Full wwPDB X-ray Structure Validation 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)

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:

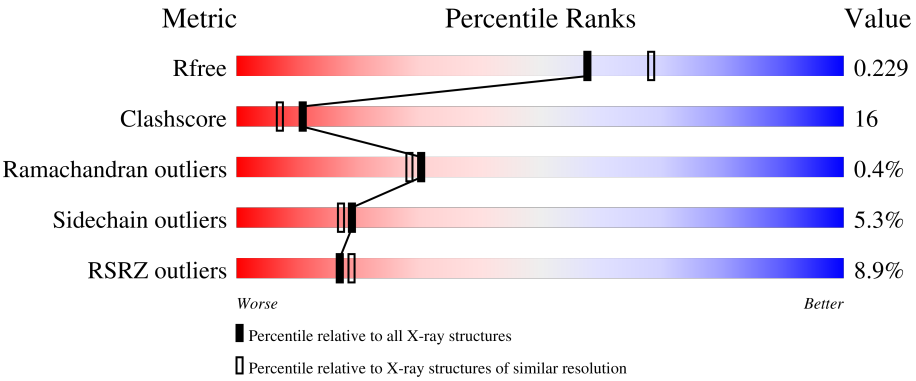
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & 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 2.11 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	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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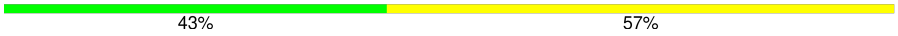
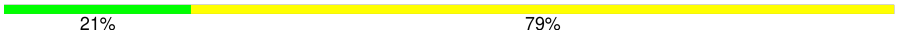
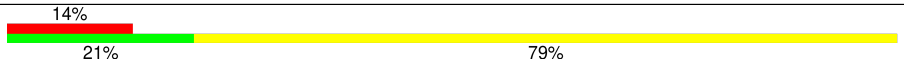
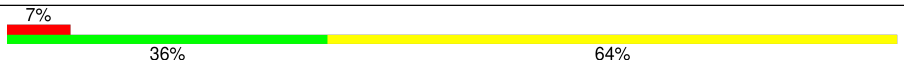
Mol	Chain	Length	Quality of chain
2	G	14	
2	I	14	
2	K	14	
3	F	14	
3	H	14	
3	J	14	
3	L	14	
4	N	2	
4	O	2	

2 Entry composition (i)

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			

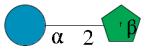
- Molecule 2 is a DNA chain called DNA1.

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.

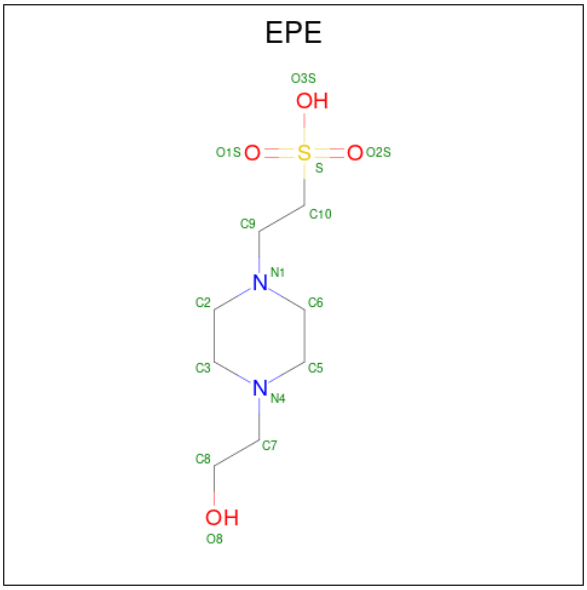
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	14	Total	C	N	O	P	0	0	0
			286	138	54	81	13			
3	H	14	Total	C	N	O	P	0	0	0
			285	138	54	80	13			
3	J	14	Total	C	N	O	P	0	0	0
			286	138	54	81	13			
3	L	14	Total	C	N	O	P	0	0	0
			286	138	54	81	13			

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



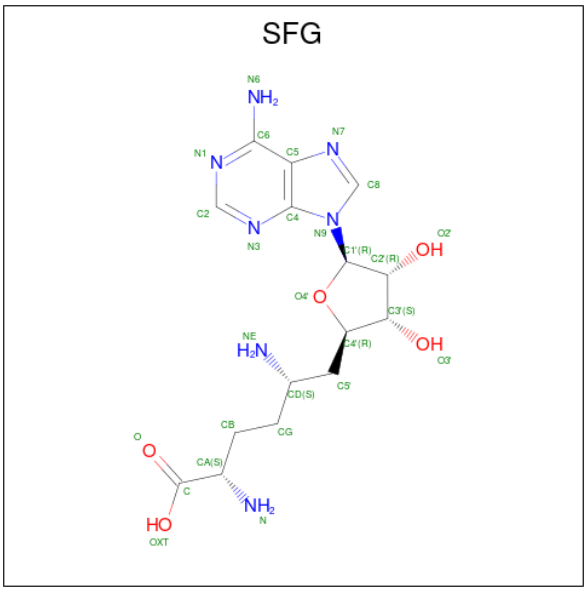
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	N	2	Total	C	H	O	0	0	0
			45	12	22	11			
4	O	2	Total	C	H	O	0	0	0
			45	12	22	11			

- 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	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 6 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
6	A	1	Total C N O 27 15 7 5	0	0
6	C	1	Total C N O 27 15 7 5	0	0
6	D	1	Total C N O 27 15 7 5	0	0
6	B	1	Total C N O 27 15 7 5	0	0

- Molecule 7 is water.

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

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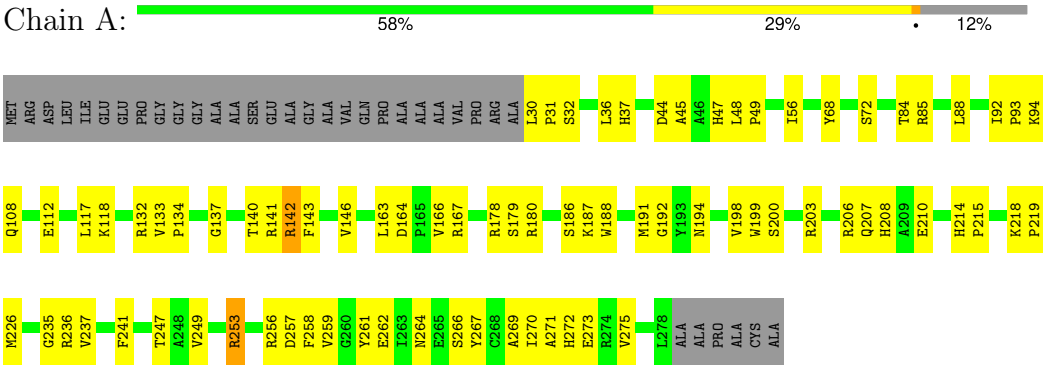
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	16	Total O 16 16	0	0
7	J	18	Total O 18 18	0	0
7	K	12	Total O 12 12	0	0
7	L	17	Total O 17 17	0	0

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.

