Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2024 – 01:28 pm BST

PDB ID	:	4C3X
Title	:	Crystal structure of 3-ketosteroid delta1-dehydrogenase from Rhodococcus erythropolis SQ1
Authors	:	Rohman, A.; van Oosterwijk, N.; Thunnissen, A.M.W.H.; Dijkstra, B.W.
Deposited on	:	2013-08-28
Resolution	:	2.00 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:

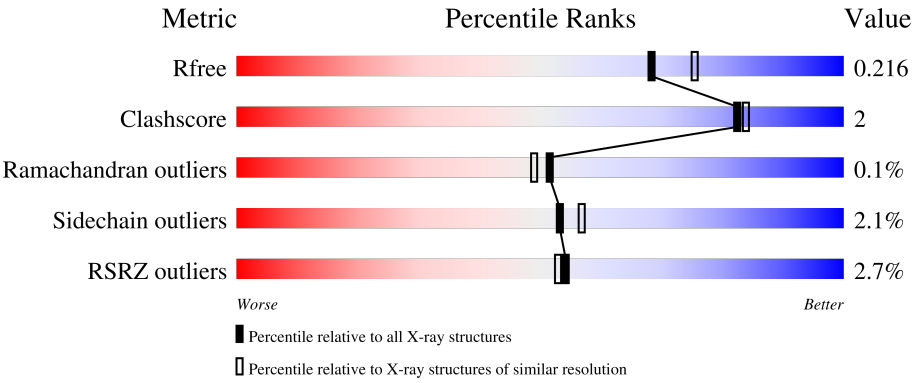
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	530	2% 89% 6% • •
1	B	530	2% 89% 6% • 5%
1	C	530	4% 88% 6% 5%
1	D	530	3% 89% 6% • •
1	E	530	3% 90% 5% • •

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Mol	Chain	Length	Quality of chain
1	F	530	4% 89% 5% • 5%
1	G	530	% 89% 5% • 5%
1	H	530	3% 90% 5% • •
2	I	2	100%
2	J	2	100%
2	K	2	100%
2	L	2	50% 50%
2	M	2	100%
2	N	2	100%
2	O	2	100%
2	P	2	100%
2	Q	2	100%
2	R	2	100%
2	S	2	100%
2	T	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PG4	E	582	-	-	-	X
6	PG4	H	582	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 33549 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 3-KETOSTEROID DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	0	0
			3712	2305	647	746	14			
1	B	505	Total	C	N	O	S	0	0	0
			3693	2294	643	742	14			
1	C	505	Total	C	N	O	S	0	0	0
			3693	2294	643	742	14			
1	D	508	Total	C	N	O	S	0	0	0
			3712	2305	647	746	14			
1	E	508	Total	C	N	O	S	0	0	0
			3712	2305	647	746	14			
1	F	505	Total	C	N	O	S	0	0	0
			3693	2294	643	742	14			
1	G	505	Total	C	N	O	S	0	0	0
			3693	2294	643	742	14			
1	H	508	Total	C	N	O	S	0	0	0
			3712	2305	647	746	14			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q9RA02
A	-18	GLY	-	expression tag	UNP Q9RA02
A	-17	SER	-	expression tag	UNP Q9RA02
A	-16	SER	-	expression tag	UNP Q9RA02
A	-15	HIS	-	expression tag	UNP Q9RA02
A	-14	HIS	-	expression tag	UNP Q9RA02
A	-13	HIS	-	expression tag	UNP Q9RA02
A	-12	HIS	-	expression tag	UNP Q9RA02
A	-11	HIS	-	expression tag	UNP Q9RA02
A	-10	HIS	-	expression tag	UNP Q9RA02
A	-9	SER	-	expression tag	UNP Q9RA02
A	-8	SER	-	expression tag	UNP Q9RA02
A	-7	GLY	-	expression tag	UNP Q9RA02

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP Q9RA02
A	-5	VAL	-	expression tag	UNP Q9RA02
A	-4	PRO	-	expression tag	UNP Q9RA02
A	-3	ARG	-	expression tag	UNP Q9RA02
A	-2	GLY	-	expression tag	UNP Q9RA02
A	-1	SER	-	expression tag	UNP Q9RA02
A	0	HIS	-	expression tag	UNP Q9RA02
B	-19	MET	-	expression tag	UNP Q9RA02
B	-18	GLY	-	expression tag	UNP Q9RA02
B	-17	SER	-	expression tag	UNP Q9RA02
B	-16	SER	-	expression tag	UNP Q9RA02
B	-15	HIS	-	expression tag	UNP Q9RA02
B	-14	HIS	-	expression tag	UNP Q9RA02
B	-13	HIS	-	expression tag	UNP Q9RA02
B	-12	HIS	-	expression tag	UNP Q9RA02
B	-11	HIS	-	expression tag	UNP Q9RA02
B	-10	HIS	-	expression tag	UNP Q9RA02
B	-9	SER	-	expression tag	UNP Q9RA02
B	-8	SER	-	expression tag	UNP Q9RA02
B	-7	GLY	-	expression tag	UNP Q9RA02
B	-6	LEU	-	expression tag	UNP Q9RA02
B	-5	VAL	-	expression tag	UNP Q9RA02
B	-4	PRO	-	expression tag	UNP Q9RA02
B	-3	ARG	-	expression tag	UNP Q9RA02
B	-2	GLY	-	expression tag	UNP Q9RA02
B	-1	SER	-	expression tag	UNP Q9RA02
B	0	HIS	-	expression tag	UNP Q9RA02
C	-19	MET	-	expression tag	UNP Q9RA02
C	-18	GLY	-	expression tag	UNP Q9RA02
C	-17	SER	-	expression tag	UNP Q9RA02
C	-16	SER	-	expression tag	UNP Q9RA02
C	-15	HIS	-	expression tag	UNP Q9RA02
C	-14	HIS	-	expression tag	UNP Q9RA02
C	-13	HIS	-	expression tag	UNP Q9RA02
C	-12	HIS	-	expression tag	UNP Q9RA02
C	-11	HIS	-	expression tag	UNP Q9RA02
C	-10	HIS	-	expression tag	UNP Q9RA02
C	-9	SER	-	expression tag	UNP Q9RA02
C	-8	SER	-	expression tag	UNP Q9RA02
C	-7	GLY	-	expression tag	UNP Q9RA02
C	-6	LEU	-	expression tag	UNP Q9RA02
C	-5	VAL	-	expression tag	UNP Q9RA02

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP Q9RA02
C	-3	ARG	-	expression tag	UNP Q9RA02
C	-2	GLY	-	expression tag	UNP Q9RA02
C	-1	SER	-	expression tag	UNP Q9RA02
C	0	HIS	-	expression tag	UNP Q9RA02
D	-19	MET	-	expression tag	UNP Q9RA02
D	-18	GLY	-	expression tag	UNP Q9RA02
D	-17	SER	-	expression tag	UNP Q9RA02
D	-16	SER	-	expression tag	UNP Q9RA02
D	-15	HIS	-	expression tag	UNP Q9RA02
D	-14	HIS	-	expression tag	UNP Q9RA02
D	-13	HIS	-	expression tag	UNP Q9RA02
D	-12	HIS	-	expression tag	UNP Q9RA02
D	-11	HIS	-	expression tag	UNP Q9RA02
D	-10	HIS	-	expression tag	UNP Q9RA02
D	-9	SER	-	expression tag	UNP Q9RA02
D	-8	SER	-	expression tag	UNP Q9RA02
D	-7	GLY	-	expression tag	UNP Q9RA02
D	-6	LEU	-	expression tag	UNP Q9RA02
D	-5	VAL	-	expression tag	UNP Q9RA02
D	-4	PRO	-	expression tag	UNP Q9RA02
D	-3	ARG	-	expression tag	UNP Q9RA02
D	-2	GLY	-	expression tag	UNP Q9RA02
D	-1	SER	-	expression tag	UNP Q9RA02
D	0	HIS	-	expression tag	UNP Q9RA02
E	-19	MET	-	expression tag	UNP Q9RA02
E	-18	GLY	-	expression tag	UNP Q9RA02
E	-17	SER	-	expression tag	UNP Q9RA02
E	-16	SER	-	expression tag	UNP Q9RA02
E	-15	HIS	-	expression tag	UNP Q9RA02
E	-14	HIS	-	expression tag	UNP Q9RA02
E	-13	HIS	-	expression tag	UNP Q9RA02
E	-12	HIS	-	expression tag	UNP Q9RA02
E	-11	HIS	-	expression tag	UNP Q9RA02
E	-10	HIS	-	expression tag	UNP Q9RA02
E	-9	SER	-	expression tag	UNP Q9RA02
E	-8	SER	-	expression tag	UNP Q9RA02
E	-7	GLY	-	expression tag	UNP Q9RA02
E	-6	LEU	-	expression tag	UNP Q9RA02
E	-5	VAL	-	expression tag	UNP Q9RA02
E	-4	PRO	-	expression tag	UNP Q9RA02
E	-3	ARG	-	expression tag	UNP Q9RA02

