WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2024 – 06:04 AM EDT

PDB ID	:	8URK
Title	:	Crystal structure of DNA N6-Adenine Methyltransferase M.BceJIV from Burkholderia cenocepacia in complex with duplex DNA substrates
Authors	:	Kottur, J.; Quintana-Feliciano, R.; Aggarwal, A.K.
Deposited on	:	2023-10-26
Resolution	:	2.11 Å(reported)

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This is a wwPDB X-ray Structure Validation Summary 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.

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

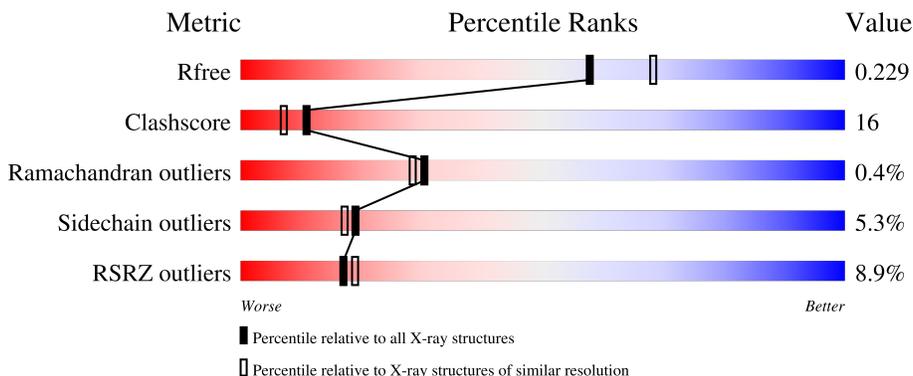|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & 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 2.11 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	Percentile Ranks	Value
Rfree		0.229
Clashscore		16
Ramachandran outliers		0.4%
Sidechain outliers		5.3%
RSRZ outliers		8.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7689 (2.14-2.10)
Clashscore	180529	8431 (2.14-2.10)
Ramachandran outliers	177936	8366 (2.14-2.10)
Sidechain outliers	177891	8367 (2.14-2.10)
RSRZ outliers	164620	7689 (2.14-2.10)

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	283	58% 29% • 12%
1	B	283	% 73% 15% 12%
1	C	283	15% 52% 34% • 12%
1	D	283	17% 57% 28% • 14%
2	E	14	43% 57%

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Mol	Chain	Length	Quality of chain
2	G	14	71% 29%
2	I	14	43% 57%
2	K	14	14% 50% 50%
3	F	14	21% 79%
3	H	14	14% 21% 79%
3	J	14	7% 50% 50%
3	L	14	7% 36% 64%
4	N	2	50% 50%
4	O	2	50% 50%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 10890 atoms, of which 61 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	249	Total	C	N	O	S	0	1	0
			1990	1269	348	363	10			
1	C	249	Total	C	N	O	S	0	1	0
			1950	1244	335	361	10			
1	D	244	Total	C	N	O	S	0	0	0
			1908	1214	329	355	10			
1	B	249	Total	C	N	O	S	0	0	0
			1992	1268	348	366	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.
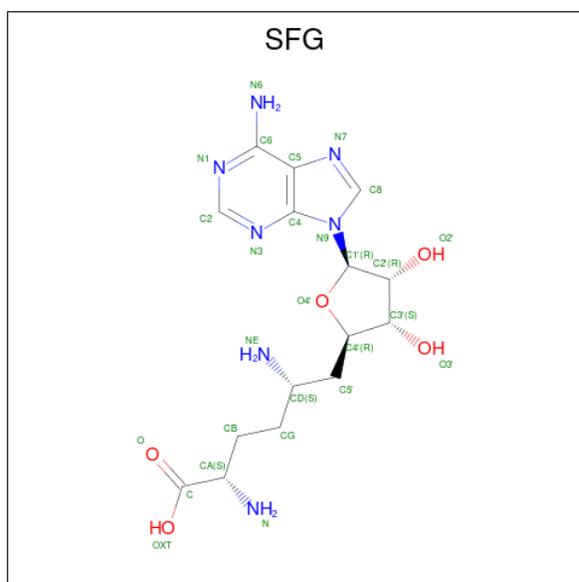

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	N	2	Total 45	C 12	H 22	O 11	0	0	0
4	O	2	Total 45	C 12	H 22	O 11	0	0	0

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).
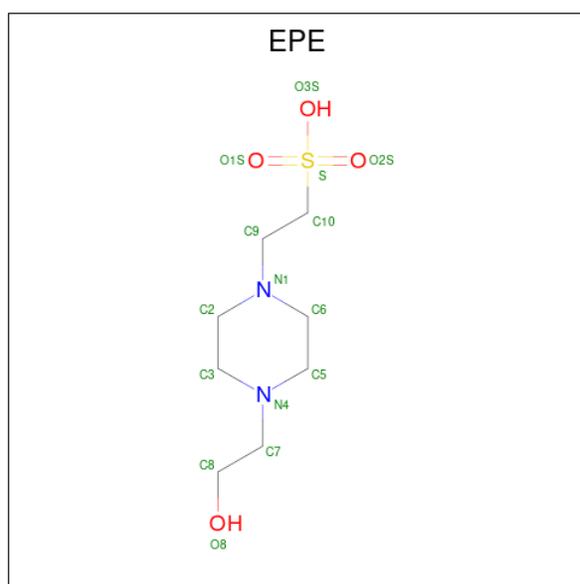
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 32	C 8	H 17	N 2	O 4	S 1	0	0

- Molecule 6 is SINEFUNGIN (three-letter code: SFG) (formula: $C_{15}H_{23}N_7O_5$) (labeled as "Ligand of Interest" by depositor).