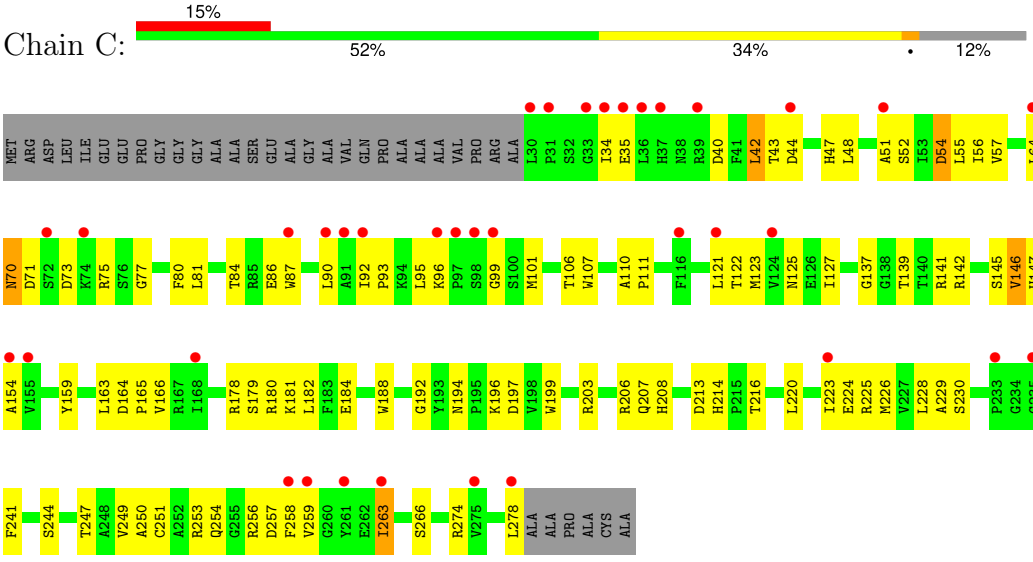
• Molecule 1: Methyltransferase

Chain A:



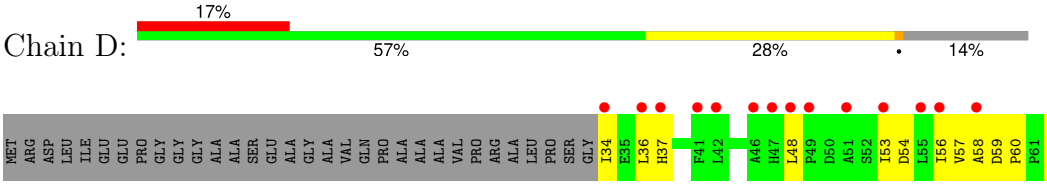
• Molecule 1: Methyltransferase

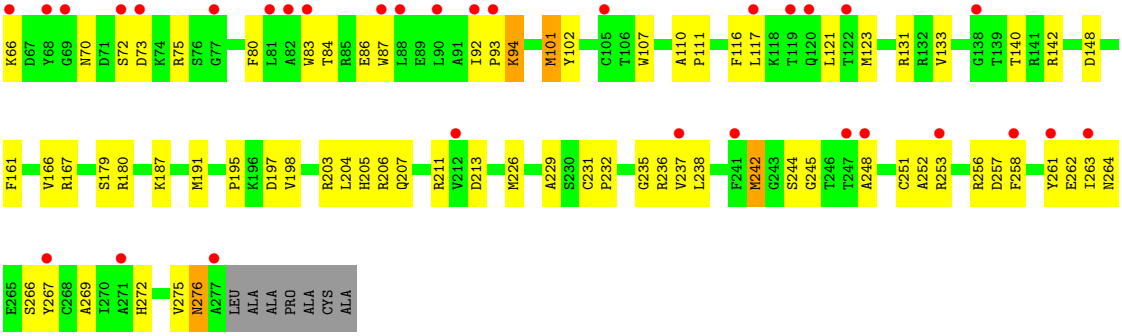
Chain C:



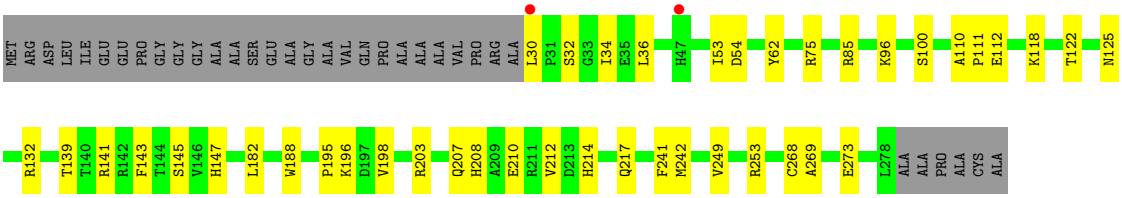
• Molecule 1: Methyltransferase

Chain D:

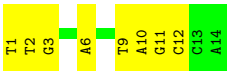




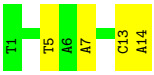
• Molecule 1: Methyltransferase



• Molecule 2: DNA1

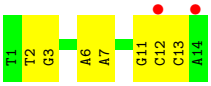


• Molecule 2: DNA1



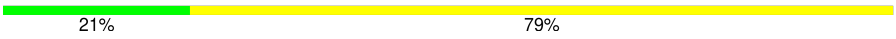
• Molecule 2: DNA1

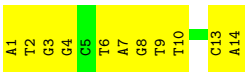
• Molecule 2: DNA1



• Molecule 3: DNA2

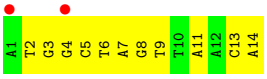
Chain F:





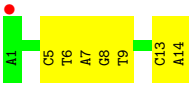
• Molecule 3: DNA2

Chain H:



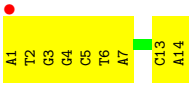
• Molecule 3: DNA2

Chain J:



• Molecule 3: DNA2

Chain L:



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

Chain N:

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

Chain O:

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)	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]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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: 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.

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.