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q9RA02
E	-1	SER	-	expression tag	UNP Q9RA02
E	0	HIS	-	expression tag	UNP Q9RA02
F	-19	MET	-	expression tag	UNP Q9RA02
F	-18	GLY	-	expression tag	UNP Q9RA02
F	-17	SER	-	expression tag	UNP Q9RA02
F	-16	SER	-	expression tag	UNP Q9RA02
F	-15	HIS	-	expression tag	UNP Q9RA02
F	-14	HIS	-	expression tag	UNP Q9RA02
F	-13	HIS	-	expression tag	UNP Q9RA02
F	-12	HIS	-	expression tag	UNP Q9RA02
F	-11	HIS	-	expression tag	UNP Q9RA02
F	-10	HIS	-	expression tag	UNP Q9RA02
F	-9	SER	-	expression tag	UNP Q9RA02
F	-8	SER	-	expression tag	UNP Q9RA02
F	-7	GLY	-	expression tag	UNP Q9RA02
F	-6	LEU	-	expression tag	UNP Q9RA02
F	-5	VAL	-	expression tag	UNP Q9RA02
F	-4	PRO	-	expression tag	UNP Q9RA02
F	-3	ARG	-	expression tag	UNP Q9RA02
F	-2	GLY	-	expression tag	UNP Q9RA02
F	-1	SER	-	expression tag	UNP Q9RA02
F	0	HIS	-	expression tag	UNP Q9RA02
G	-19	MET	-	expression tag	UNP Q9RA02
G	-18	GLY	-	expression tag	UNP Q9RA02
G	-17	SER	-	expression tag	UNP Q9RA02
G	-16	SER	-	expression tag	UNP Q9RA02
G	-15	HIS	-	expression tag	UNP Q9RA02
G	-14	HIS	-	expression tag	UNP Q9RA02
G	-13	HIS	-	expression tag	UNP Q9RA02
G	-12	HIS	-	expression tag	UNP Q9RA02
G	-11	HIS	-	expression tag	UNP Q9RA02
G	-10	HIS	-	expression tag	UNP Q9RA02
G	-9	SER	-	expression tag	UNP Q9RA02
G	-8	SER	-	expression tag	UNP Q9RA02
G	-7	GLY	-	expression tag	UNP Q9RA02
G	-6	LEU	-	expression tag	UNP Q9RA02
G	-5	VAL	-	expression tag	UNP Q9RA02
G	-4	PRO	-	expression tag	UNP Q9RA02
G	-3	ARG	-	expression tag	UNP Q9RA02
G	-2	GLY	-	expression tag	UNP Q9RA02
G	-1	SER	-	expression tag	UNP Q9RA02

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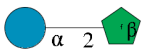
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q9RA02
H	-19	MET	-	expression tag	UNP Q9RA02
H	-18	GLY	-	expression tag	UNP Q9RA02
H	-17	SER	-	expression tag	UNP Q9RA02
H	-16	SER	-	expression tag	UNP Q9RA02
H	-15	HIS	-	expression tag	UNP Q9RA02
H	-14	HIS	-	expression tag	UNP Q9RA02
H	-13	HIS	-	expression tag	UNP Q9RA02
H	-12	HIS	-	expression tag	UNP Q9RA02
H	-11	HIS	-	expression tag	UNP Q9RA02
H	-10	HIS	-	expression tag	UNP Q9RA02
H	-9	SER	-	expression tag	UNP Q9RA02
H	-8	SER	-	expression tag	UNP Q9RA02
H	-7	GLY	-	expression tag	UNP Q9RA02
H	-6	LEU	-	expression tag	UNP Q9RA02
H	-5	VAL	-	expression tag	UNP Q9RA02
H	-4	PRO	-	expression tag	UNP Q9RA02
H	-3	ARG	-	expression tag	UNP Q9RA02
H	-2	GLY	-	expression tag	UNP Q9RA02
H	-1	SER	-	expression tag	UNP Q9RA02
H	0	HIS	-	expression tag	UNP Q9RA02

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	I	2	Total	C	O	0	0	0
			23	12	11			
2	J	2	Total	C	O	0	0	0
			23	12	11			
2	K	2	Total	C	O	0	0	0
			23	12	11			
2	L	2	Total	C	O	0	0	0
			23	12	11			
2	M	2	Total	C	O	0	0	0
			23	12	11			
2	N	2	Total	C	O	0	0	0
			23	12	11			

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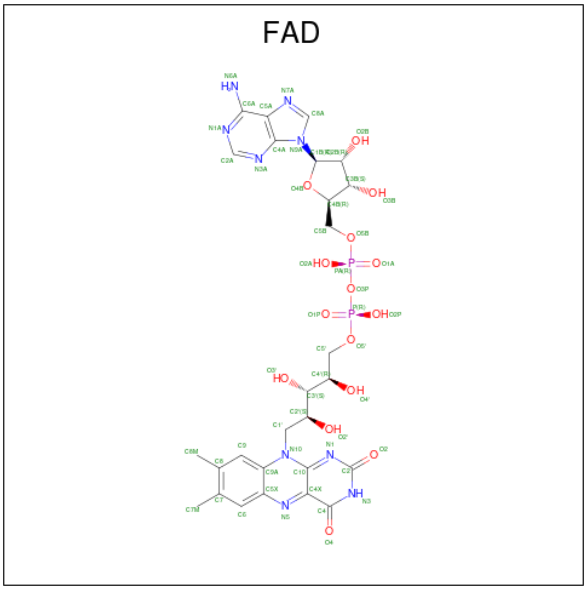
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	O	2	Total C O 23 12 11	0	0	0
2	P	2	Total C O 23 12 11	0	0	0
2	Q	2	Total C O 23 12 11	0	0	0
2	R	2	Total C O 23 12 11	0	0	0
2	S	2	Total C O 23 12 11	0	0	0
2	T	2	Total C O 23 12 11	0	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 53 27 9 15 2	0	0
3	B	1	Total C N O P 53 27 9 15 2	0	0
3	C	1	Total C N O P 53 27 9 15 2	0	0
3	D	1	Total C N O P 53 27 9 15 2	0	0
3	E	1	Total C N O P 53 27 9 15 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

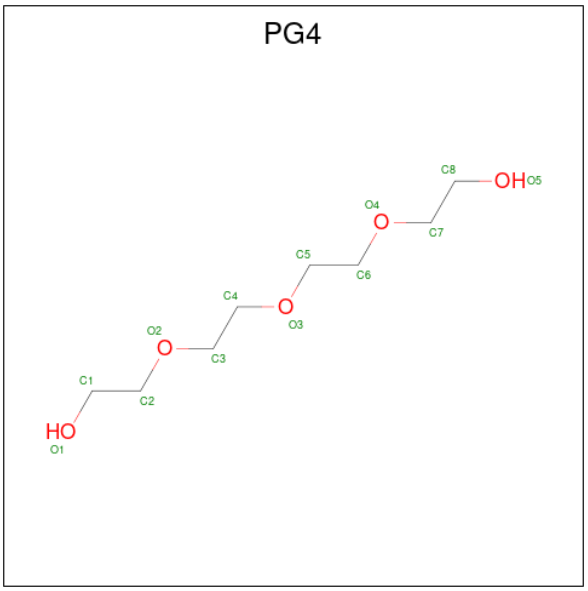
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		
4	E	1	Total	Na	0	0
			1	1		
4	G	1	Total	Na	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	E	1	Total	Cl	0	0
			1	1		
5	F	1	Total	Cl	0	0
			1	1		
5	G	1	Total	Cl	0	0
			1	1		
5	H	1	Total	Cl	0	0
			1	1		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0
6	B	1	Total C O 13 8 5	0	0
6	B	1	Total C O 13 8 5	0	0
6	B	1	Total C O 13 8 5	0	0
6	C	1	Total C O 13 8 5	0	0
6	C	1	Total C O 13 8 5	0	0
6	D	1	Total C O 13 8 5	0	0
6	D	1	Total C O 13 8 5	0	0
6	E	1	Total C O 13 8 5	0	0
6	E	1	Total C O 13 8 5	0	0
6	E	1	Total C O 13 8 5	0	0
6	F	1	Total C O 13 8 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C O 13 8 5	0	0
6	G	1	Total C O 13 8 5	0	0
6	G	1	Total C O 13 8 5	0	0
6	H	1	Total C O 13 8 5	0	0
6	H	1	Total C O 13 8 5	0	0

- Molecule 7 is water.

