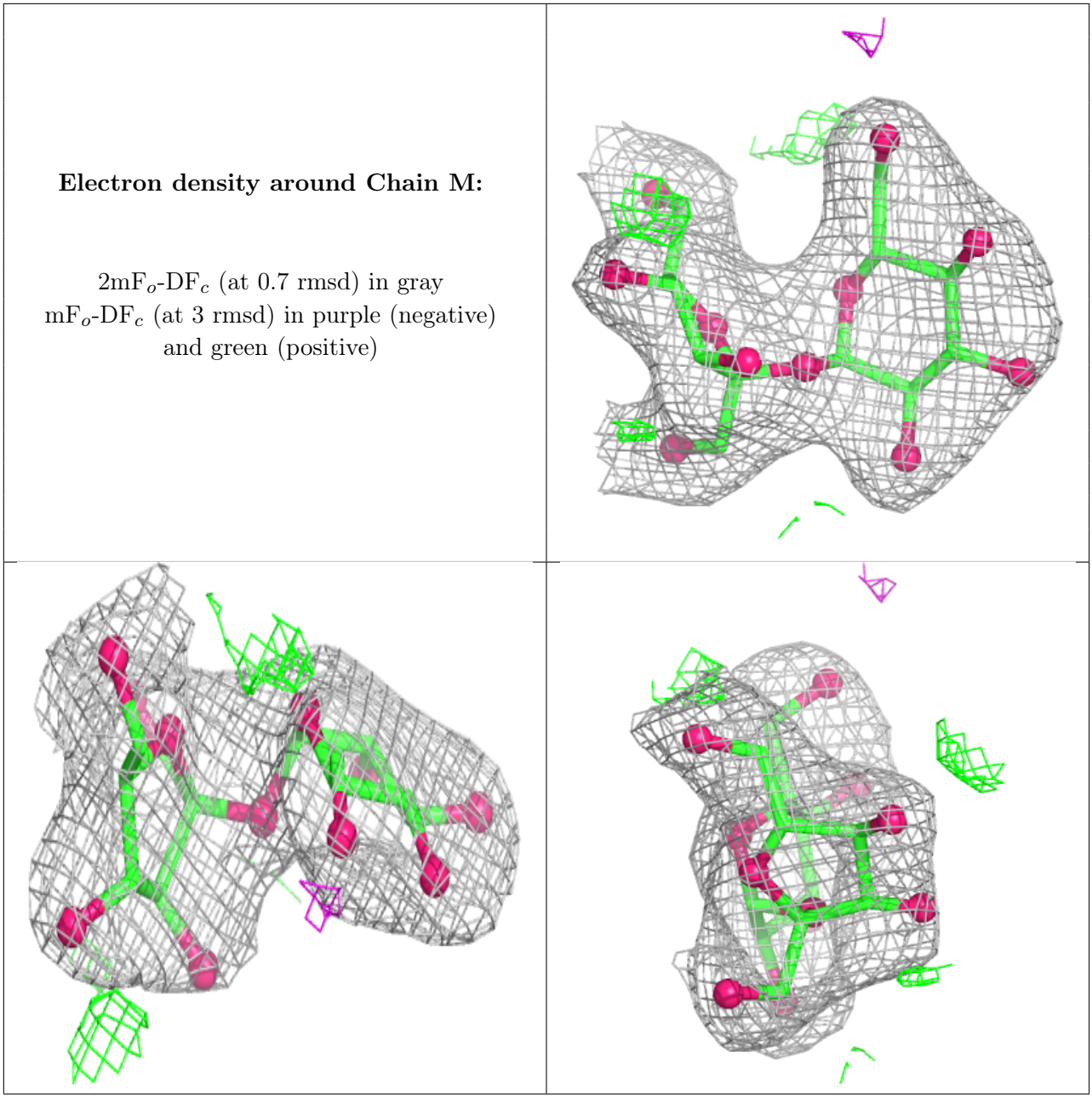
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	GLC	M	1	11/12	0.88	0.10	42,53,61,61	0
4	FRU	M	2	12/12	0.90	0.09	31,42,52,60	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 M:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SFG	D	301	27/27	0.85	0.13	53,75,95,97	0
5	SFG	C	301	27/27	0.86	0.12	40,71,82,94	0
5	SFG	A	301	27/27	0.94	0.07	27,37,42,50	0