All (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
1:B:208:HIS:CD2	1:B:210:GLU:H	1.94	0.85
1:D:75:ARG:HD2	1:D:80:PHE:HA	1.57	0.84
1:A:208:HIS:HD2	1:A:210:GLU:H	1.20	0.84
2:E:12:DC:H6	2:E:12:DC:H5'	1.42	0.84
2:I:1:DT:H5"	2:I:1:DT:H6	1.40	0.84
1:C:214:HIS:CE1	6:C:601:SFG:HB1	2.16	0.80
1:D:133:VAL:HG11	1:D:203:ARG:HH21	1.47	0.80
1:A:141:ARG:HH11	1:A:141:ARG:HG2	1.48	0.78
3:F:3:DG:H2"	3:F:4:DG:C8	2.18	0.78
1:D:56:ILE:HB	1:D:101:MET:HG2	1.66	0.77
2:K:12:DC:H2"	2:K:13:DC:H5'	1.66	0.76
1:A:112:GLU:OE2	1:B:118:LYS:HE2	1.86	0.76
3:L:3:DG:H2"	3:L:4:DG:C8	2.20	0.76
1:C:84:THR:HA	1:C:87:TRP:CD1	2.21	0.76
1:B:141:ARG:HG2	1:B:141:ARG:HH11	1.50	0.76
3:J:6:DT:H2"	3:J:7:DA:H5'	1.68	0.76
1:C:166:VAL:HG11	1:C:229:ALA:HB2	1.69	0.75
2:E:10:DA:H2"	2:E:11:DG:C8	2.22	0.75
3:L:5:DC:H2'	3:L:6:DT:C6	2.22	0.74
1:D:205:HIS:CE1	1:D:207:GLN:HG3	2.21	0.74
1:C:181:LYS:HA	1:C:184:GLU:HG3	1.69	0.73
3:F:6:DT:H4'	3:F:7:DA:OP1	1.89	0.72
1:D:166:VAL:HG21	1:D:229:ALA:HB2	1.71	0.72
2:E:2:DT:H2"	2:E:3:DG:C8	2.24	0.72
1:D:84:THR:HA	1:D:87:TRP:CD1	2.24	0.72
2:I:1:DT:H5"	2:I:1:DT:C6	2.23	0.72
2:K:2:DT:H2'	2:K:3:DG:C8	2.24	0.71
3:F:6:DT:H2'	3:F:7:DA:C8	2.25	0.71
1:C:77:GLY:O	1:C:81:LEU:HG	1.91	0.71
1:C:56:ILE:HB	1:C:101:MET:HG3	1.73	0.71
2:E:12:DC:H5'	2:E:12:DC:C6	2.24	0.70
1:D:242:MET:HE2	1:D:245:GLY:HA2	1.73	0.70
3:H:13:DC:H2'	3:H:14:DA:C8	2.26	0.70
2:I:1:DT:H2"	2:I:2:DT:H5'	1.73	0.70
3:L:3:DG:H2"	3:L:4:DG:H8	1.55	0.70
1:D:48:LEU:O	1:D:94:LYS:HE3	1.93	0.69
1:D:75:ARG:HB3	1:D:80:PHE:HB2	1.73	0.68
3:L:6:DT:H2'	3:L:7:DA:C8	2.29	0.68
1:D:248:ALA:HB2	1:D:258:PHE:CE2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:HE3	1:A:191:MET:SD	2.35	0.67
1:A:85:ARG:HD2	7:A:915:HOH:O	1.95	0.66
3:L:13:DC:H2'	3:L:14:DA:C8	2.30	0.66
1:A:241:PHE:HB3	6:A:802:SFG:O4'	1.96	0.65
1:A:206:ARG:HD2	2:E:6:DA:OP1	1.97	0.65
1:C:75:ARG:HB3	1:C:80:PHE:HB2	1.79	0.64
1:A:141:ARG:HG2	1:A:141:ARG:NH1	2.12	0.64
1:B:208:HIS:HD2	1:B:210:GLU:N	1.88	0.63
2:E:10:DA:H4'	2:E:11:DG:OP1	1.97	0.63
1:C:220:LEU:HG	1:C:224:GLU:HG3	1.81	0.62
1:D:205:HIS:HE1	1:D:207:GLN:HG3	1.61	0.62
1:A:56:ILE:HG13	1:A:95:LEU:HD21	1.79	0.62
1:A:214:HIS:CE1	6:A:802:SFG:HB1	2.35	0.62
1:C:145:SER:HA	1:D:197:ASP:OD2	1.99	0.62
3:F:8:DG:C2'	3:F:9:DT:H5'	2.27	0.62
3:J:6:DT:H2"	3:J:7:DA:C5'	2.29	0.62
1:A:236:ARG:HA	1:A:257:ASP:HB2	1.82	0.61
1:C:228:LEU:HD21	1:C:254:GLN:CG	2.30	0.61
1:C:223:ILE:HA	1:C:226:MET:HE2	1.82	0.61
1:B:141:ARG:HG2	1:B:141:ARG:NH1	2.13	0.61
1:C:121:LEU:HB3	1:C:154:ALA:O	2.00	0.61
3:H:6:DT:H2'	3:H:7:DA:C8	2.36	0.61
1:A:223:ILE:HA	1:A:226:MET:HE2	1.81	0.61
1:D:110:ALA:N	1:D:111:PRO:HD2	2.15	0.61
3:H:6:DT:H1'	7:H:101:HOH:O	2.00	0.61
2:E:1:DT:H5"	2:E:1:DT:H6	1.65	0.61
1:A:214:HIS:CG	1:A:215:PRO:HD2	2.36	0.61
1:D:167:ARG:NH2	3:J:9:DT:OP1	2.28	0.61
1:C:182:LEU:HD23	1:C:182:LEU:O	2.01	0.61
1:A:30:LEU:HD21	1:A:272:HIS:ND1	2.16	0.60
1:A:269:ALA:O	1:A:273:GLU:HG3	2.01	0.60
3:F:13:DC:H2'	3:F:14:DA:C8	2.37	0.60
3:L:2:DT:H2"	3:L:3:DG:O5'	2.01	0.60
1:C:188:TRP:HA	1:C:192:GLY:O	2.02	0.59
1:B:182:LEU:O	1:B:182:LEU:HD12	2.03	0.59
1:C:54:ASP:O	1:C:99:GLY:HA2	2.02	0.59
1:C:123:MET:HG2	1:D:107:TRP:HZ3	1.67	0.59
1:B:241:PHE:HB3	6:B:601:SFG:O4'	2.02	0.59
3:L:2:DT:H4'	3:L:3:DG:OP1	2.02	0.59
1:A:48:LEU:HD12	1:A:49:PRO:HD2	1.84	0.58
1:C:54:ASP:HB3	7:C:712:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ASP:OD2	1:B:96:LYS:HD2	2.02	0.58
1:C:34:ILE:HG23	1:C:258:PHE:HB3	1.84	0.58
1:D:36:LEU:HD22	1:D:36:LEU:H	1.67	0.58
2:I:9:DT:H2"	2:I:10:DA:C8	2.39	0.58
1:C:86:GLU:O	1:C:90:LEU:HG	2.03	0.57
2:I:9:DT:H5'	2:I:9:DT:H6	1.69	0.57
1:D:59:ASP:HB3	6:D:601:SFG:HG1	1.85	0.57
1:C:139:THR:OG1	2:I:10:DA:H5'	2.03	0.57
1:D:133:VAL:HG21	1:D:203:ARG:NH2	2.20	0.57
3:J:14:DA:N7	7:J:101:HOH:O	2.32	0.57
1:B:269:ALA:O	1:B:273:GLU:HG3	2.04	0.57
1:A:208:HIS:CD2	1:A:210:GLU:H	2.11	0.57
3:H:6:DT:H4'	3:H:7:DA:OP1	2.05	0.56
1:D:242:MET:HG3	1:D:262:GLU:HB2	1.87	0.56
1:C:263:ILE:HD11	6:C:601:SFG:C5	2.35	0.56
1:D:236:ARG:HG3	1:D:257:ASP:CB	2.36	0.56
3:J:13:DC:H2'	3:J:14:DA:C8	2.41	0.56
1:C:163:LEU:O	1:C:166:VAL:HG22	2.06	0.55
1:C:107:TRP:HZ3	1:D:123:MET:HG2	1.71	0.55
1:D:83:TRP:O	1:D:86:GLU:HB2	2.06	0.55
1:D:236:ARG:HA	1:D:257:ASP:HB2	1.87	0.55
1:D:58:ALA:O	1:D:60:PRO:HD3	2.07	0.55
1:C:249:VAL:HG13	1:C:278:LEU:HD11	1.89	0.55
1:C:146:VAL:HG12	1:D:197:ASP:OD1	2.06	0.55
1:A:167:ARG:NH2	3:H:9:DT:OP1	2.39	0.55
1:C:194:ASN:O	1:C:196:LYS:HG3	2.08	0.54
1:D:187:LYS:NZ	3:J:8:DG:OP1	2.38	0.54
1:D:236:ARG:HG3	1:D:257:ASP:HB2	1.89	0.53
1:D:92:ILE:HB	1:D:93:PRO:HD3	1.90	0.53
3:J:5:DC:H2"	3:J:6:DT:O5'	2.09	0.53
1:C:47:HIS:N	7:C:701:HOH:O	2.40	0.53
1:C:249:VAL:HG12	1:C:253:ARG:HD3	1.90	0.53
2:E:9:DT:H2"	2:E:10:DA:C8	2.43	0.53
3:F:2:DT:H4'	3:F:3:DG:OP1	2.09	0.53
1:A:88:LEU:HD22	1:A:117:LEU:HD21	1.91	0.53
1:D:244:SER:HB3	6:D:601:SFG:O	2.09	0.53
1:A:271:ALA:O	1:A:275:VAL:HG23	2.09	0.53
1:C:179:SER:O	1:C:180:ARG:HG2	2.08	0.53
1:A:30:LEU:HD11	1:A:272:HIS:CE1	2.43	0.52
1:C:73:ASP:OD2	2:I:7:DA:H2	1.93	0.52
1:C:241:PHE:HB3	6:C:601:SFG:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:9:DT:H5'	2:I:9:DT:C6	2.44	0.52
1:C:137:GLY:O	3:J:8:DG:N2	2.39	0.52
1:B:208:HIS:CD2	1:B:210:GLU:HB3	2.45	0.52
2:K:12:DC:H2'	2:K:13:DC:C6	2.45	0.52
1:A:249:VAL:O	1:A:253:ARG:HG2	2.09	0.52
5:A:801:EPE:H102	3:F:9:DT:H3	1.74	0.52
1:C:224:GLU:HG2	1:C:250:ALA:HB1	1.92	0.52
1:D:187:LYS:HG2	1:D:191:MET:SD	2.50	0.51
1:C:127:ILE:HG21	1:C:199:TRP:CE2	2.46	0.51
1:C:141:ARG:NE	2:I:11:DG:OP1	2.41	0.51
2:I:5:DT:H2"	2:I:6:DA:N7	2.26	0.51
1:A:164:ASP:HA	1:A:167:ARG:HD2	1.92	0.50
2:E:10:DA:C2'	2:E:11:DG:C8	2.94	0.50
1:B:53:ILE:O	1:B:96:LYS:HG2	2.10	0.50
1:D:203:ARG:HD3	2:K:6:DA:H4'	1.93	0.50
1:D:237:VAL:N	1:D:257:ASP:O	2.37	0.50
1:B:30:LEU:HD21	1:B:36:LEU:HD13	1.94	0.50
1:A:199:TRP:CE3	1:A:222:ILE:HG23	2.46	0.50
1:C:57:VAL:HG12	1:C:57:VAL:O	2.11	0.50
1:D:231:CYS:SG	1:D:256:ARG:HG2	2.51	0.50
1:C:142:ARG:NH1	2:I:10:DA:OP1	2.39	0.49
1:B:214:HIS:CE1	6:B:601:SFG:HB1	2.47	0.49
3:H:4:DG:H2"	3:H:5:DC:OP2	2.12	0.49
1:A:241:PHE:HD1	6:A:802:SFG:C4	2.26	0.49
1:D:251:CYS:HB3	1:D:256:ARG:O	2.11	0.49
2:E:1:DT:H5"	2:E:1:DT:C6	2.47	0.49
1:D:179:SER:O	1:D:180:ARG:HG2	2.13	0.49
1:C:56:ILE:HG12	1:C:238:LEU:HD23	1.95	0.49
1:A:45:ALA:O	1:A:94:LYS:HE3	2.11	0.49
1:C:141:ARG:HA	1:D:161:PHE:HD2	1.78	0.49
1:D:264:ASN:HB3	1:D:267:TYR:CD2	2.48	0.49
1:A:262:GLU:HG2	1:A:267:TYR:HB2	1.95	0.48
2:G:5:DT:H6	4:O:1:GLC:H62	1.78	0.48
3:J:6:DT:H4'	3:J:7:DA:OP1	2.13	0.48
1:C:178:ARG:NH1	7:C:703:HOH:O	2.45	0.48
3:L:1:DA:H2"	3:L:2:DT:O5'	2.13	0.48