SFG

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	154	Total 154	O 154	0	0
7	E	19	Total 19	O 19	0	0
7	F	12	Total 12	O 12	0	0
7	C	46	Total 46	O 46	0	0
7	D	75	Total 75	O 75	0	0
7	B	149	Total 149	O 149	0	0
7	G	17	Total 17	O 17	0	0
7	H	16	Total 16	O 16	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	16	Total 16	O 16	0	0
7	J	18	Total 18	O 18	0	0
7	K	12	Total 12	O 12	0	0
7	L	17	Total 17	O 17	0	0

3 Residue-property plots ⓘ

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 C:

- Molecule 1: Methyltransferase

Chain D:

K66 D67 Y68 G69 N70 D71 S72 D73 K74 R75 S76 G77 F80 L81 A82 W83 T84 R85 E86 W87 L88 E89 L90 A91 I92 P93 K94 M101 Y102 C105 T106 W107 A110 P111 F116 L117 K118 T119 Q120 L121 T122 M123 R131 R132 V133 G138 T139 T140 R141 R142 D148

F161 V166 R167 S179 R180 K187 M191 P195 K196 D197 V198 R203 L204 H205 R206 Q207 R211 V212 D213 M226 A229 S230 C231 P232 G235 R236 V237 L238 F241 M242 G243 S244 G245 T246 T247 A248 C251 A252 R253 R256 D257 F258 Y261 E262 I263 N264

E265 S266 Y267 C268 A269 I270 A271 H272 V275 N276 A277 LEU ALA ALA PRO ALA CYS ALA

• Molecule 1: Methyltransferase

Chain B:

%

73%   15%   12%

MET ARG ASP LEU ILE GLU GLU PRO GLY GLY GLY ALA ALA SER GLU ALA GLY ALA VAL GLN PRO ALA ALA ALA VAL PRO ARG ALA L30 P31 S32 G33 I34 E35 L36 H47 I53 D54 Y62 R75 R85 K96 S100 A110 P111 E112 K118 T122 N125

R132 T139 T140 R141 R142 F143 T144 S145 V146 H147 L182 W188 P195 K196 D197 V198 R203 Q207 H208 A209 E210 R211 V212 D213 H214 Q217 F241 M242 V249 R253 C268 A269 E273 L278 ALA ALA PRO ALA CYS ALA

• Molecule 2: DNA1

Chain E:

43%   57%

T1 T2 G3 A6 T9 A10 G11 C12 C13 A14

• Molecule 2: DNA1

Chain G:

71%   29%

T1 T5 A6 A7 C13 A14

• Molecule 2: DNA1

Chain I:

43%   57%

T1 T2 T5 A6 A7 C8 T9 A10 G11 A14

• Molecule 2: DNA1

Chain K:

14%

50%   50%

T1 T2 G3 A6 A7 G11 C12 C13 A14

• Molecule 3: DNA2

Chain F:
21%   79%

A1 T2 G3 G4 C5 T6 A7 G8 T9 T10 C13 A14

• Molecule 3: DNA2

Chain H:
14%
21%   79%

A1 T2 G3 G4 C5 T6 A7 G8 T9 T10 A11 A12 C13 A14
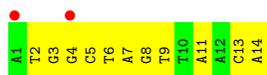
• Molecule 3: DNA2

Chain J:
7%
50%   50%

A1 C5 T6 A7 G8 T9 C13 A14

• Molecule 3: DNA2

Chain L:
7%
36%   64%

A1 T2 G3 G4 C5 T6 A7 C13 A14
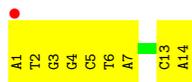
• Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain N:
50%   50%

GLC1 FRU2

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

Chain O:
50%   50%

GLC1 FRU2

4 Data and refinement statistics ⓘ

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)	44.27　–　2.11 44.27　–　2.11	Depositor EDS
% Data completeness (in resolution range)	55.2 (44.27-2.11) 55.3 (44.27-2.11)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.20rc3_4406: ???)	Depositor
R, R_{free}	0.184　,　0.234 0.191　,　0.229	Depositor DCC
R_{free} test set	4543 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 75.5	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10890	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: FRU, GLC, EPE, SFG

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	0.59	0/2049	0.63	0/2782
1	B	0.64	0/2048	0.66	0/2781
1	C	0.54	0/2009	0.59	0/2736
1	D	0.51	0/1961	0.60	0/2667
2	E	0.59	0/315	0.81	0/484
2	G	0.54	0/314	0.78	0/482
2	I	0.56	0/315	0.83	0/484
2	K	0.52	0/314	0.93	1/482 (0.2%)
3	F	0.63	0/321	0.91	0/494
3	H	0.45	0/320	0.76	0/493
3	J	0.72	0/321	0.97	0/494
3	L	0.56	0/321	0.82	0/494
All	All	0.58	0/10608	0.69	1/14873 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	11	DG	C1'-O4'-C4'	-5.51	104.59	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1990	0	1926	68	0
1	B	1992	0	1928	33	0
1	C	1950	0	1831	77	0
1	D	1908	0	1790	79	0
2	E	282	0	161	16	0
2	G	281	0	159	5	0
2	I	282	0	161	11	0
2	K	281	0	159	7	0
3	F	286	0	160	12	0
3	H	285	0	157	17	0
3	J	286	0	160	13	0
3	L	286	0	160	12	0
4	N	23	22	21	1	0
4	O	23	22	21	2	0
5	A	15	17	17	3	0
6	A	27	0	22	3	0
6	B	27	0	22	3	0
6	C	27	0	22	4	0
6	D	27	0	22	6	0
7	A	154	0	0	2	0
7	B	149	0	0	3	0
7	C	46	0	0	5	0
7	D	75	0	0	3	0
7	E	19	0	0	1	0
7	F	12	0	0	0	0
7	G	17	0	0	0	0
7	H	16	0	0	3	0
7	I	16	0	0	0	0
7	J	18	0	0	1	0
7	K	12	0	0	0	0
7	L	17	0	0	0	0
All	All	10829	61	8899	311	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 16.