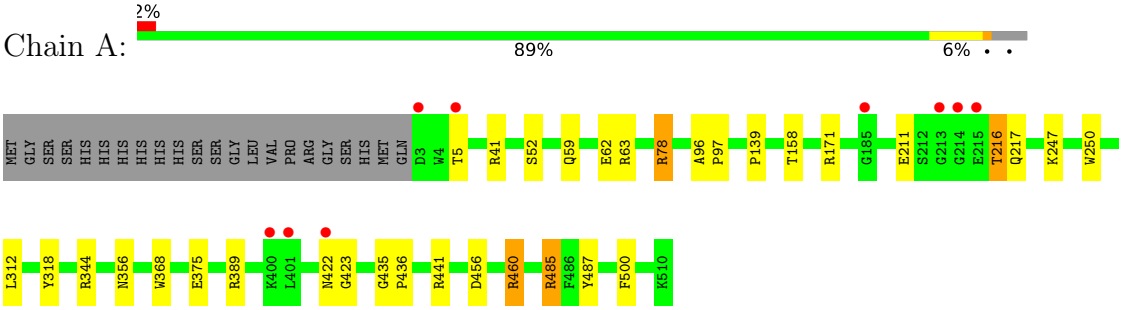
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	473	Total O 473 473	0	0
7	B	405	Total O 405 405	0	0
7	C	315	Total O 315 315	0	0
7	D	321	Total O 321 321	0	0
7	E	359	Total O 359 359	0	0
7	F	296	Total O 296 296	0	0
7	G	440	Total O 440 440	0	0
7	H	361	Total O 361 361	0	0

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.

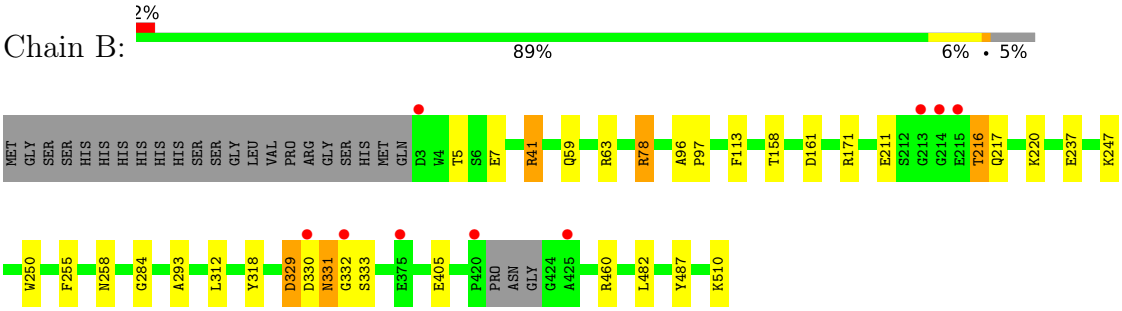
• Molecule 1: 3-KETOSTEROID DEHYDROGENASE

Chain A:



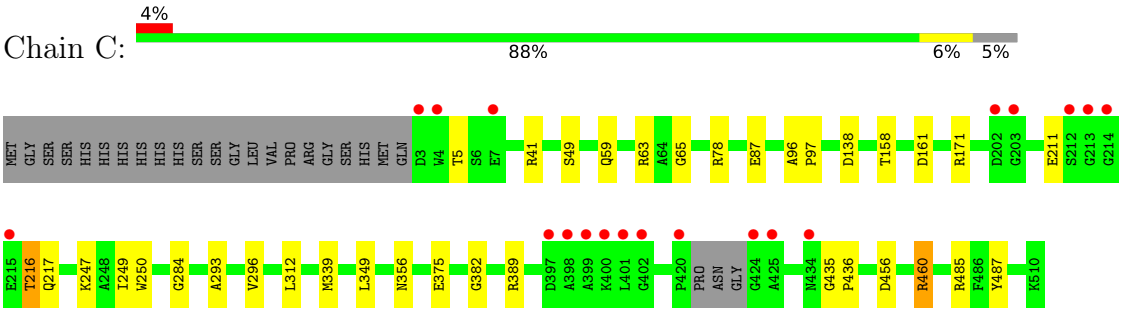
• Molecule 1: 3-KETOSTEROID DEHYDROGENASE

Chain B:



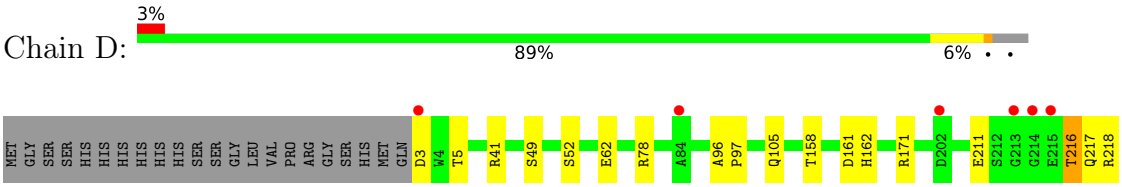
• Molecule 1: 3-KETOSTEROID DEHYDROGENASE

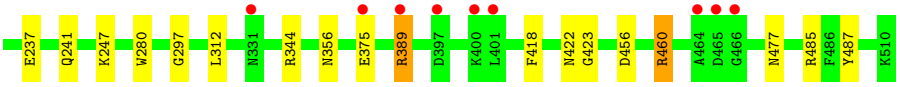
Chain C:



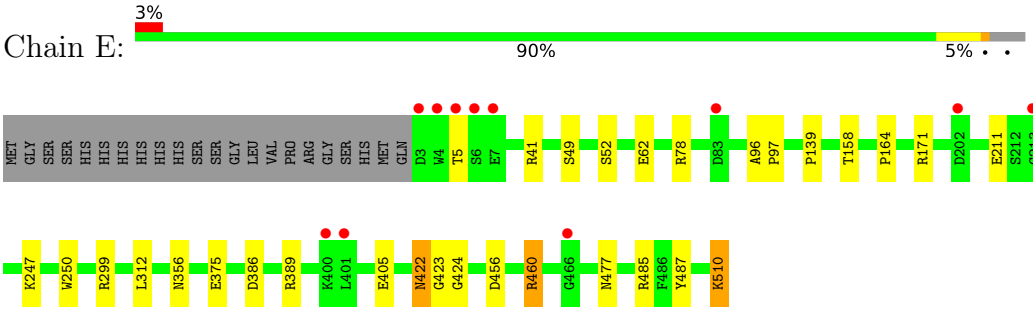
• Molecule 1: 3-KETOSTEROID DEHYDROGENASE

Chain D:

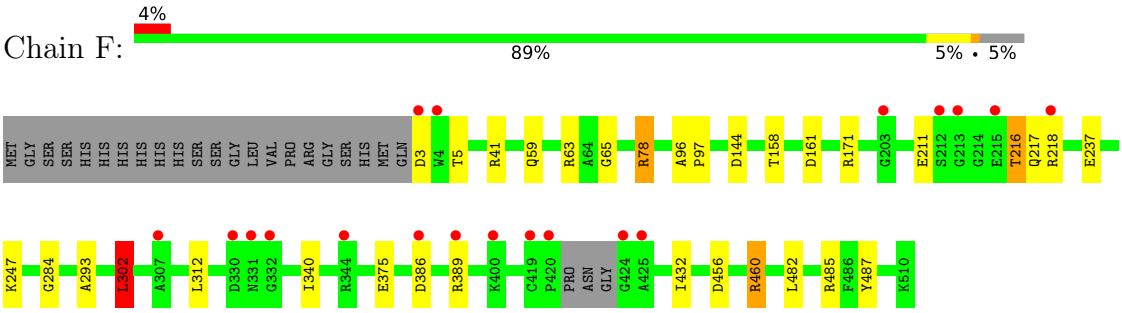




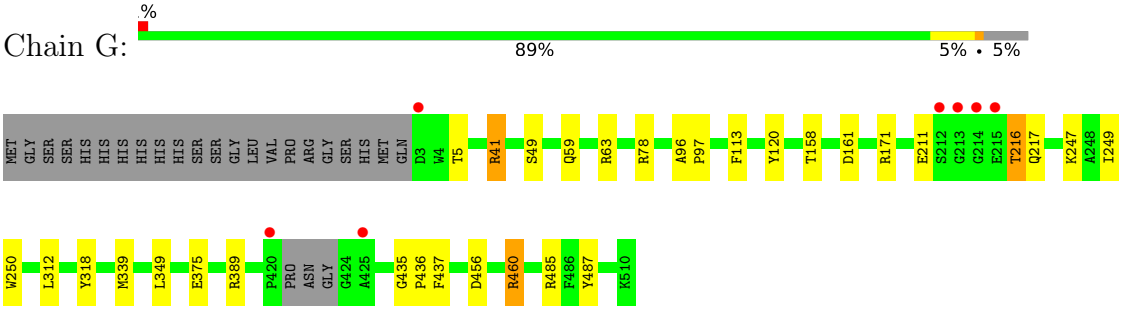
• Molecule 1: 3-KETOSTEROID DEHYDROGENASE