1:A:179:SER:O	1:A:180:ARG:HG2	2.13	0.48
1:D:59:ASP:O	6:D:601:SFG:HG1	2.13	0.48
2:G:13:DC:H2"	2:G:14:DA:N7	2.28	0.48
1:C:181:LYS:CA	1:C:184:GLU:HG3	2.42	0.48
1:D:252:ALA:O	1:D:253:ARG:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:HG3	1:A:257:ASP:HB3	1.95	0.48
3:L:6:DT:H4'	3:L:7:DA:OP1	2.14	0.48
1:A:92:ILE:N	1:A:93:PRO:HD2	2.28	0.48
1:D:59:ASP:HB3	6:D:601:SFG:CG	2.44	0.48
1:D:66:LYS:HB2	1:D:73:ASP:OD2	2.14	0.48
1:A:164:ASP:HA	1:A:167:ARG:HG3	1.96	0.47
3:H:6:DT:H2"	3:H:7:DA:O5'	2.13	0.47
1:A:47:HIS:N	1:A:47:HIS:CD2	2.83	0.47
1:C:55:LEU:HD13	1:C:230:SER:HB3	1.96	0.47
1:C:57:VAL:HG22	1:C:226:MET:HE3	1.95	0.47
1:D:36:LEU:HD12	1:D:242:MET:HE1	1.96	0.47
3:H:5:DC:H2'	3:H:6:DT:H72	1.96	0.47
1:A:88:LEU:O	1:A:92:ILE:HG13	2.14	0.47
1:A:178:ARG:NH1	7:A:907:HOH:O	2.44	0.47
1:C:213:ASP:N	7:C:704:HOH:O	2.46	0.47
1:A:137:GLY:N	5:A:801:EPE:O2S	2.48	0.47
1:C:123:MET:HG2	1:D:107:TRP:CZ3	2.49	0.47
1:B:249:VAL:O	1:B:253:ARG:HG3	2.14	0.47
1:D:206:ARG:HD2	1:D:206:ARG:HA	1.66	0.47
1:B:30:LEU:HD12	1:B:30:LEU:HA	1.74	0.47
1:C:141:ARG:HG2	1:C:141:ARG:HH11	1.80	0.47
1:C:164:ASP:N	1:C:165:PRO:HD2	2.30	0.46
1:C:199:TRP:CZ2	1:C:225:ARG:HD2	2.50	0.46
2:G:5:DT:H73	4:O:1:GLC:O6	2.15	0.46
3:H:2:DT:H2"	3:H:3:DG:C8	2.51	0.46
1:A:118:LYS:NZ	1:B:112:GLU:OE1	2.47	0.46
3:H:2:DT:H2"	3:H:3:DG:O5'	2.13	0.46
1:A:143:PHE:CD1	1:B:195:PRO:HG2	2.50	0.46
2:E:2:DT:H3'	7:E:101:HOH:O	2.15	0.46
3:L:1:DA:C8	3:L:1:DA:H5"	2.50	0.46
1:A:235:GLY:O	1:A:257:ASP:HB2	2.16	0.46
3:J:7:DA:H1'	3:J:8:DG:H5'	1.98	0.46
1:C:154:ALA:HB1	1:C:159:TYR:HB3	1.98	0.46
1:A:142:ARG:HB2	1:B:125:ASN:OD1	2.16	0.46
1:C:42:LEU:HD13	1:C:90:LEU:HD12	1.98	0.46
1:C:44:ASP:OD1	1:C:44:ASP:O	2.34	0.46
1:C:141:ARG:HA	1:D:161:PHE:CD2	2.50	0.46
1:D:272:HIS:HA	1:D:275:VAL:HG22	1.98	0.46
1:A:132[A]:ARG:HE	1:A:200:SER:HB3	1.81	0.46
1:A:198:VAL:CG2	1:B:147:HIS:HB3	2.46	0.46
1:D:84:THR:HA	1:D:87:TRP:NE1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:THR:HA	1:C:87:TRP:NE1	2.31	0.45
1:C:92:ILE:N	1:C:93:PRO:HD2	2.31	0.45
1:D:37:HIS:O	1:D:261:TYR:HA	2.16	0.45
3:H:9:DT:H5"	7:H:105:HOH:O	2.17	0.45
1:B:207:GLN:O	3:H:14:DA:H5'	2.16	0.45
1:C:208:HIS:CD2	3:J:13:DC:H5"	2.52	0.45
1:D:207:GLN:NE2	2:K:3:DG:H21	2.14	0.45
1:C:70:ASN:HB2	1:C:71:ASP:H	1.65	0.45
1:A:214:HIS:CD2	1:A:215:PRO:HD2	2.51	0.45
1:C:147:HIS:HB3	1:D:198:VAL:CG2	2.46	0.45
1:C:207:GLN:O	3:J:14:DA:H5'	2.17	0.45
1:A:164:ASP:HA	1:A:167:ARG:CD	2.47	0.45
1:D:110:ALA:N	1:D:111:PRO:CD	2.79	0.45
1:B:110:ALA:N	1:B:111:PRO:HD2	2.31	0.45
3:J:6:DT:H2'	3:J:7:DA:C8	2.53	0.44
7:B:747:HOH:O	2:G:7:DA:H5"	2.18	0.44
1:A:133:VAL:HA	1:A:134:PRO:HD3	1.88	0.44
1:D:116:PHE:HD2	1:D:117:LEU:HD12	1.82	0.44
1:A:146:VAL:CG1	1:B:198:VAL:HG23	2.48	0.44
2:E:1:DT:H2"	2:E:2:DT:O5'	2.16	0.44
1:C:40:ASP:HB3	1:C:43:THR:HG23	1.99	0.44
1:A:163:LEU:HG	1:A:167:ARG:HG2	2.00	0.44
1:C:214:HIS:HE1	1:C:216:THR:OG1	2.01	0.44
1:B:212:VAL:HG22	1:B:217:GLN:OE1	2.18	0.44
1:C:42:LEU:HD13	1:C:90:LEU:CD1	2.48	0.44
1:D:272:HIS:O	1:D:276:ASN:HB2	2.18	0.44
1:A:143:PHE:CE1	1:B:195:PRO:HG2	2.53	0.43
1:C:244:SER:O	1:C:274:ARG:HD3	2.17	0.43
1:A:68:TYR:HD2	1:A:72:SER:OG	2.01	0.43
1:A:142:ARG:HD2	2:E:10:DA:OP1	2.18	0.43
1:A:186:SER:HB3	1:A:188:TRP:CD1	2.53	0.43
1:A:207:GLN:O	3:F:14:DA:H5'	2.18	0.43
3:F:2:DT:H2"	3:F:3:DG:O5'	2.17	0.43
1:D:56:ILE:HG12	1:D:238:LEU:HD23	2.00	0.43
1:C:251:CYS:HB3	1:C:256:ARG:O	2.17	0.43
1:D:203:ARG:HD2	1:D:204:LEU:C	2.39	0.43
1:D:266:SER:O	1:D:269:ALA:HB3	2.18	0.43
2:E:12:DC:C6	2:E:12:DC:C5'	3.00	0.43
1:D:242:MET:HE2	1:D:242:MET:HB2	1.63	0.43
1:A:141:ARG:HD3	2:E:11:DG:OP1	2.19	0.43
3:H:6:DT:O2	7:H:101:HOH:O	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:TRP:HE3	1:A:222:ILE:HG23	1.83	0.43
1:A:194:ASN:HD21	1:B:143:PHE:HA	1.84	0.43
1:C:110:ALA:O	1:C:111:PRO:C	2.57	0.43
1:D:236:ARG:HG3	1:D:257:ASP:HB3	2.01	0.43
1:D:133:VAL:HG11	1:D:203:ARG:NH2	2.26	0.43
1:D:242:MET:HE3	1:D:258:PHE:CE2	2.54	0.43
1:D:34:ILE:N	7:D:708:HOH:O	2.52	0.42
2:E:11:DG:H2"	2:E:12:DC:C5'	2.49	0.42
1:D:131:ARG:HD3	7:D:707:HOH:O	2.18	0.42
1:D:203:ARG:HD3	2:K:6:DA:C4'	2.49	0.42
6:B:601:SFG:HG2	6:B:601:SFG:H4'	1.89	0.42
3:F:1:DA:C8	3:F:1:DA:H5"	2.54	0.42
1:C:47:HIS:HB2	7:C:701:HOH:O	2.20	0.42
1:D:203:ARG:HH11	1:D:205:HIS:N	2.18	0.42
1:A:134:PRO:HG3	1:B:196:LYS:HD3	2.01	0.42
1:C:141:ARG:HG2	1:C:141:ARG:NH1	2.33	0.42
1:B:139:THR:HA	7:B:783:HOH:O	2.19	0.42
1:A:137:GLY:CA	5:A:801:EPE:O2S	2.67	0.42
1:A:237:VAL:HG22	1:A:258:PHE:HD1	1.84	0.42
1:D:102:TYR:CD2	1:D:226:MET:HB3	2.54	0.42
1:D:236:ARG:HG3	1:D:236:ARG:HH11	1.84	0.42
1:B:30:LEU:N	7:B:709:HOH:O	2.52	0.42
1:A:37:HIS:O	1:A:261:TYR:HA	2.18	0.42
3:F:10:DT:H72	1:B:188:TRP:CZ2	2.55	0.42
1:C:35:GLU:O	1:C:259:VAL:HA	2.19	0.42
1:D:148:ASP:HA	7:D:705:HOH:O	2.19	0.42
1:B:132:ARG:O	3:H:11:DA:H4'	2.20	0.42
3:H:6:DT:H2"	3:H:7:DA:C5'	2.50	0.42
1:C:56:ILE:CB	1:C:101:MET:HG3	2.47	0.42
1:A:264:ASN:HB3	1:A:267:TYR:CD2	2.54	0.42
1:A:36:LEU:N	1:A:36:LEU:CD1	2.83	0.41
1:A:84:THR:HG22	1:A:88:LEU:HD12	2.02	0.41
1:A:218:LYS:HA	1:A:219:PRO:HD3	1.95	0.41
6:C:601:SFG:H4'	6:C:601:SFG:HG2	1.67	0.41
3:H:2:DT:C2'	3:H:3:DG:C8	3.03	0.41
1:D:57:VAL:HG22	1:D:226:MET:HE3	2.02	0.41
1:D:166:VAL:CG1	1:D:195:PRO:HG2	2.50	0.41
1:A:188:TRP:HA	1:A:192:GLY:O	2.21	0.41
1:C:80:PHE:CD2	1:C:81:LEU:HD23	2.56	0.41
1:C:92:ILE:HG23	1:C:121:LEU:HD21	2.03	0.41
1:A:108:GLN:HG2	4:N:2:FRU:O4	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ILE:HG23	1:D:236:ARG:O	2.20	0.41
1:D:62:TYR:HB2	2:K:7:DA:C2	2.55	0.41
1:D:179:SER:C	1:D:180:ARG:HG2	2.40	0.41
1:D:235:GLY:O	1:D:257:ASP:N	2.43	0.41
1:A:187:LYS:HD2	3:H:8:DG:OP1	2.20	0.41
1:C:52:SER:C	1:C:96:LYS:HE2	2.40	0.41
1:C:122:THR:O	1:C:153:PHE:HA	2.20	0.41
1:D:206:ARG:HA	1:D:211:ARG:HG2	2.02	0.41
1:A:163:LEU:HD12	1:A:166:VAL:HG23	2.03	0.41
1:C:68:TYR:HD1	1:C:68:TYR:HA	1.78	0.41
1:C:107:TRP:CZ3	1:D:123:MET:HG2	2.55	0.41
1:D:231:CYS:HA	1:D:232:PRO:HD3	1.95	0.41
1:A:48:LEU:HA	1:A:49:PRO:HD3	1.91	0.41
1:D:102:TYR:CE2	1:D:226:MET:HB3	2.56	0.41
1:C:125:ASN:HB2	1:C:152:PHE:HD2	1.86	0.40
1:D:263:ILE:HG22	6:D:601:SFG:C4	2.50	0.40
1:B:34:ILE:HG22	1:B:36:LEU:HD11	2.04	0.40
1:B:62:TYR:CD1	2:G:7:DA:C6	3.09	0.40
1:A:208:HIS:CD2	1:A:210:GLU:HB2	2.56	0.40
3:L:5:DC:H2'	3:L:6:DT:C5	2.56	0.40
1:D:262:GLU:OE1	6:D:601:SFG:H1'	2.21	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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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 (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	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