The worst 5 of 311 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:B:208:HIS:HD2	1:B:210:GLU:H	1.05	0.98
3:F:8:DG:H2"	3:F:9:DT:H5'	1.48	0.95
3:L:2:DT:H2'	3:L:3:DG:C8	2.07	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ALA:HA	1:C:95:LEU:O	1.76	0.86
1:C:228:LEU:HD21	1:C:254:GLN:HG3	1.58	0.86

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	248/283 (88%)	232 (94%)	14 (6%)	2 (1%)	16	12
1	B	247/283 (87%)	232 (94%)	15 (6%)	0	100	100
1	C	248/283 (88%)	223 (90%)	23 (9%)	2 (1%)	16	12
1	D	242/283 (86%)	219 (90%)	23 (10%)	0	100	100
All	All	985/1132 (87%)	906 (92%)	75 (8%)	4 (0%)	30	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	31	PRO
1	C	48	LEU
1	C	146	VAL

5.3.2 Protein sidechains ⓘ

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	210/231 (91%)	199 (95%)	11 (5%)	19	18
1	B	212/231 (92%)	203 (96%)	9 (4%)	25	25
1	C	199/231 (86%)	187 (94%)	12 (6%)	16	13
1	D	194/231 (84%)	183 (94%)	11 (6%)	17	15
All	All	815/924 (88%)	772 (95%)	43 (5%)	19	17

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	121	LEU
1	B	75	ARG
1	D	140	THR
1	D	242	MET
1	B	100	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	208	HIS
1	C	38	ASN
1	C	214	HIS
1	B	208	HIS

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 ⓘ

4 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	N	1	4	11,11,12	0.38	0	15,15,17	0.58	0
4	FRU	N	2	4	11,12,12	0.41	0	10,18,18	1.04	1 (10%)
4	GLC	O	1	4	11,11,12	0.33	0	15,15,17	1.15	1 (6%)
4	FRU	O	2	4	11,12,12	0.46	0	10,18,18	1.60	2 (20%)

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	N	1	4	-	1/2/19/22	0/1/1/1
4	FRU	N	2	4	-	5/5/24/24	0/1/1/1
4	GLC	O	1	4	-	2/2/19/22	0/1/1/1
4	FRU	O	2	4	-	5/5/24/24	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	2	FRU	O2-C2-O5	3.77	116.56	109.33
4	O	1	GLC	C2-C3-C4	-2.43	106.59	110.86
4	N	2	FRU	C6-C5-C4	-2.34	109.58	115.10
4	O	2	FRU	O6-C6-C5	-2.12	104.12	111.33

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	2	FRU	1	0
4	O	1	GLC	2	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 N