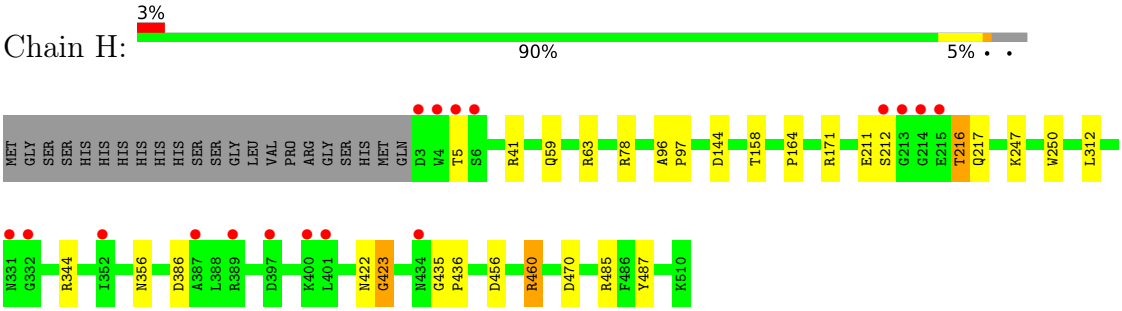
• Molecule 1: 3-KETOSTEROID DEHYDROGENASE



• Molecule 1: 3-KETOSTEROID DEHYDROGENASE



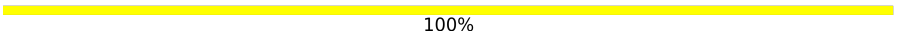
• Molecule 1: 3-KETOSTEROID DEHYDROGENASE



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

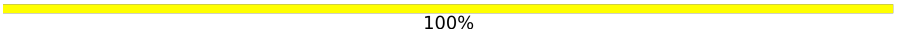
• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain J:



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

Chain K:

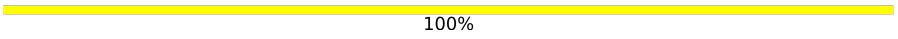


• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain L:

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

Chain M:

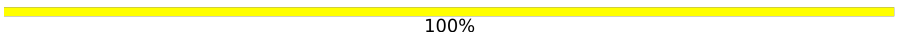


• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain N:

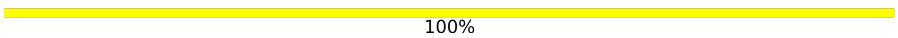
• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain O:



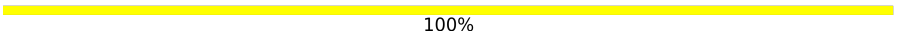
• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain P:



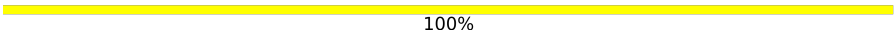
• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Q:



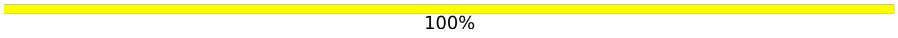
• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain R:



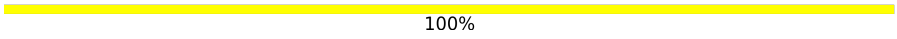
• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain S:



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

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.39Å 131.62Å 363.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.26 – 2.00 49.26 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.26-2.00) 99.8 (49.26-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.177 , 0.208 0.186 , 0.216	Depositor DCC
R_{free} test set	17446 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	33549	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: FAD, GLC, CL, NA, FRU, PG4

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	0.76	4/3782 (0.1%)	1.02	7/5138 (0.1%)
1	B	0.75	1/3761 (0.0%)	0.89	11/5107 (0.2%)
1	C	0.65	1/3761 (0.0%)	0.96	7/5107 (0.1%)
1	D	0.66	1/3782 (0.0%)	0.82	7/5138 (0.1%)
1	E	0.68	1/3782 (0.0%)	0.81	8/5138 (0.2%)
1	F	0.63	0/3761	1.01	11/5107 (0.2%)
1	G	0.76	6/3761 (0.2%)	0.82	6/5107 (0.1%)
1	H	0.72	1/3782 (0.0%)	0.99	9/5138 (0.2%)
All	All	0.70	15/30172 (0.0%)	0.92	66/40980 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	120	TYR	CG-CD1	7.88	1.49	1.39
1	G	437	PHE	CG-CD1	6.82	1.49	1.38
1	B	405	GLU	CG-CD	6.35	1.61	1.51
1	H	41	ARG	CZ-NH1	6.28	1.41	1.33
1	G	120	TYR	CE1-CZ	6.24	1.46	1.38
1	G	120	TYR	CE2-CZ	6.22	1.46	1.38
1	A	500	PHE	CG-CD2	5.89	1.47	1.38
1	A	500	PHE	CE2-CZ	5.83	1.48	1.37
1	G	437	PHE	CE1-CZ	5.82	1.48	1.37
1	G	437	PHE	CG-CD2	5.61	1.47	1.38
1	A	500	PHE	CG-CD1	5.37	1.46	1.38
1	D	280	TRP	CD2-CE2	5.33	1.47	1.41
1	E	405	GLU	CD-OE2	5.19	1.31	1.25
1	C	41	ARG	CZ-NH1	5.16	1.39	1.33
1	A	368	TRP	CD2-CE2	5.04	1.47	1.41