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASP
1	A	100	SER
1	A	140	THR
1	A	142	ARG
1	A	203	ARG
1	A	247	THR
1	A	253	ARG
1	A	256	ARG
1	A	259	VAL
1	A	266	SER
1	A	270	ILE

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Mol	Chain	Res	Type
1	C	42	LEU
1	C	54	ASP
1	C	64	LEU
1	C	70	ASN
1	C	106	THR
1	C	197	ASP
1	C	203	ARG
1	C	206	ARG
1	C	247	THR
1	C	257	ASP
1	C	263	ILE
1	C	266	SER
1	D	54	ASP
1	D	70	ASN
1	D	72	SER
1	D	94	LYS
1	D	101	MET
1	D	121	LEU
1	D	140	THR
1	D	142	ARG
1	D	213	ASP
1	D	242	MET
1	D	276	ASN
1	B	32	SER
1	B	75	ARG
1	B	85	ARG
1	B	100	SER
1	B	122	THR
1	B	145	SER
1	B	203	ARG
1	B	242	MET
1	B	268	CYS

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 (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)

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.

All (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
4	N	2	FRU	C4-C5-C6-O6
4	N	1	GLC	O5-C5-C6-O6
4	O	2	FRU	O1-C1-C2-C3
4	N	2	FRU	O1-C1-C2-O5
4	O	2	FRU	O1-C1-C2-O5
4	N	2	FRU	O5-C5-C6-O6
4	O	2	FRU	O1-C1-C2-O2
4	N	2	FRU	O1-C1-C2-C3

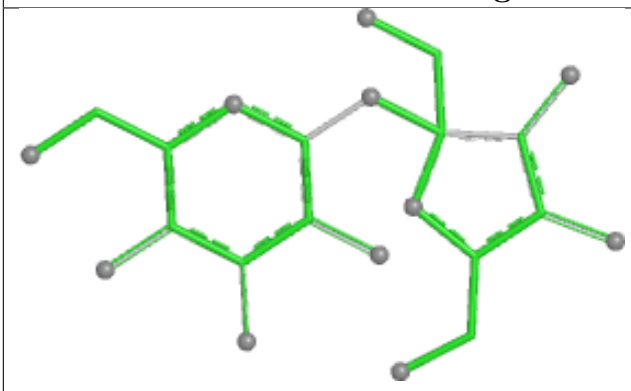
There are no ring outliers.