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain O
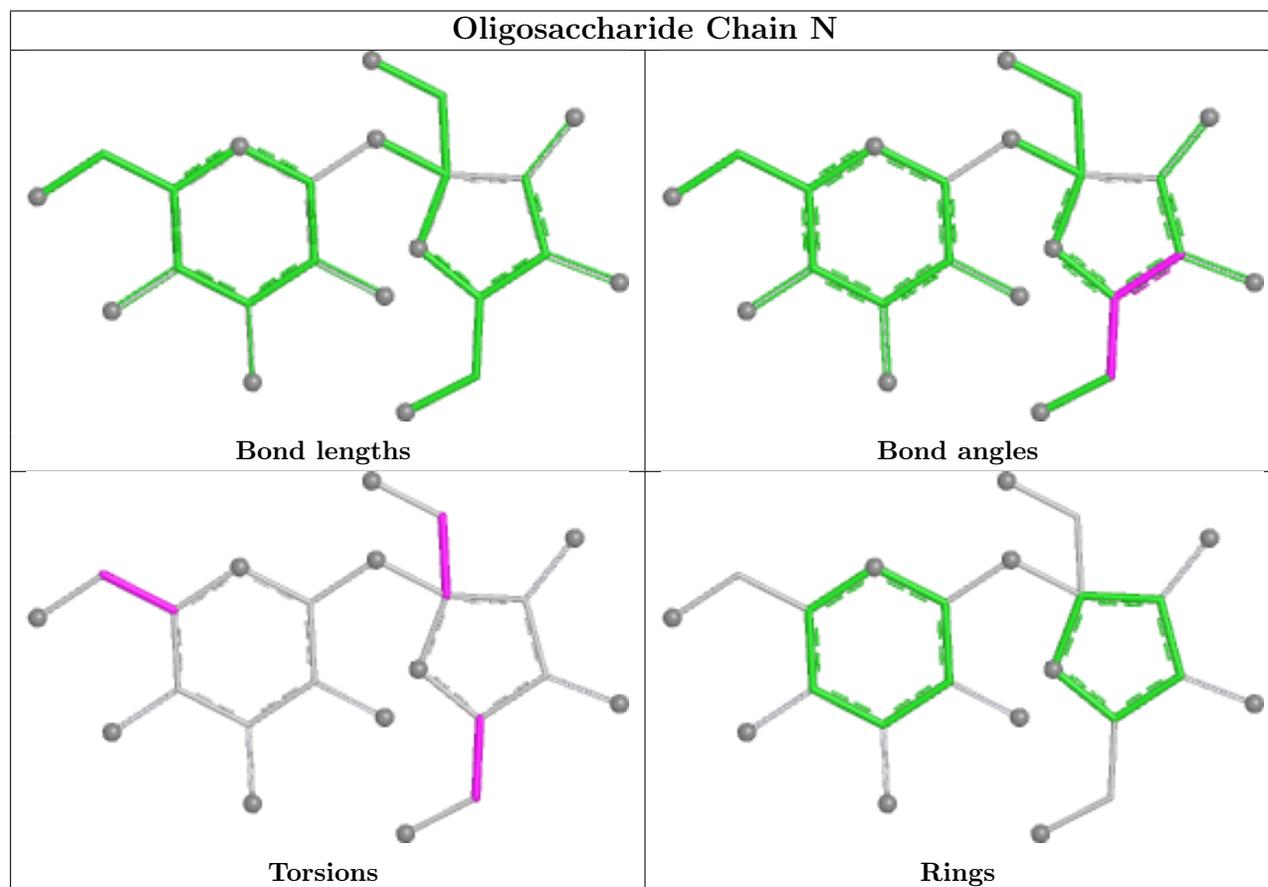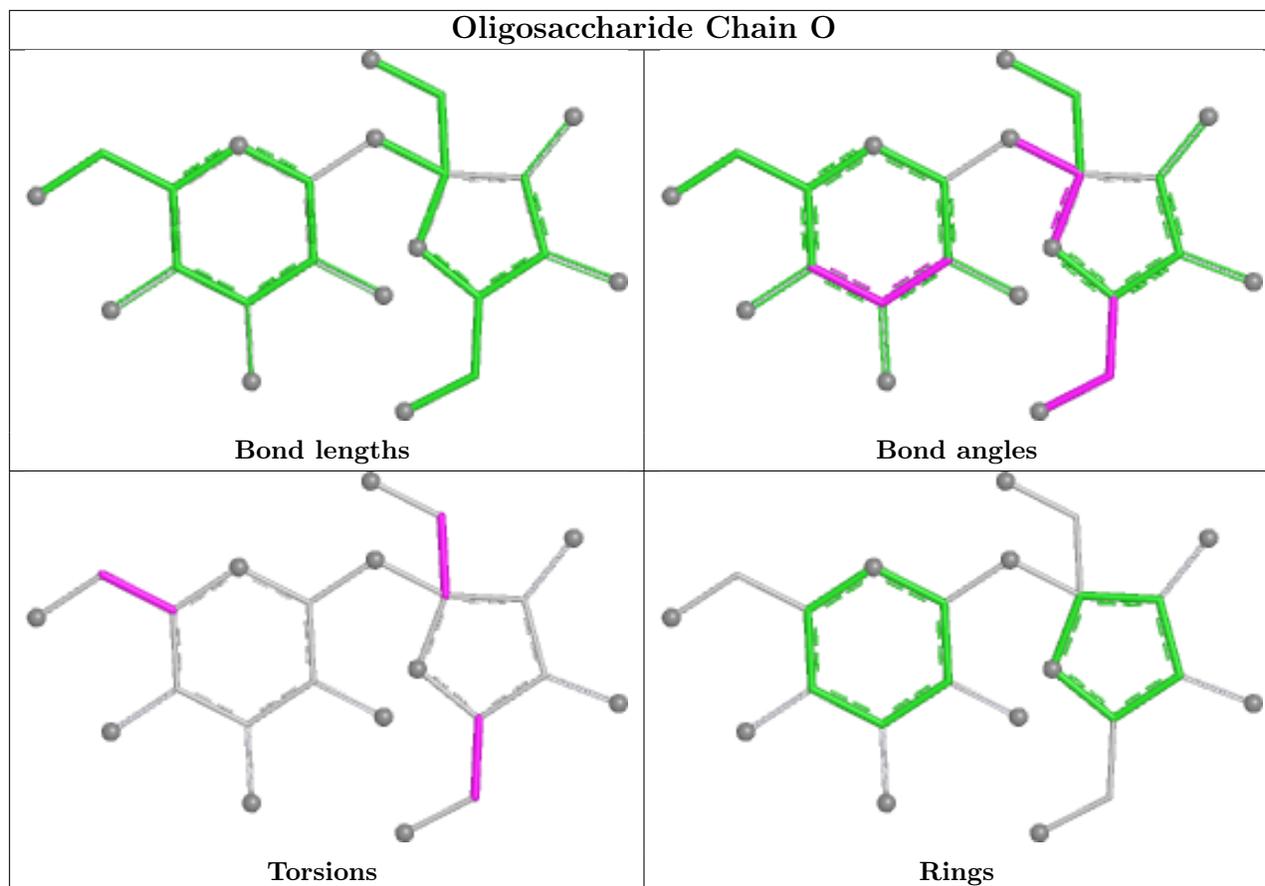
5.6 Ligand geometry ⓘ