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	78	ARG	NE-CZ-NH1	33.04	136.82	120.30
1	F	78	ARG	NE-CZ-NH1	31.73	136.17	120.30
1	C	41	ARG	NE-CZ-NH1	30.25	135.42	120.30
1	H	41	ARG	NE-CZ-NH1	30.19	135.40	120.30
1	H	41	ARG	NE-CZ-NH2	-29.71	105.45	120.30
1	C	41	ARG	NE-CZ-NH2	-28.55	106.03	120.30
1	A	78	ARG	NE-CZ-NH2	-28.14	106.23	120.30
1	F	78	ARG	NE-CZ-NH2	-27.30	106.65	120.30
1	G	41	ARG	NE-CZ-NH2	-13.41	113.60	120.30
1	B	41	ARG	NE-CZ-NH2	-13.26	113.67	120.30
1	F	41	ARG	NE-CZ-NH2	-13.03	113.78	120.30
1	B	460	ARG	NE-CZ-NH2	-12.99	113.81	120.30
1	D	41	ARG	NE-CZ-NH2	-12.78	113.91	120.30
1	E	41	ARG	NE-CZ-NH2	-12.31	114.14	120.30
1	D	41	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	G	41	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	F	78	ARG	CD-NE-CZ	11.52	139.72	123.60
1	B	41	ARG	NE-CZ-NH1	11.45	126.02	120.30
1	A	41	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	F	41	ARG	NE-CZ-NH1	11.37	125.98	120.30
1	A	78	ARG	CD-NE-CZ	11.23	139.32	123.60
1	A	41	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	E	41	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	B	78	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	A	460	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	G	460	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	B	460	ARG	NE-CZ-NH1	8.69	124.65	120.30
1	F	460	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	G	78	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	H	460	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	E	78	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	C	460	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	D	78	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	F	302	LEU	CA-CB-CG	8.10	133.94	115.30
1	E	460	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	H	78	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	B	78	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	460	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	H	460	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	D	460	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	G	460	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	E	78	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	E	460	ARG	NE-CZ-NH2	-7.08	116.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	78	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	F	460	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	C	460	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	510	LYS	CD-CE-NZ	6.68	127.06	111.70
1	H	78	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	F	302	LEU	CB-CG-CD2	6.64	122.30	111.00
1	D	460	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	G	78	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	B	329	ASP	CB-CA-C	-6.23	97.95	110.40
1	C	78	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	C	41	ARG	CD-NE-CZ	5.98	131.97	123.60
1	H	144	ASP	CB-CA-C	-5.96	98.49	110.40
1	F	247	LYS	CG-CD-CE	5.91	129.62	111.90
1	D	247	LYS	CG-CD-CE	5.75	129.16	111.90
1	B	331	ASN	N-CA-C	5.74	126.51	111.00
1	H	41	ARG	CD-NE-CZ	5.55	131.37	123.60
1	C	138	ASP	CB-CG-OD1	5.48	123.23	118.30
1	E	299	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	405	GLU	OE1-CD-OE2	-5.24	117.02	123.30
1	B	510	LYS	CG-CD-CE	5.20	127.51	111.90
1	H	470	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	E	405	GLU	CG-CD-OE2	5.18	128.66	118.30
1	F	144	ASP	CB-CA-C	-5.15	100.10	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3712	0	3579	16	0
1	B	3693	0	3562	19	0
1	C	3693	0	3562	26	0
1	D	3712	0	3579	17	0
1	E	3712	0	3579	18	0
1	F	3693	0	3562	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3693	0	3562	21	0
1	H	3712	0	3579	17	0
2	I	23	0	21	0	0
2	J	23	0	21	0	0
2	K	23	0	21	0	0
2	L	23	0	21	0	0
2	M	23	0	20	0	0
2	N	23	0	21	1	0
2	O	23	0	21	0	0
2	P	23	0	21	0	0
2	Q	23	0	21	0	0
2	R	23	0	21	0	0
2	S	23	0	21	0	0
2	T	23	0	21	0	0
3	A	53	0	31	0	0
3	B	53	0	31	1	0
3	C	53	0	31	1	0
3	D	53	0	31	3	0
3	E	53	0	31	2	0
3	F	53	0	31	0	0
3	G	53	0	31	2	0
3	H	53	0	31	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	39	0	54	1	0
6	B	39	0	54	2	0
6	C	26	0	36	3	0
6	D	26	0	36	4	0
6	E	39	0	54	4	0
6	F	26	0	36	3	0
6	G	26	0	36	2	0
6	H	26	0	36	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	473	0	0	3	0
7	B	405	0	0	4	0
7	C	315	0	0	3	0
7	D	321	0	0	1	0
7	E	359	0	0	1	0
7	F	296	0	0	2	0
7	G	440	0	0	2	0
7	H	361	0	0	3	0
All	All	33549	0	29405	148	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 2.