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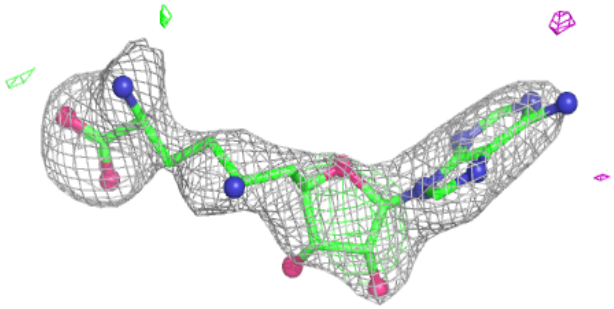
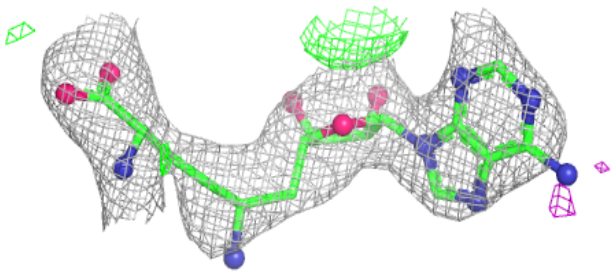
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SFG	B	301	27/27	0.94	0.07	21,35,45,50	0

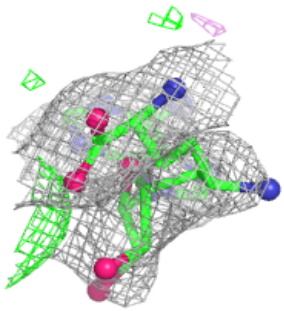
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SFG D 301:

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

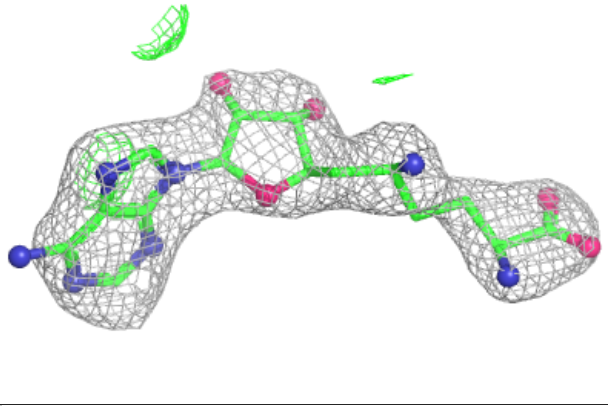


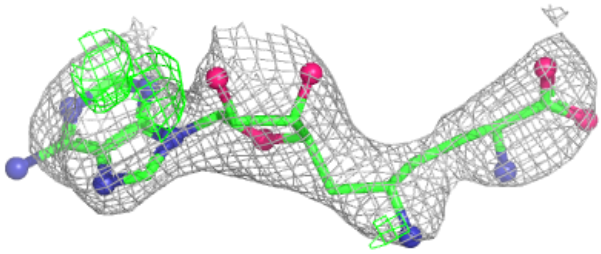


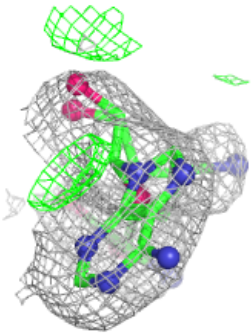


Electron density around SFG C 301:

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

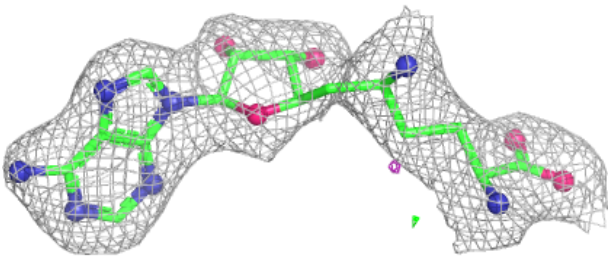


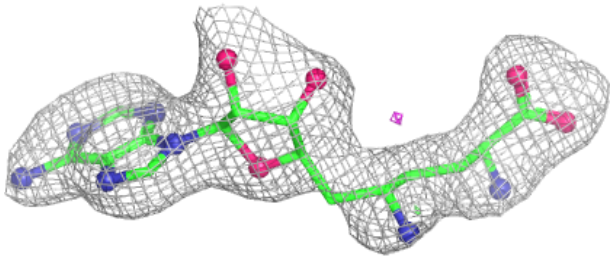


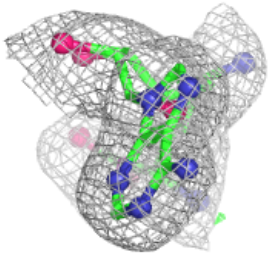


Electron density around SFG A 301:

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

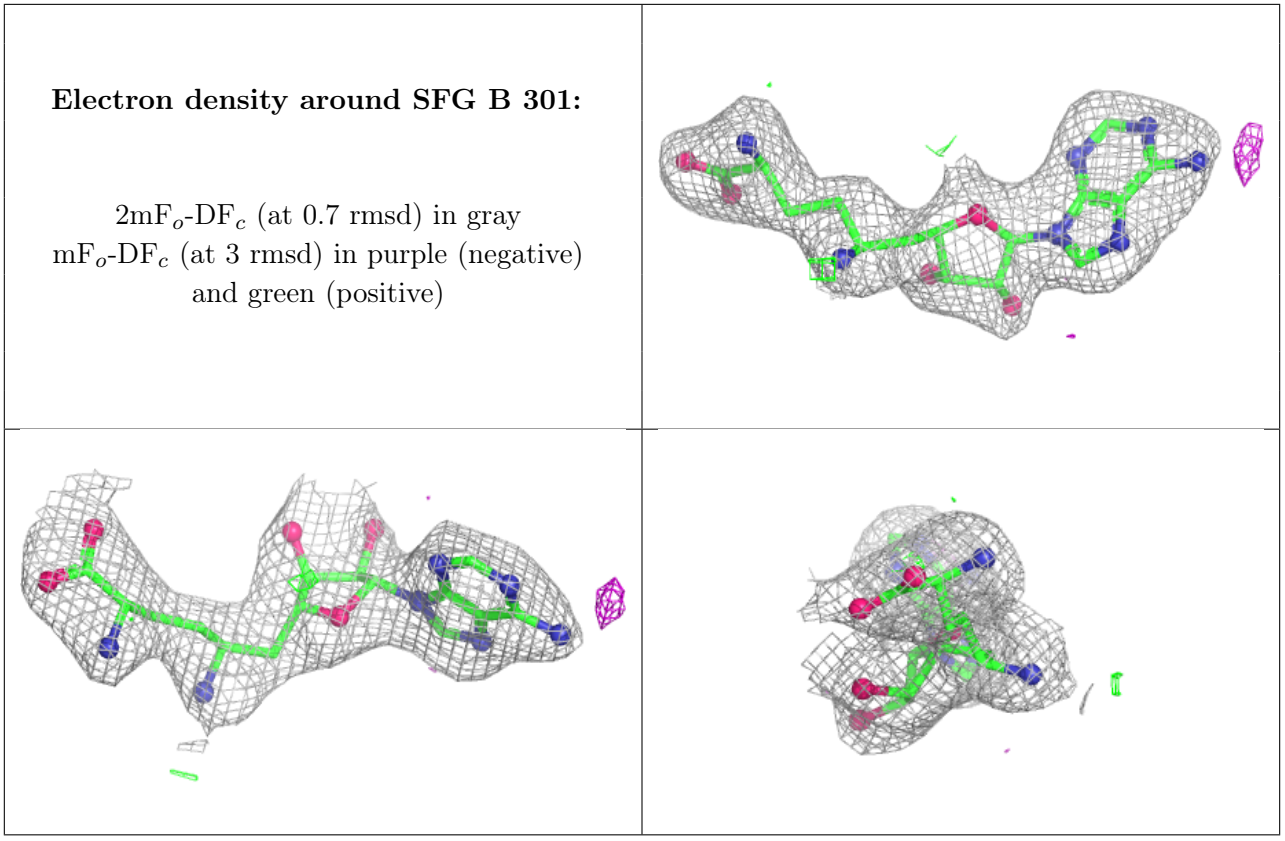






Electron density around SFG B 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.