5 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	$\#|Z| > 2$
6	SFG	B	601	-	24,29,29	0.89	1 (4%)	20,42,42	1.42	4 (20%)
6	SFG	C	601	-	24,29,29	0.95	1 (4%)	20,42,42	1.27	2 (10%)
6	SFG	A	802	-	24,29,29	0.93	1 (4%)	20,42,42	1.40	3 (15%)
5	EPE	A	801	-	15,15,15	0.94	1 (6%)	19,20,20	1.89	7 (36%)
6	SFG	D	601	-	24,29,29	1.07	1 (4%)	20,42,42	1.57	4 (20%)

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
6	SFG	B	601	-	-	1/13/33/33	0/3/3/3
6	SFG	C	601	-	-	3/13/33/33	0/3/3/3
6	SFG	A	802	-	-	0/13/33/33	0/3/3/3
5	EPE	A	801	-	-	7/9/19/19	0/1/1/1
6	SFG	D	601	-	-	8/13/33/33	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	801	EPE	C10-S	3.23	1.82	1.77
6	D	601	SFG	OXT-C	-3.22	1.20	1.30
6	A	802	SFG	OXT-C	-2.74	1.21	1.30
6	C	601	SFG	OXT-C	-2.54	1.22	1.30
6	B	601	SFG	OXT-C	-2.52	1.22	1.30

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	801	EPE	C5-N4-C3	4.25	117.99	108.84
5	A	801	EPE	C7-N4-C5	3.85	121.51	111.24
6	D	601	SFG	N3-C2-N1	-3.74	123.60	128.67
6	D	601	SFG	CB-CA-N	-3.74	100.38	110.12
6	C	601	SFG	N3-C2-N1	-3.66	123.70	128.67

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	801	EPE	C9-C10-S-O1S
5	A	801	EPE	C9-C10-S-O3S
6	D	601	SFG	O-C-CA-N
6	D	601	SFG	C4'-C5'-CD-CG
6	D	601	SFG	OXT-C-CA-N

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	601	SFG	3	0
6	C	601	SFG	4	0
6	A	802	SFG	3	0
5	A	801	EPE	3	0
6	D	601	SFG	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 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 B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SFG C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SFG A 802