All (148) 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:339:MET:HE1	1:C:349:LEU:HD21	1.25	1.17
1:G:339:MET:HE1	1:G:349:LEU:HD21	1.27	1.15
1:G:339:MET:CE	1:G:349:LEU:HD21	2.04	0.88
1:F:302:LEU:HD13	1:F:432:ILE:HD12	1.62	0.82
1:F:302:LEU:HD22	1:F:340:ILE:HB	1.68	0.76
1:F:302:LEU:HD13	1:F:432:ILE:CD1	2.16	0.76
1:C:339:MET:HE1	1:C:349:LEU:CD2	2.14	0.72
1:C:339:MET:CE	1:C:349:LEU:HD21	2.12	0.71
1:C:249:ILE:HB	7:C:2178:HOH:O	1.89	0.71
1:C:339:MET:CE	1:C:349:LEU:HD11	2.24	0.67
1:B:41:ARG:HD3	7:B:2034:HOH:O	1.96	0.65
6:D:581:PG4:O1	6:D:581:PG4:C5	2.46	0.64
1:A:139:PRO:HG3	6:B:582:PG4:H42	1.80	0.63
1:E:456:ASP:OD2	1:E:460:ARG:HD3	1.99	0.62
1:C:456:ASP:OD2	1:C:460:ARG:HD3	1.99	0.62
1:F:456:ASP:OD2	1:F:460:ARG:HD3	2.00	0.62
1:G:456:ASP:OD2	1:G:460:ARG:HD3	1.99	0.62
1:D:456:ASP:OD2	1:D:460:ARG:HD3	2.00	0.62
1:H:344:ARG:NH1	7:H:2281:HOH:O	2.27	0.61
1:H:456:ASP:OD2	1:H:460:ARG:HD3	2.00	0.61
1:A:456:ASP:OD2	1:A:460:ARG:HD3	2.00	0.61
1:E:139:PRO:HB3	6:F:582:PG4:H42	1.83	0.60
1:A:62:GLU:OE2	1:D:422:ASN:OD1	2.18	0.60
1:E:5:THR:HG21	1:E:217:GLN:HG2	1.85	0.59
1:B:113:PHE:HE2	1:C:65:GLY:HA3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:GLU:OE2	1:D:389:ARG:NE	2.32	0.58
1:D:344:ARG:NH1	7:D:2238:HOH:O	2.35	0.57
1:B:5:THR:HG21	1:B:217:GLN:HG2	1.86	0.56
1:H:212:SER:OG	1:H:217:GLN:NE2	2.36	0.56
6:B:582:PG4:H51	7:B:2405:HOH:O	2.05	0.55
1:A:485:ARG:HD3	7:A:2295:HOH:O	2.06	0.55
1:H:212:SER:HG	1:H:217:GLN:HE22	1.55	0.54
6:D:581:PG4:O1	6:D:581:PG4:H51	2.07	0.53
1:D:5:THR:HG21	1:D:217:GLN:HG2	1.90	0.53
1:E:422:ASN:ND2	1:E:424:GLY:H	2.06	0.53
1:A:441:ARG:NH1	7:A:2421:HOH:O	2.41	0.53
1:G:5:THR:HG21	1:G:217:GLN:HG2	1.90	0.53
1:E:386:ASP:HB3	7:E:2302:HOH:O	2.08	0.53
1:A:5:THR:HG21	1:A:217:GLN:HG2	1.91	0.53
1:F:5:THR:HG21	1:F:217:GLN:HG2	1.91	0.52
1:A:344:ARG:NH1	7:A:2358:HOH:O	2.36	0.51
1:C:5:THR:HG21	1:C:217:GLN:HG2	1.91	0.51
1:H:423:GLY:HA3	7:H:2320:HOH:O	2.10	0.51
1:G:339:MET:CE	1:G:349:LEU:HD11	2.40	0.51
1:B:330:ASP:C	1:B:331:ASN:OD1	2.48	0.51
1:A:375:GLU:OE2	1:A:389:ARG:NE	2.39	0.51
1:A:356:ASN:ND2	1:B:161:ASP:HB3	2.26	0.50
1:G:49:SER:HA	3:G:551:FAD:C6	2.40	0.50
1:D:3:ASP:OD1	1:D:218:ARG:NH1	2.45	0.50
1:F:375:GLU:OE2	1:F:389:ARG:NE	2.36	0.50
1:B:332:GLY:HA2	7:B:2304:HOH:O	2.11	0.50
1:G:339:MET:CE	1:G:349:LEU:CD2	2.84	0.50
1:E:139:PRO:HG3	6:F:582:PG4:H32	1.94	0.50
1:F:386:ASP:HB2	7:F:2256:HOH:O	2.11	0.49
1:G:41:ARG:HD3	7:G:2034:HOH:O	2.12	0.49
1:H:5:THR:HG21	1:H:217:GLN:HG2	1.93	0.49
1:A:422:ASN:ND2	1:D:62:GLU:OE2	2.44	0.49
6:C:582:PG4:H32	1:D:162:HIS:HB2	1.94	0.49
1:C:296:VAL:HG21	6:C:581:PG4:H51	1.94	0.49
1:F:65:GLY:HA3	1:G:113:PHE:HE2	1.78	0.49
1:F:3:ASP:OD1	1:F:218:ARG:NH1	2.45	0.49
1:B:255:PHE:HB2	7:B:2241:HOH:O	2.13	0.49
1:C:87:GLU:HG3	7:C:2060:HOH:O	2.13	0.48
1:G:339:MET:HE1	1:G:349:LEU:CD2	2.19	0.48
1:B:258:ASN:OD1	3:B:551:FAD:H2B	2.14	0.48
1:B:247:LYS:HE2	1:B:250:TRP:CH2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:GLU:OE2	1:C:389:ARG:NE	2.40	0.48
1:B:329:ASP:CG	1:B:329:ASP:O	2.51	0.48
1:H:247:LYS:HE2	1:H:250:TRP:CH2	2.48	0.48
1:A:52:SER:HB2	6:A:581:PG4:H82	1.95	0.48
1:G:49:SER:HB2	3:G:551:FAD:C4X	2.44	0.47
1:C:339:MET:HE3	1:C:349:LEU:HG	1.97	0.47
6:D:581:PG4:O1	6:D:581:PG4:H52	2.15	0.47
1:G:339:MET:HE3	1:G:349:LEU:CG	2.45	0.47
1:C:382:GLY:HA2	7:C:2264:HOH:O	2.15	0.47
1:C:339:MET:HE3	1:C:349:LEU:CG	2.46	0.46
6:E:581:PG4:O1	6:E:581:PG4:C5	2.64	0.46
1:E:96:ALA:HB3	1:E:97:PRO:HD3	1.98	0.46
1:E:247:LYS:HE2	1:E:250:TRP:CH2	2.51	0.46
1:D:96:ALA:HB3	1:D:97:PRO:HD3	1.98	0.46
1:E:62:GLU:OE2	1:H:422:ASN:OD1	2.34	0.45
1:E:356:ASN:ND2	1:F:161:ASP:HB3	2.32	0.45
1:G:96:ALA:HB3	1:G:97:PRO:HD3	1.98	0.45
1:E:510:LYS:HB2	1:E:510:LYS:HE3	1.62	0.45
1:B:7:GLU:HG2	1:B:220:LYS:HB3	1.98	0.45
1:B:7:GLU:HG2	1:B:220:LYS:HD3	1.99	0.45
6:C:581:PG4:O3	6:C:581:PG4:O1	2.35	0.45
1:G:247:LYS:HE2	1:G:250:TRP:CH2	2.51	0.45
1:B:96:ALA:HB3	1:B:97:PRO:HD3	1.99	0.45
1:D:49:SER:HA	3:D:551:FAD:C6	2.47	0.44
1:E:477:ASN:ND2	3:E:551:FAD:H5'2	2.31	0.44
6:G:582:PG4:H11	1:H:164:PRO:HA	1.98	0.44
1:C:435:GLY:HA2	1:C:436:PRO:C	2.38	0.44
1:A:435:GLY:HA2	1:A:436:PRO:C	2.38	0.44
1:G:375:GLU:OE2	1:G:389:ARG:NE	2.39	0.44
1:H:96:ALA:HB3	1:H:97:PRO:HD3	1.99	0.44
1:C:161:ASP:HB3	1:D:356:ASN:ND2	2.32	0.44
1:C:247:LYS:HE2	1:C:250:TRP:CH2	2.52	0.44
1:F:96:ALA:HB3	1:F:97:PRO:HD3	1.99	0.44
1:A:96:ALA:HB3	1:A:97:PRO:HD3	1.98	0.44
1:E:164:PRO:HG3	7:F:2120:HOH:O	2.16	0.44
1:G:161:ASP:HB3	1:H:356:ASN:ND2	2.32	0.43
1:D:52:SER:HB2	6:D:581:PG4:H82	2.00	0.43
1:B:482:LEU:C	1:B:482:LEU:HD12	2.39	0.43
1:G:339:MET:HE3	1:G:349:LEU:HG	2.00	0.43
1:C:339:MET:CE	1:C:349:LEU:CG	2.97	0.43
1:H:211:GLU:OE2	1:H:216:THR:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:GLU:OE2	1:E:216:THR:HB	2.19	0.43
1:F:211:GLU:OE2	1:F:216:THR:HB	2.19	0.42
1:D:211:GLU:OE2	1:D:216:THR:HB	2.20	0.42
1:B:211:GLU:OE2	1:B:216:THR:HB	2.19	0.42
1:C:49:SER:HA	3:C:551:FAD:C6	2.49	0.42
1:E:49:SER:HB2	3:E:551:FAD:C4X	2.49	0.42
2:N:1:GLC:O5	2:N:2:FRU:H61	2.19	0.42
1:A:211:GLU:OE2	1:A:216:THR:HB	2.19	0.42
1:C:96:ALA:HB3	1:C:97:PRO:HD3	2.01	0.42
1:D:49:SER:HB2	3:D:551:FAD:C4X	2.49	0.42
1:G:211:GLU:OE2	1:G:216:THR:HB	2.20	0.42
6:G:582:PG4:C1	1:H:164:PRO:HA	2.50	0.42
1:A:247:LYS:HE2	1:A:250:TRP:CH2	2.54	0.42
1:C:211:GLU:OE2	1:C:216:THR:HB	2.20	0.42
1:H:435:GLY:HA2	1:H:436:PRO:C	2.40	0.42
1:C:59:GLN:O	1:C:63:ARG:HG3	2.20	0.41
1:C:356:ASN:ND2	1:D:161:ASP:HB3	2.35	0.41
1:F:59:GLN:O	1:F:63:ARG:HG3	2.20	0.41
1:G:249:ILE:HB	7:G:2245:HOH:O	2.20	0.41
1:A:59:GLN:O	1:A:63:ARG:HG3	2.21	0.41
1:G:59:GLN:O	1:G:63:ARG:HG3	2.20	0.41
1:H:456:ASP:HB2	7:H:2329:HOH:O	2.20	0.41
1:C:339:MET:HE2	1:C:349:LEU:HD11	2.03	0.41
1:H:59:GLN:O	1:H:63:ARG:HG3	2.20	0.41
1:D:477:ASN:ND2	3:D:551:FAD:H5'2	2.36	0.41
1:F:482:LEU:C	1:F:482:LEU:HD12	2.41	0.41
1:B:331:ASN:HB2	1:B:333:SER:HB3	2.03	0.41
1:C:339:MET:CE	1:C:349:LEU:CD2	2.88	0.41
1:E:52:SER:HB2	6:E:581:PG4:H81	2.01	0.41
1:H:422:ASN:C	1:H:423:GLY:O	2.58	0.41
1:B:284:GLY:HA2	1:B:293:ALA:O	2.22	0.40
1:E:139:PRO:CB	6:F:582:PG4:H42	2.51	0.40
1:E:375:GLU:OE2	1:E:389:ARG:NE	2.40	0.40
6:E:581:PG4:O1	6:E:581:PG4:H51	2.21	0.40
1:B:59:GLN:O	1:B:63:ARG:HG3	2.20	0.40
6:E:581:PG4:O1	6:E:581:PG4:H52	2.21	0.40
1:G:435:GLY:HA2	1:G:436:PRO:C	2.42	0.40
1:D:297:GLY:HA2	1:D:418:PHE:CG	2.57	0.40
1:B:330:ASP:O	1:B:331:ASN:OD1	2.39	0.40
1:C:284:GLY:HA2	1:C:293:ALA:O	2.21	0.40
1:F:284:GLY:HA2	1:F:293:ALA:O	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	506/530 (96%)	493 (97%)	12 (2%)	1 (0%)	47	44
1	B	501/530 (94%)	487 (97%)	14 (3%)	0	100	100
1	C	501/530 (94%)	489 (98%)	12 (2%)	0	100	100
1	D	506/530 (96%)	493 (97%)	12 (2%)	1 (0%)	47	44
1	E	506/530 (96%)	494 (98%)	11 (2%)	1 (0%)	47	44
1	F	501/530 (94%)	489 (98%)	12 (2%)	0	100	100
1	G	501/530 (94%)	490 (98%)	11 (2%)	0	100	100
1	H	506/530 (96%)	495 (98%)	10 (2%)	1 (0%)	47	44
All	All	4028/4240 (95%)	3930 (98%)	94 (2%)	4 (0%)	51	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	GLY
1	H	423	GLY
1	D	423	GLY
1	E	423	GLY

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	369/388 (95%)	361 (98%)	8 (2%)	52	55
1	B	367/388 (95%)	359 (98%)	8 (2%)	52	55
1	C	367/388 (95%)	361 (98%)	6 (2%)	62	67
1	D	369/388 (95%)	359 (97%)	10 (3%)	44	46
1	E	369/388 (95%)	361 (98%)	8 (2%)	52	55
1	F	367/388 (95%)	358 (98%)	9 (2%)	47	49
1	G	367/388 (95%)	360 (98%)	7 (2%)	57	61
1	H	369/388 (95%)	362 (98%)	7 (2%)	57	61
All	All	2944/3104 (95%)	2881 (98%)	63 (2%)	53	57

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	158	THR
1	A	171	ARG
1	A	216	THR
1	A	312	LEU
1	A	318	TYR
1	A	485	ARG
1	A	487	TYR
1	B	78	ARG
1	B	158	THR
1	B	171	ARG
1	B	216	THR
1	B	237	GLU
1	B	312	LEU
1	B	318	TYR
1	B	487	TYR
1	C	158	THR
1	C	171	ARG
1	C	216	THR
1	C	312	LEU
1	C	485	ARG
1	C	487	TYR
1	D	105	GLN
1	D	158	THR
1	D	171	ARG
1	D	216	THR
1	D	237	GLU