2 monomers are involved in 3 short contacts:

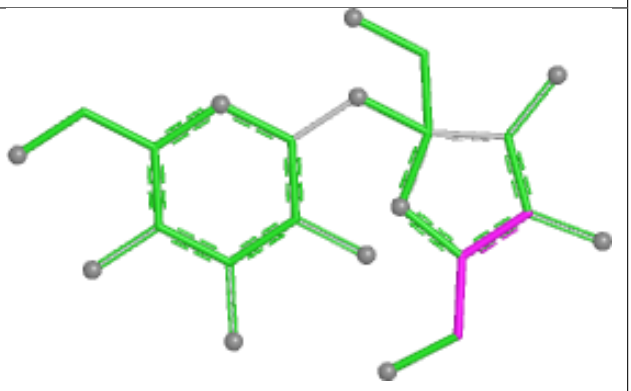
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	2	FRU	1	0
4	O	1	GLC	2	0

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

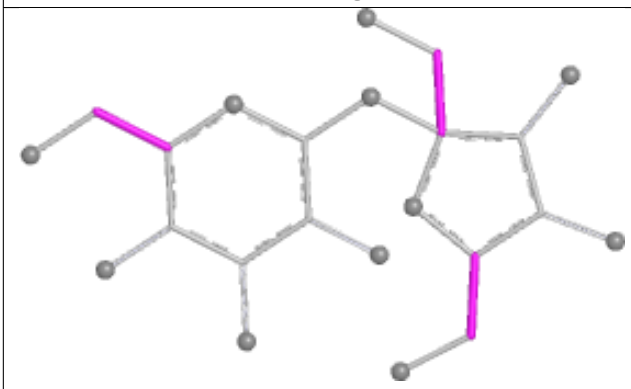
Oligosaccharide Chain N



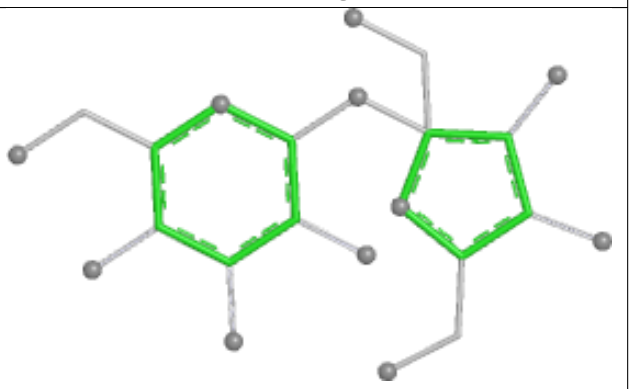
Bond lengths



Bond angles

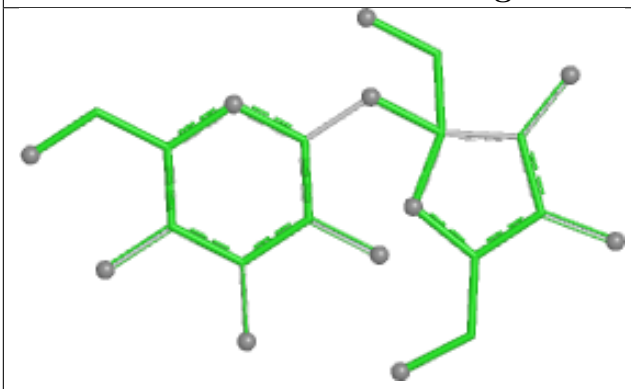


Torsions

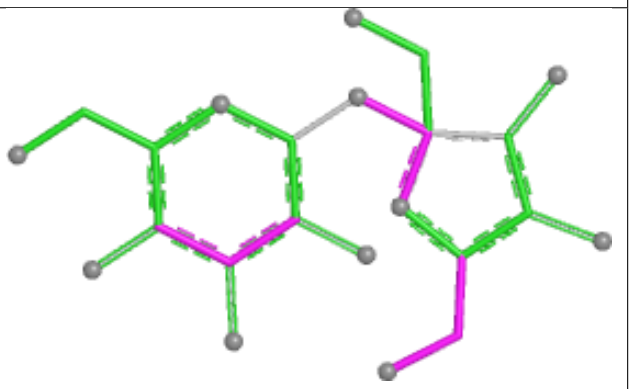


Rings

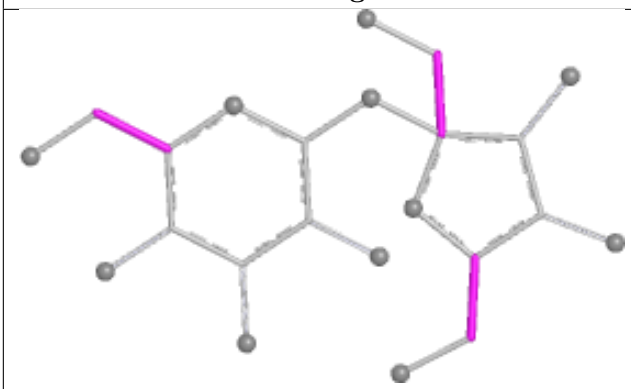
Oligosaccharide Chain O



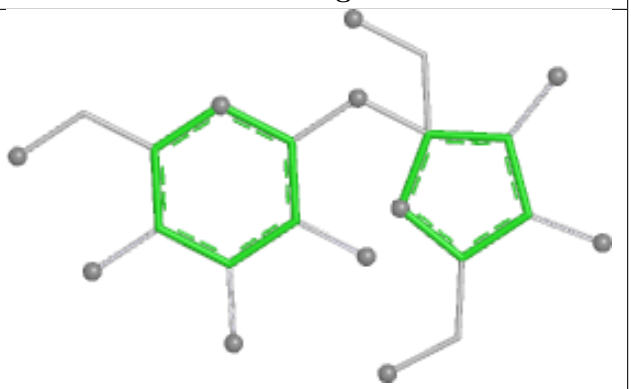
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

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

All (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
6	A	802	SFG	N3-C2-N1	-3.63	123.74	128.67
6	B	601	SFG	N3-C2-N1	-3.49	123.93	128.67
5	A	801	EPE	C7-N4-C3	3.26	119.93	111.24
6	A	802	SFG	C4-C5-N7	-2.83	106.35	109.34
6	B	601	SFG	C4-C5-N7	-2.74	106.44	109.34
6	D	601	SFG	C4-C5-N7	-2.50	106.70	109.34
6	B	601	SFG	C4'-O4'-C1'	-2.42	107.71	109.92
6	B	601	SFG	C1'-N9-C4	-2.23	122.72	126.64
5	A	801	EPE	O1S-S-C10	2.21	110.06	106.73
6	A	802	SFG	C4'-O4'-C1'	-2.20	107.91	109.92
5	A	801	EPE	O3S-S-C10	2.19	110.29	106.00
6	C	601	SFG	C4-C5-N7	-2.18	107.04	109.34
5	A	801	EPE	C6-N1-C2	2.06	113.29	108.84
5	A	801	EPE	O2S-S-O1S	-2.04	107.20	113.82
6	D	601	SFG	C2'-C3'-C4'	2.01	106.50	102.61

There are no chirality outliers.

All (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
5	A	801	EPE	C8-C7-N4-C3
5	A	801	EPE	C10-C9-N1-C2
5	A	801	EPE	C9-C10-S-O2S
6	D	601	SFG	O-C-CA-CB
6	D	601	SFG	OXT-C-CA-CB
6	D	601	SFG	C4'-C5'-CD-NE
5	A	801	EPE	N4-C7-C8-O8
5	A	801	EPE	C10-C9-N1-C6
6	C	601	SFG	O4'-C4'-C5'-CD
6	D	601	SFG	O4'-C4'-C5'-CD
6	C	601	SFG	C4'-C5'-CD-CG
6	B	601	SFG	C4'-C5'-CD-CG
6	C	601	SFG	C3'-C4'-C5'-CD

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Mol	Chain	Res	Type	Atoms
6	D	601	SFG	C3'-C4'-C5'-CD