Bond lengths

Bond angles

Torsions

Rings

Ligand SFG D 601

Bond lengths

Bond angles

Torsions

Rings
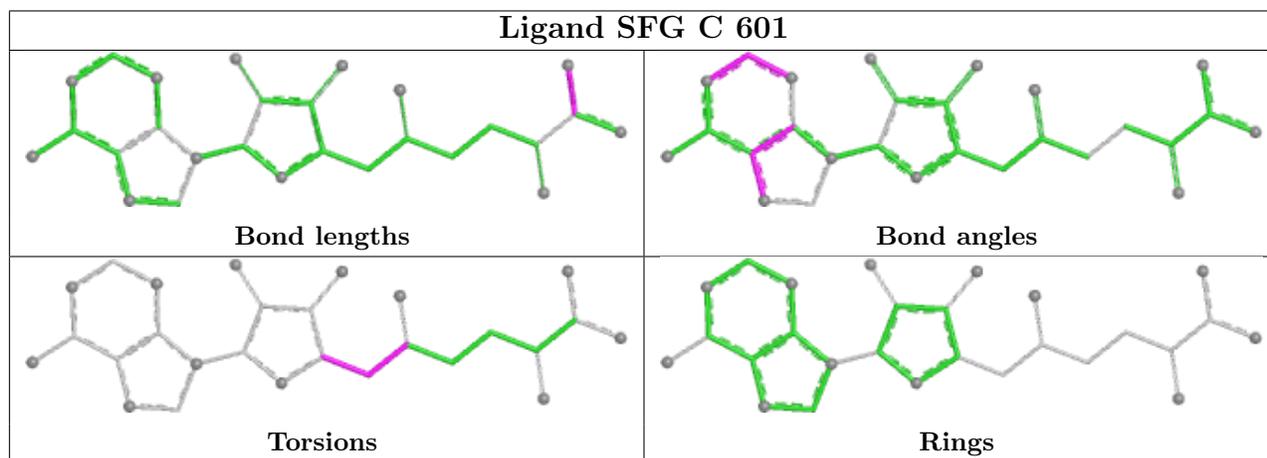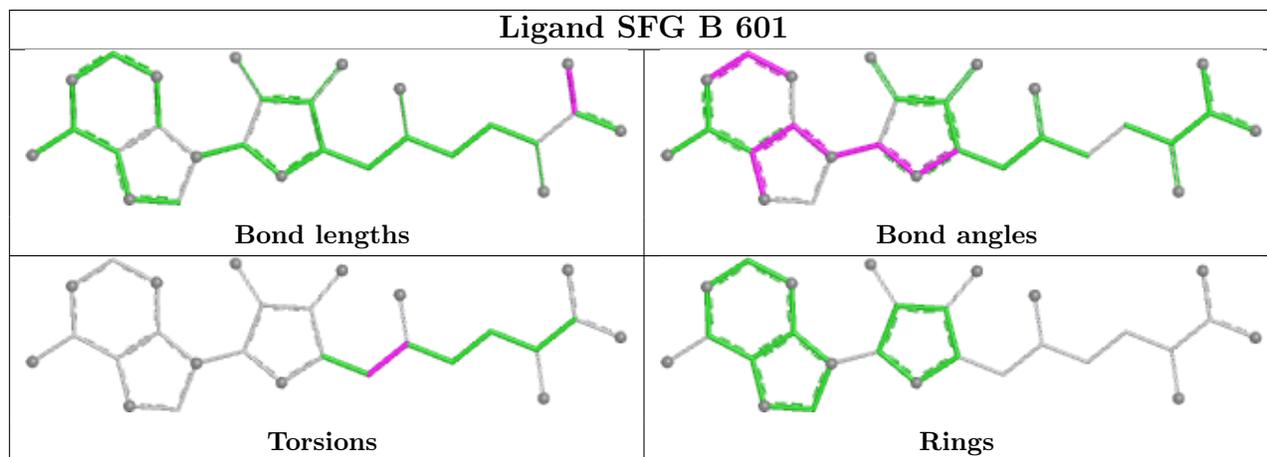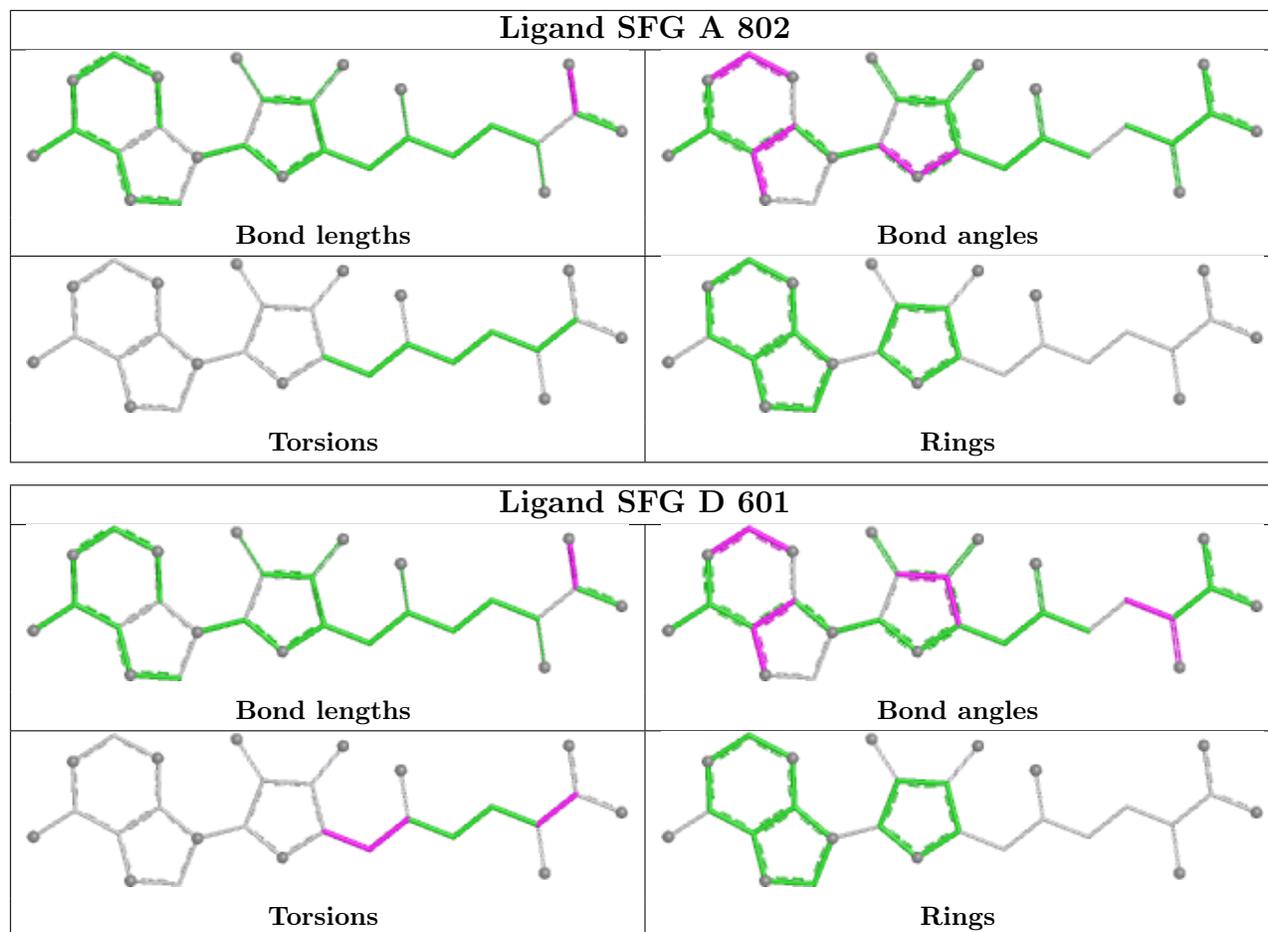
5.7   Other polymers ⓘ

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, 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	249/283 (87%)	-0.00	0	100	100	10, 31, 48, 61	1 (0%)
1	B	249/283 (87%)	-0.11	2 (0%)	82	84	14, 26, 41, 59	0
1	C	249/283 (87%)	1.12	42 (16%)	5	6	16, 52, 74, 96	1 (0%)
1	D	244/283 (86%)	1.20	48 (19%)	3	4	29, 54, 76, 85	0
2	E	14/14 (100%)	-0.40	0	100	100	25, 36, 55, 60	0
2	G	14/14 (100%)	0.07	0	100	100	22, 37, 67, 69	0
2	I	14/14 (100%)	0.16	0	100	100	37, 45, 58, 62	0
2	K	14/14 (100%)	0.93	2 (14%)	7	8	51, 58, 87, 91	0
3	F	14/14 (100%)	-0.28	0	100	100	24, 37, 65, 66	0
3	H	14/14 (100%)	0.46	2 (14%)	7	8	22, 34, 64, 64	0
3	J	14/14 (100%)	0.23	1 (7%)	23	26	29, 42, 60, 63	0
3	L	14/14 (100%)	0.71	1 (7%)	23	26	41, 56, 72, 74	0
All	All	1103/1244 (88%)	0.52	98 (8%)	17	19	10, 39, 72, 96	2 (0%)