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Mol	Chain	Res	Type
1	D	241	GLN
1	D	312	LEU
1	D	389	ARG
1	D	485	ARG
1	D	487	TYR
1	E	158	THR
1	E	171	ARG
1	E	216	THR
1	E	312	LEU
1	E	422	ASN
1	E	485	ARG
1	E	487	TYR
1	E	510	LYS
1	F	78	ARG
1	F	158	THR
1	F	171	ARG
1	F	216	THR
1	F	237	GLU
1	F	302	LEU
1	F	312	LEU
1	F	485	ARG
1	F	487	TYR
1	G	158	THR
1	G	171	ARG
1	G	216	THR
1	G	312	LEU
1	G	318	TYR
1	G	485	ARG
1	G	487	TYR
1	H	158	THR
1	H	171	ARG
1	H	216	THR
1	H	312	LEU
1	H	386	ASP
1	H	485	ARG
1	H	487	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	217	GLN
1	D	422	ASN

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Mol	Chain	Res	Type
1	E	217	GLN
1	E	422	ASN
1	H	217	GLN
1	H	241	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)

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLC	I	1	2	11,11,12	1.38	2 (18%)	15,15,17	0.93	1 (6%)
2	FRU	I	2	2	11,12,12	1.17	1 (9%)	10,18,18	0.84	0
2	GLC	J	1	2	11,11,12	1.26	2 (18%)	15,15,17	1.86	4 (26%)
2	FRU	J	2	2	11,12,12	2.26	3 (27%)	10,18,18	2.12	3 (30%)
2	GLC	K	1	2	11,11,12	2.27	7 (63%)	15,15,17	1.38	1 (6%)
2	FRU	K	2	2	11,12,12	2.82	3 (27%)	10,18,18	1.10	1 (10%)
2	GLC	L	1	2	11,11,12	0.89	0	15,15,17	0.93	0
2	FRU	L	2	2	11,12,12	2.12	3 (27%)	10,18,18	1.64	2 (20%)
2	GLC	M	1	2	11,11,12	1.54	2 (18%)	15,15,17	0.83	0
2	FRU	M	2	2	11,12,12	1.82	3 (27%)	10,18,18	1.46	3 (30%)
2	GLC	N	1	2	11,11,12	2.00	5 (45%)	15,15,17	2.13	2 (13%)
2	FRU	N	2	2	11,12,12	1.49	3 (27%)	10,18,18	1.42	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLC	O	1	2	11,11,12	1.68	3 (27%)	15,15,17	0.96	0
2	FRU	O	2	2	11,12,12	1.26	2 (18%)	10,18,18	1.44	2 (20%)
2	GLC	P	1	2	11,11,12	1.62	3 (27%)	15,15,17	1.66	3 (20%)
2	FRU	P	2	2	11,12,12	2.58	4 (36%)	10,18,18	1.44	2 (20%)
2	GLC	Q	1	2	11,11,12	2.15	4 (36%)	15,15,17	1.33	1 (6%)
2	FRU	Q	2	2	11,12,12	1.64	2 (18%)	10,18,18	1.56	2 (20%)
2	GLC	R	1	2	11,11,12	1.17	1 (9%)	15,15,17	1.23	1 (6%)
2	FRU	R	2	2	11,12,12	1.46	2 (18%)	10,18,18	0.79	0
2	GLC	S	1	2	11,11,12	0.95	1 (9%)	15,15,17	1.34	2 (13%)
2	FRU	S	2	2	11,12,12	2.00	3 (27%)	10,18,18	1.52	3 (30%)
2	GLC	T	1	2	11,11,12	2.11	5 (45%)	15,15,17	1.07	2 (13%)
2	FRU	T	2	2	11,12,12	1.80	3 (27%)	10,18,18	1.65	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
2	GLC	I	1	2	-	0/2/19/22	0/1/1/1
2	FRU	I	2	2	-	0/5/24/24	0/1/1/1
2	GLC	J	1	2	-	0/2/19/22	0/1/1/1
2	FRU	J	2	2	-	0/5/24/24	0/1/1/1
2	GLC	K	1	2	-	2/2/19/22	0/1/1/1
2	FRU	K	2	2	-	0/5/24/24	0/1/1/1
2	GLC	L	1	2	-	0/2/19/22	0/1/1/1
2	FRU	L	2	2	-	2/5/24/24	0/1/1/1
2	GLC	M	1	2	-	0/2/19/22	0/1/1/1
2	FRU	M	2	2	-	1/5/24/24	0/1/1/1
2	GLC	N	1	2	-	2/2/19/22	0/1/1/1
2	FRU	N	2	2	-	2/5/24/24	0/1/1/1
2	GLC	O	1	2	-	0/2/19/22	0/1/1/1
2	FRU	O	2	2	-	0/5/24/24	0/1/1/1
2	GLC	P	1	2	-	0/2/19/22	0/1/1/1
2	FRU	P	2	2	-	2/5/24/24	0/1/1/1
2	GLC	Q	1	2	-	1/2/19/22	0/1/1/1
2	FRU	Q	2	2	-	0/5/24/24	0/1/1/1
2	GLC	R	1	2	-	0/2/19/22	0/1/1/1
2	FRU	R	2	2	-	0/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	S	1	2	-	0/2/19/22	0/1/1/1
2	FRU	S	2	2	-	0/5/24/24	0/1/1/1
2	GLC	T	1	2	-	2/2/19/22	0/1/1/1
2	FRU	T	2	2	-	0/5/24/24	0/1/1/1