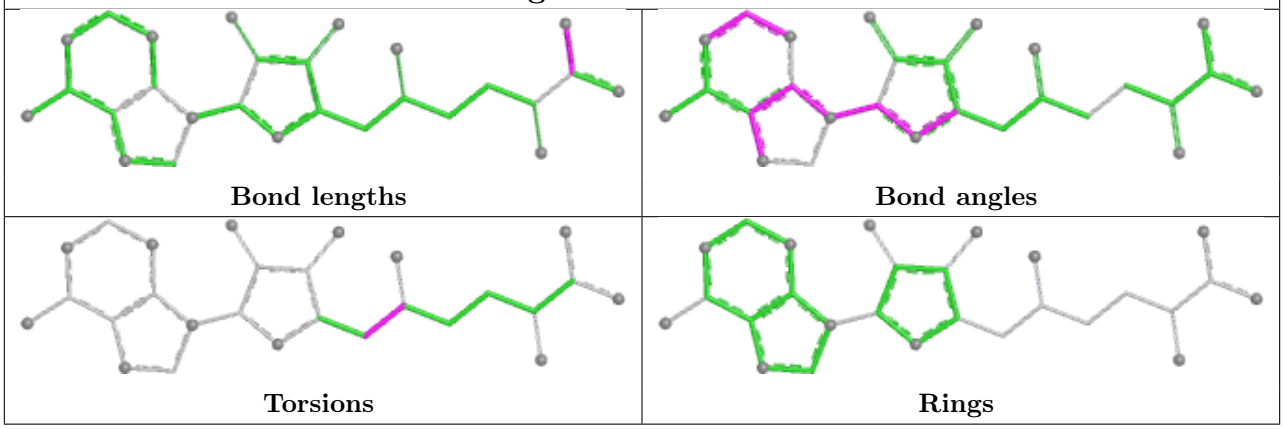
There are no ring outliers.

5 monomers are involved in 19 short contacts:

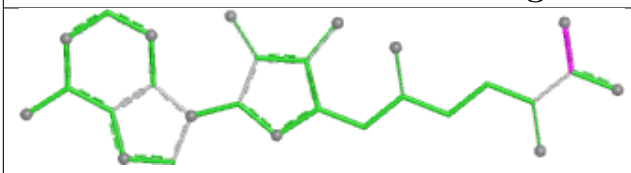
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	601	SFG	3	0
6	C	601	SFG	4	0
6	A	802	SFG	3	0
5	A	801	EPE	3	0
6	D	601	SFG	6	0

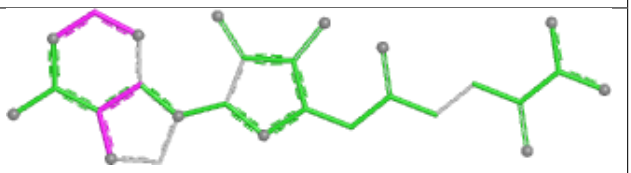
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

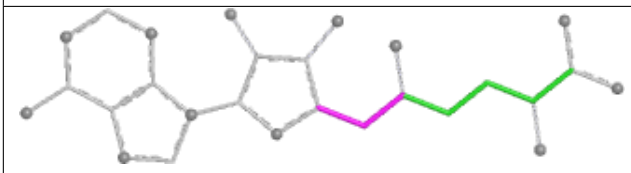
Ligand SFG B 601

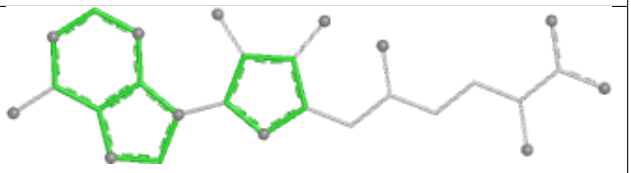


Ligand SFG C 601

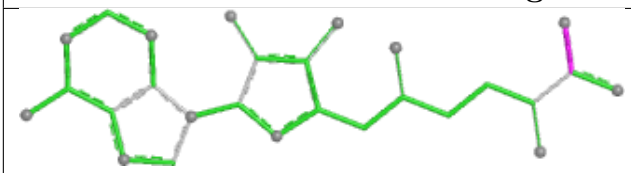

Bond lengths

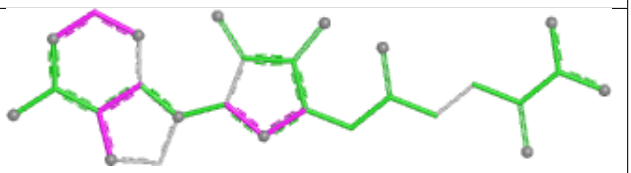

Bond angles

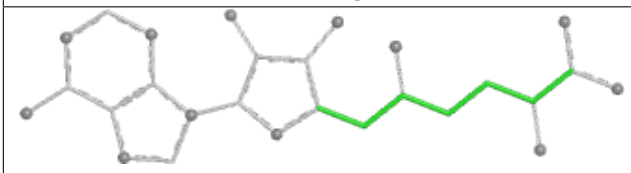

Torsions

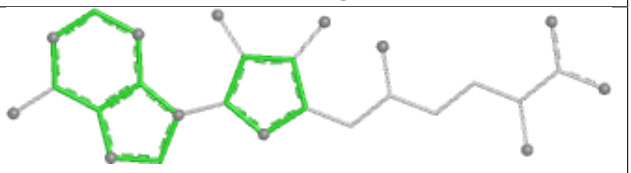

Rings

Ligand SFG A 802

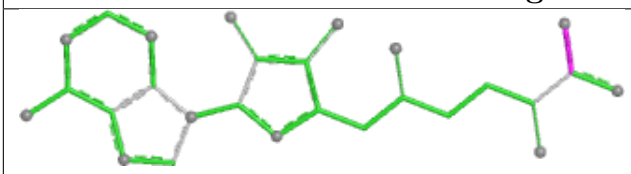

Bond lengths

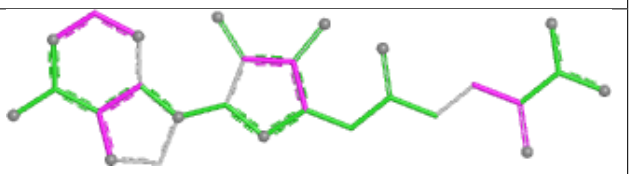

Bond angles

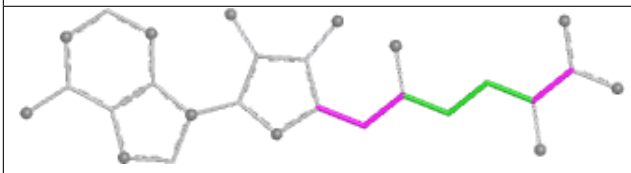

Torsions

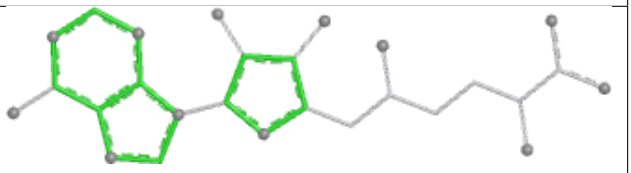

Rings

Ligand SFG D 601


Bond lengths


Bond angles


Torsions


Rings

5.7 Other polymers (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	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%)