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	51	ALA	4.6
1	D	65	GLY	4.5
1	D	41	PHE	4.4
1	C	259	VAL	3.9
1	D	105	CYS	3.9

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

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

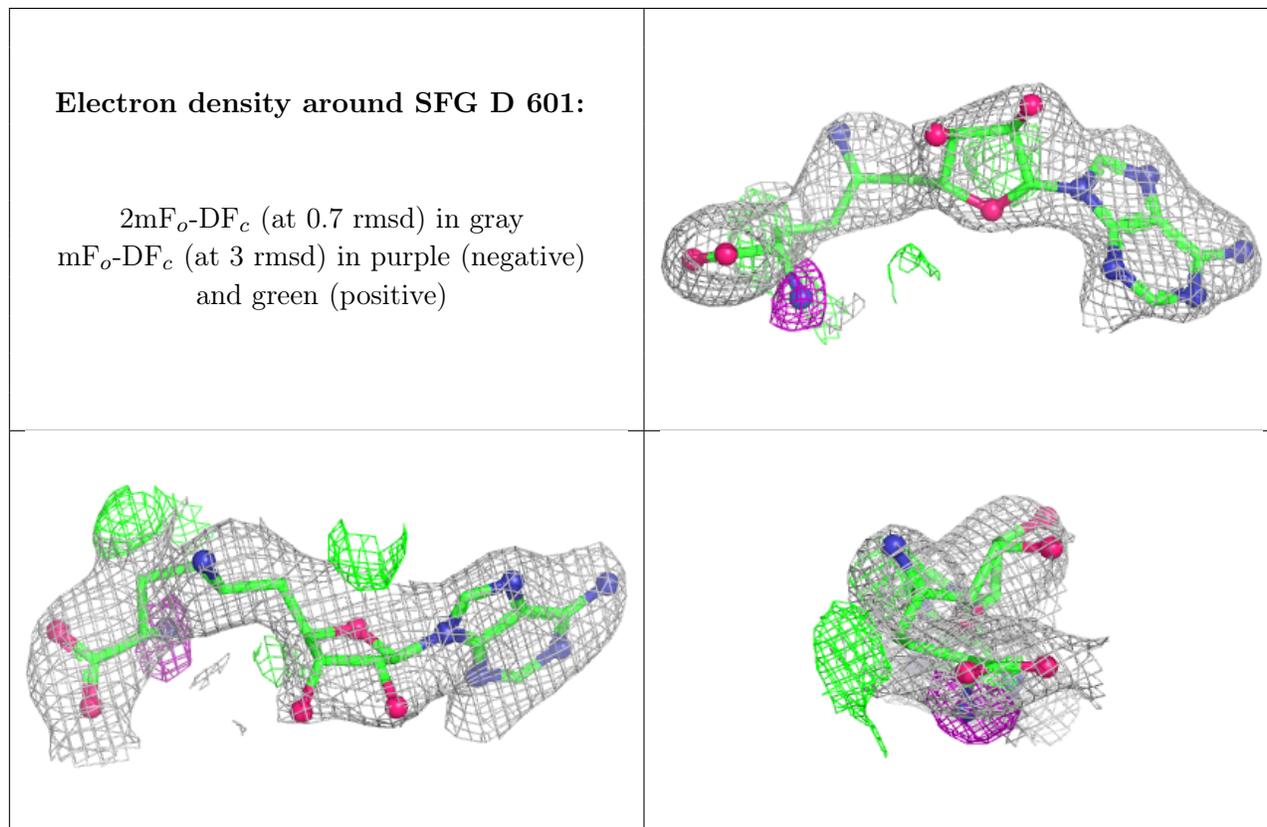WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.3 Carbohydrates (i)

SUGAR-RSR INFOmissingINFO

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
5	EPE	A	801	15/15	0.66	0.22	67,81,84,86	0
6	SFG	D	601	27/27	0.73	0.16	56,66,72,73	0
6	SFG	C	601	27/27	0.87	0.09	44,46,48,49	0
6	SFG	A	802	27/27	0.94	0.06	22,24,27,27	0
6	SFG	B	601	27/27	0.94	0.07	22,24,28,28	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 601:

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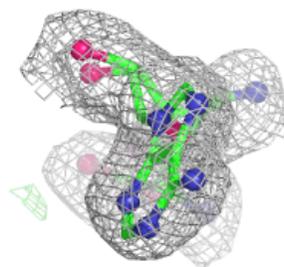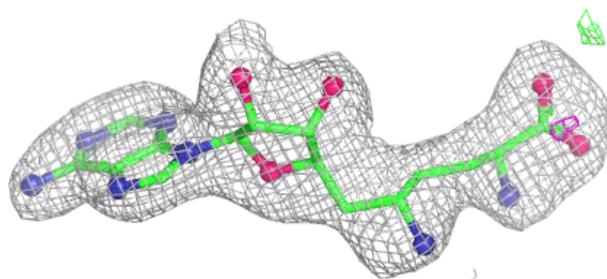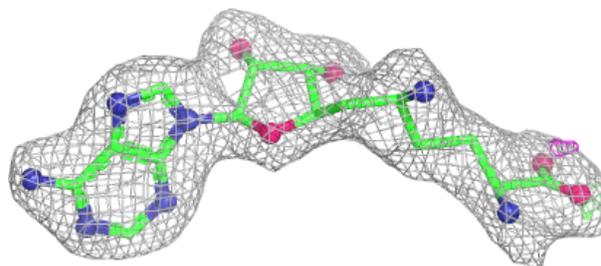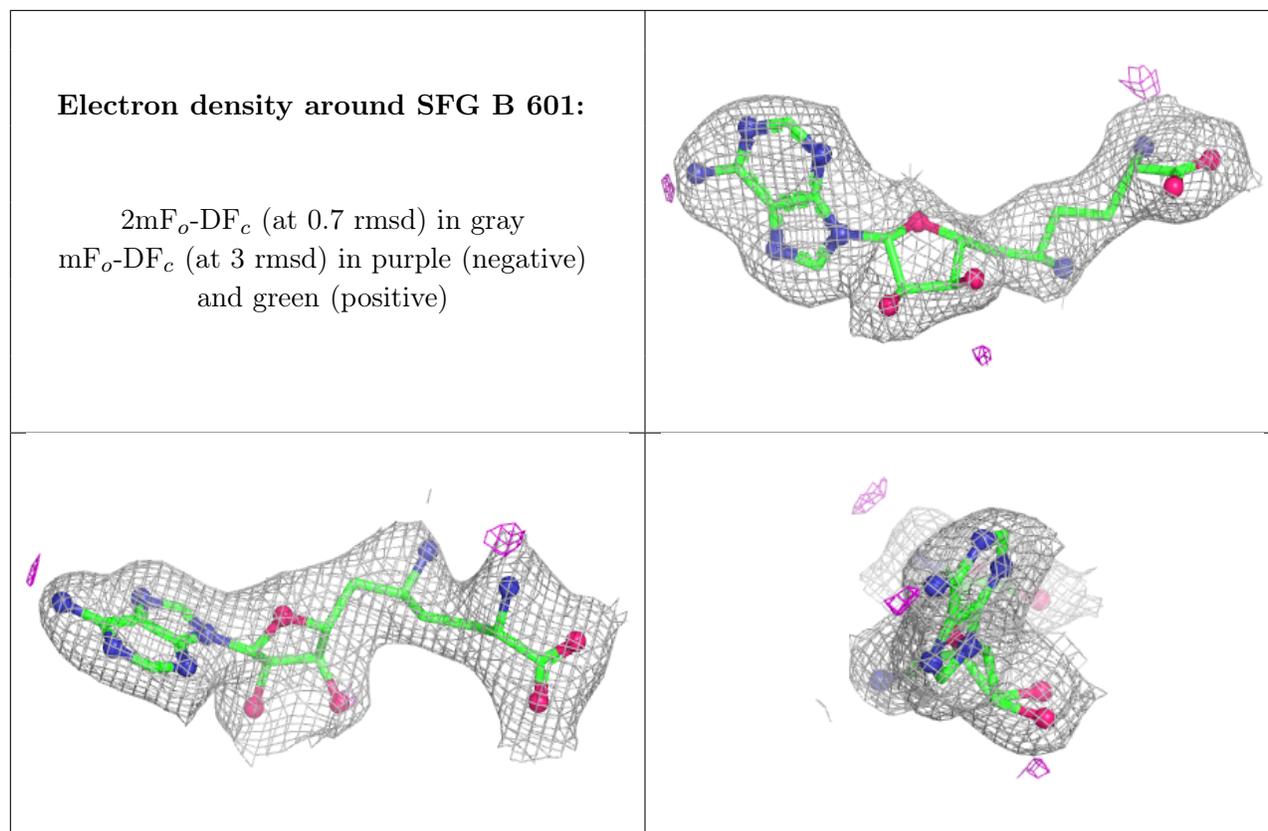$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around SFG C 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
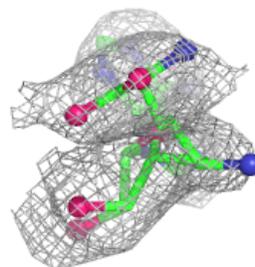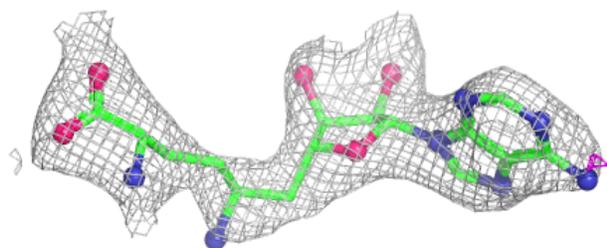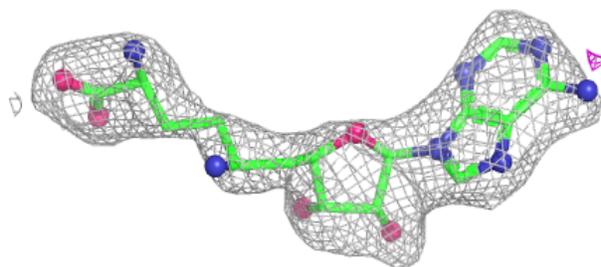
Electron density around SFG A 802:

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

Electron density around SFG B 601:

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 ⓘ

There are no such residues in this entry.