All (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
1	D	48	LEU	3.7
1	D	261	TYR	3.6
1	D	258	PHE	3.6
1	D	66	LYS	3.6
1	C	261	TYR	3.6
1	D	34	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	74	LYS	3.4
1	C	263	ILE	3.2
1	D	263	ILE	3.1
1	D	68	TYR	3.1
1	D	47	HIS	3.0
1	D	42	LEU	3.0
1	C	87	TRP	2.9
1	D	49	PRO	2.9
1	D	64	LEU	2.9
1	C	116	PHE	2.9
3	L	1	DA	2.9
1	C	258	PHE	2.9
1	C	151	GLY	2.9
1	C	36	LEU	2.8
1	C	168	ILE	2.8
1	C	35	GLU	2.8
3	H	1	DA	2.8
1	D	56	ILE	2.8
1	C	278	LEU	2.8
1	C	68	TYR	2.7
1	D	53	ILE	2.7
2	K	14	DA	2.7
1	C	44	ASP	2.7
1	D	81	LEU	2.7
1	C	72	SER	2.7
1	D	69	GLY	2.7
1	C	31	PRO	2.6
1	D	36	LEU	2.6
1	C	65	GLY	2.6
1	D	241	PHE	2.6
1	C	90	LEU	2.6
1	D	55	LEU	2.6
1	D	267	TYR	2.6
1	D	82	ALA	2.6
1	C	237	VAL	2.6
1	D	247	THR	2.6
1	D	90	LEU	2.6
1	C	223	ILE	2.5
1	C	124	VAL	2.5
1	C	64	LEU	2.4
1	D	88	LEU	2.4
1	D	271	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	237	VAL	2.4
1	D	117	LEU	2.4
1	C	39	ARG	2.4
1	D	77	GLY	2.4
1	D	138	GLY	2.4
1	D	46	ALA	2.4
1	D	51	ALA	2.4
1	C	34	ILE	2.4
1	D	93	PRO	2.3
1	D	73	ASP	2.3
1	C	121	LEU	2.3
1	D	248	ALA	2.3
1	B	30	LEU	2.3
1	D	72	SER	2.3
1	C	92	ILE	2.2
1	D	92	ILE	2.2
1	D	122	THR	2.2
1	C	154	ALA	2.2
1	C	98	SER	2.2
3	J	1	DA	2.2
1	B	47	HIS	2.2
1	D	83	TRP	2.2
3	H	4	DG	2.2
1	C	153	PHE	2.1
1	D	119	THR	2.1
1	D	87	TRP	2.1
1	C	235	GLY	2.1
1	C	238	LEU	2.1
1	D	253	ARG	2.1
1	C	91	ALA	2.1
1	D	37	HIS	2.1
2	K	12	DC	2.1
1	C	30	LEU	2.1
1	D	277	ALA	2.1
1	C	97	PRO	2.1
1	C	99	GLY	2.1
1	C	37	HIS	2.1
1	C	33	GLY	2.0
1	C	233	PRO	2.0
1	D	120	GLN	2.0
1	D	58	ALA	2.0
1	C	96	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	155	VAL	2.0
1	C	275	VAL	2.0
1	D	212	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)

SUGAR-RSR INFOmissingINFO

6.4 Ligands (i)

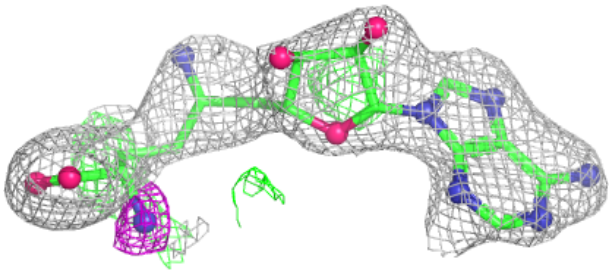
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

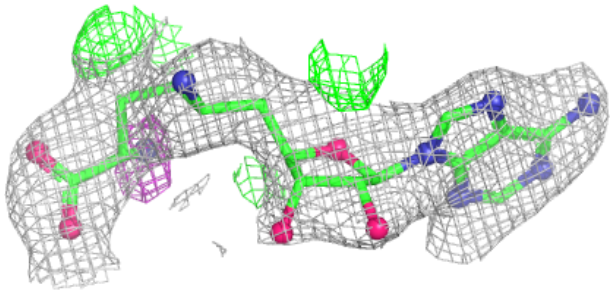
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EPE	A	801	15/15	0.66	0.22	67,81,84,86	0
6	SFG	D	601	27/27	0.73	0.16	56,66,72,73	0
6	SFG	C	601	27/27	0.87	0.09	44,46,48,49	0
6	SFG	A	802	27/27	0.94	0.06	22,24,27,27	0
6	SFG	B	601	27/27	0.94	0.07	22,24,28,28	0

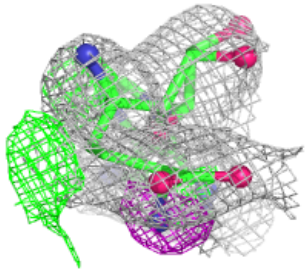
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SFG D 601:

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

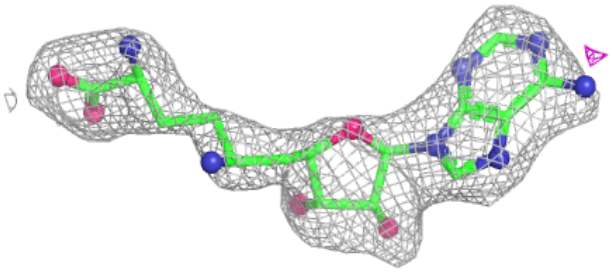


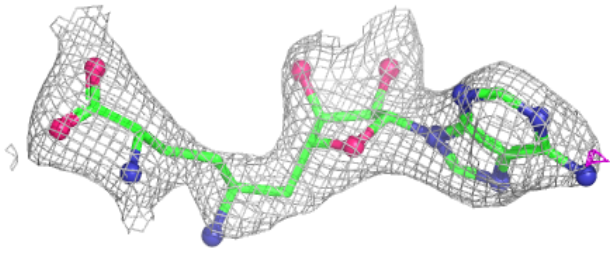


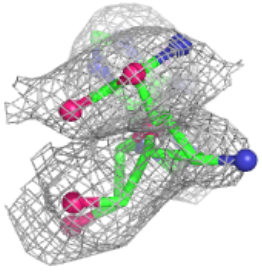


Electron density around SFG C 601:

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

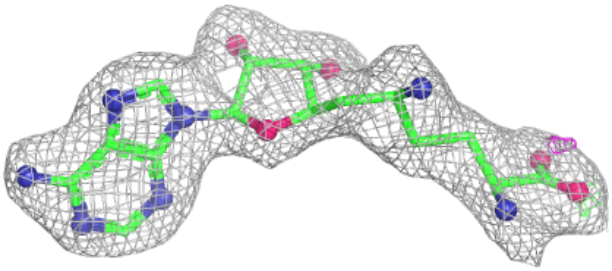


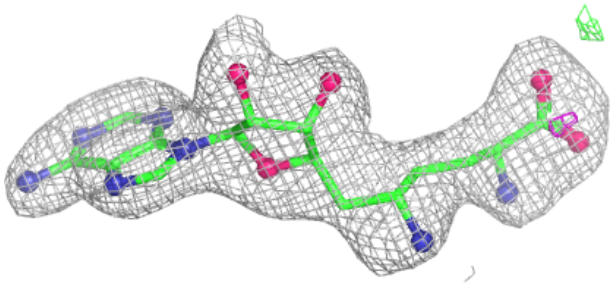


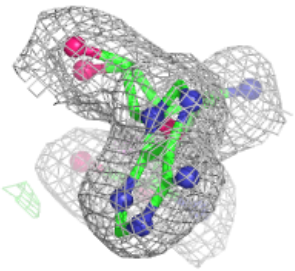


Electron density around SFG A 802:

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

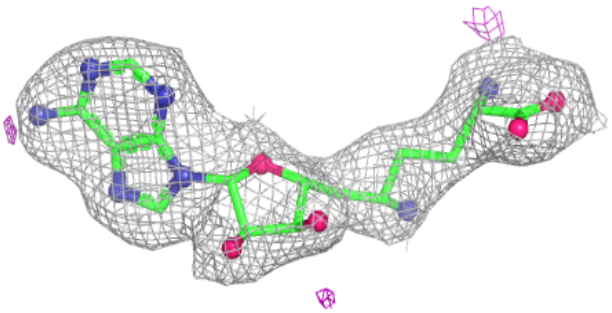


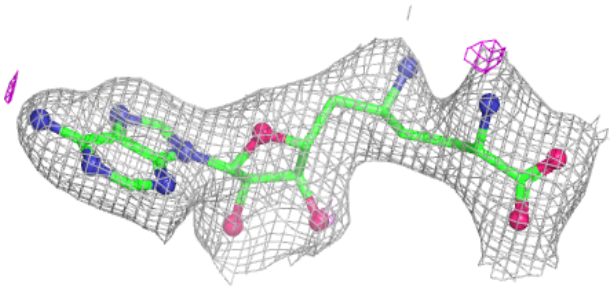


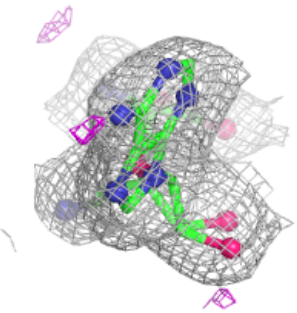


Electron density around SFG B 601:

$2mF_o$-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 (i)

There are no such residues in this entry.