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	FRU	O2-C2	6.91	1.52	1.40
2	P	2	FRU	O5-C2	5.88	1.52	1.43
2	K	2	FRU	O5-C2	4.86	1.50	1.43
2	J	2	FRU	O2-C2	4.83	1.49	1.40
2	L	2	FRU	O2-C2	4.52	1.48	1.40
2	Q	1	GLC	O5-C5	4.26	1.52	1.43
2	Q	2	FRU	O5-C2	4.09	1.49	1.43
2	P	2	FRU	O2-C2	3.92	1.47	1.40
2	T	2	FRU	O5-C2	3.89	1.49	1.43
2	T	1	GLC	O5-C1	3.84	1.49	1.43
2	Q	1	GLC	O2-C2	3.82	1.51	1.43
2	J	2	FRU	O5-C2	3.80	1.49	1.43
2	S	2	FRU	O5-C2	3.78	1.49	1.43
2	S	2	FRU	O2-C2	3.72	1.47	1.40
2	L	2	FRU	O5-C2	3.62	1.48	1.43
2	N	1	GLC	O5-C5	3.57	1.50	1.43
2	J	2	FRU	O5-C5	3.49	1.51	1.43
2	K	1	GLC	C2-C3	3.39	1.57	1.52
2	O	1	GLC	O5-C5	3.32	1.50	1.43
2	N	2	FRU	O2-C2	3.16	1.46	1.40
2	K	2	FRU	C1-C2	3.15	1.57	1.52
2	T	1	GLC	O2-C2	3.14	1.50	1.43
2	P	1	GLC	O5-C1	3.10	1.48	1.43
2	M	1	GLC	O2-C2	-3.10	1.36	1.43
2	M	2	FRU	O5-C2	3.08	1.48	1.43
2	P	2	FRU	O5-C5	3.08	1.50	1.43
2	K	1	GLC	O2-C2	3.02	1.49	1.43
2	M	2	FRU	O2-C2	3.01	1.45	1.40
2	M	1	GLC	O5-C5	2.91	1.49	1.43
2	N	1	GLC	C2-C3	2.84	1.56	1.52
2	R	2	FRU	O2-C2	2.82	1.45	1.40
2	Q	1	GLC	C4-C3	2.79	1.59	1.52
2	L	2	FRU	C4-C5	2.77	1.60	1.53
2	T	2	FRU	O2-C2	2.74	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	1	GLC	O3-C3	2.72	1.49	1.43
2	O	1	GLC	O4-C4	2.67	1.49	1.43
2	Q	1	GLC	C2-C3	2.65	1.56	1.52
2	Q	2	FRU	O2-C2	2.62	1.45	1.40
2	M	2	FRU	O5-C5	2.62	1.49	1.43
2	N	1	GLC	O2-C2	2.61	1.48	1.43
2	K	1	GLC	O3-C3	2.59	1.49	1.43
2	K	1	GLC	O5-C1	2.56	1.47	1.43
2	O	1	GLC	C2-C3	2.54	1.56	1.52
2	O	2	FRU	O5-C5	2.54	1.49	1.43
2	I	1	GLC	O2-C2	-2.51	1.38	1.43
2	T	1	GLC	C2-C3	2.49	1.56	1.52
2	K	1	GLC	C4-C5	2.45	1.58	1.53
2	I	1	GLC	O5-C1	2.44	1.47	1.43
2	T	1	GLC	C4-C3	2.41	1.58	1.52
2	P	1	GLC	C4-C3	2.40	1.58	1.52
2	S	1	GLC	C2-C3	-2.38	1.49	1.52
2	N	2	FRU	O5-C2	2.37	1.47	1.43
2	S	2	FRU	O5-C5	2.36	1.49	1.43
2	N	1	GLC	C4-C5	2.32	1.57	1.53
2	K	1	GLC	O5-C5	2.32	1.48	1.43
2	J	1	GLC	C4-C3	2.31	1.58	1.52
2	I	2	FRU	O3-C3	-2.30	1.38	1.42
2	K	1	GLC	O4-C4	2.29	1.48	1.43
2	T	2	FRU	C1-C2	2.19	1.55	1.52
2	N	2	FRU	C1-C2	2.17	1.55	1.52
2	J	1	GLC	C2-C3	2.10	1.55	1.52
2	P	1	GLC	O4-C4	2.08	1.47	1.43
2	N	1	GLC	O3-C3	2.06	1.47	1.43
2	O	2	FRU	O4-C4	2.05	1.47	1.43
2	P	2	FRU	C1-C2	2.04	1.55	1.52
2	R	2	FRU	O5-C2	2.02	1.46	1.43
2	R	1	GLC	O4-C4	2.02	1.47	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	1	GLC	O5-C5-C6	7.22	118.53	107.20
2	J	1	GLC	C1-O5-C5	4.55	118.36	112.19
2	K	1	GLC	O5-C5-C6	4.47	114.22	107.20
2	T	2	FRU	O2-C2-O5	4.40	117.99	109.50
2	P	1	GLC	C1-O5-C5	4.34	118.07	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	2	FRU	C6-C5-C4	-4.30	104.71	115.09
2	J	2	FRU	O2-C2-O5	3.77	116.79	109.50
2	Q	2	FRU	O2-C2-O5	3.59	116.43	109.50
2	Q	1	GLC	O5-C5-C6	3.38	112.51	107.20
2	L	2	FRU	O2-C2-O5	3.32	115.91	109.50
2	O	2	FRU	O2-C2-O5	3.21	115.70	109.50
2	S	1	GLC	C1-O5-C5	3.17	116.48	112.19
2	K	2	FRU	O2-C2-O5	3.10	115.48	109.50
2	S	2	FRU	O2-C2-O5	2.97	115.23	109.50
2	P	2	FRU	O2-C2-O5	2.87	115.05	109.50
2	O	2	FRU	O1-C1-C2	-2.71	106.09	111.86
2	P	2	FRU	O5-C5-C6	2.70	116.36	108.85
2	J	1	GLC	C1-C2-C3	2.64	112.91	109.67
2	N	2	FRU	O1-C1-C2	-2.60	106.33	111.86
2	J	1	GLC	C6-C5-C4	-2.59	106.94	113.00
2	Q	2	FRU	O1-C1-C2	-2.55	106.44	111.86
2	J	2	FRU	O5-C5-C6	2.52	115.86	108.85
2	T	1	GLC	O5-C5-C6	2.44	111.02	107.20
2	P	1	GLC	O4-C4-C3	2.43	115.98	110.35
2	I	1	GLC	C1-O5-C5	2.41	115.46	112.19
2	R	1	GLC	O2-C2-C1	-2.37	104.31	109.15
2	M	2	FRU	O5-C5-C6	2.35	115.38	108.85
2	L	2	FRU	O5-C5-C6	-2.33	102.38	108.85
2	P	1	GLC	C6-C5-C4	-2.31	107.60	113.00
2	M	2	FRU	O6-C6-C5	-2.30	103.41	111.29
2	J	1	GLC	O4-C4-C3	2.26	115.58	110.35
2	T	1	GLC	O2-C2-C3	2.25	114.64	110.14
2	S	2	FRU	C6-C5-C4	-2.14	109.94	115.09
2	M	2	FRU	O2-C2-O5	2.10	113.56	109.50
2	N	2	FRU	O2-C2-O5	2.04	113.45	109.50
2	S	1	GLC	C6-C5-C4	-2.03	108.25	113.00
2	N	1	GLC	O3-C3-C2	2.00	113.83	109.99
2	N	2	FRU	C6-C5-C4	-2.00	110.26	115.09
2	S	2	FRU	O6-C6-C5	-2.00	104.43	111.29

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	2	FRU	O5-C5-C6-O6
2	N	2	FRU	C4-C5-C6-O6
2	L	2	FRU	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	L	2	FRU	O5-C5-C6-O6
2	N	1	GLC	O5-C5-C6-O6
2	K	1	GLC	C4-C5-C6-O6
2	K	1	GLC	O5-C5-C6-O6
2	N	1	GLC	C4-C5-C6-O6
2	T	1	GLC	C4-C5-C6-O6
2	T	1	GLC	O5-C5-C6-O6
2	P	2	FRU	O5-C5-C6-O6
2	Q	1	GLC	C4-C5-C6-O6
2	M	2	FRU	O1-C1-C2-O2
2	P	2	FRU	C4-C5-C6-O6

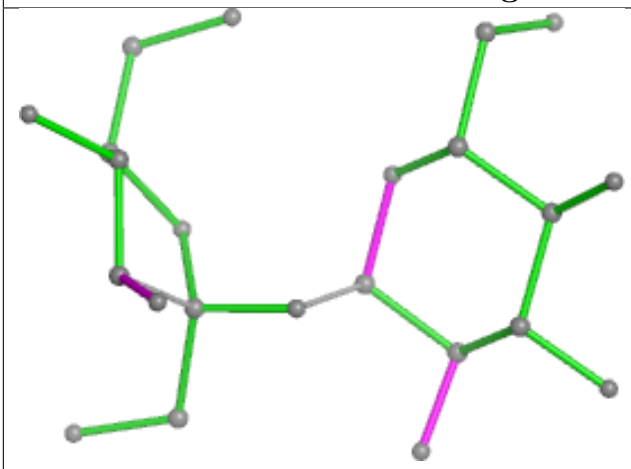
There are no ring outliers.

2 monomers are involved in 1 short contact:

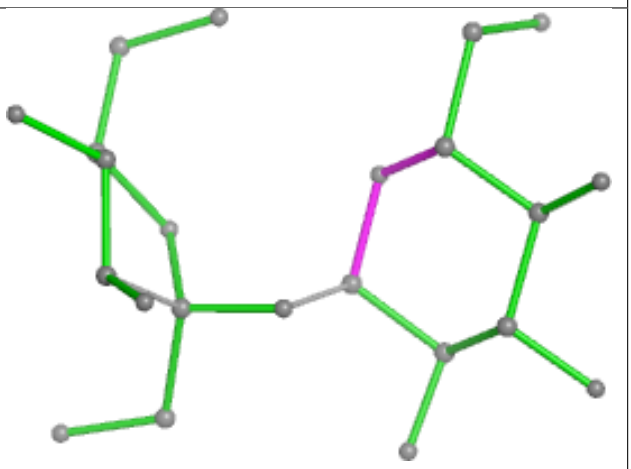
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	1	GLC	1	0
2	N	2	FRU	1	0

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

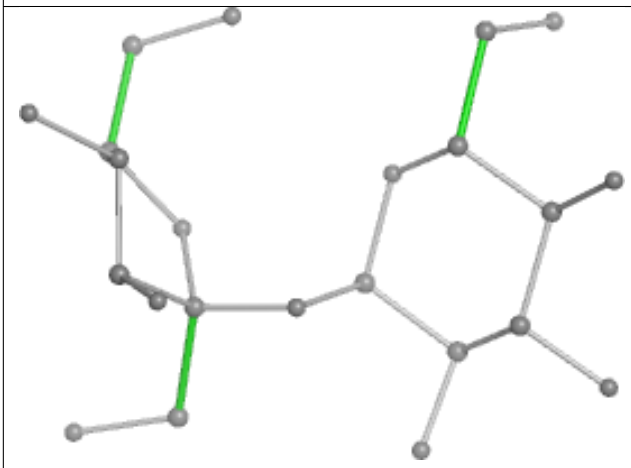
Oligosaccharide Chain I



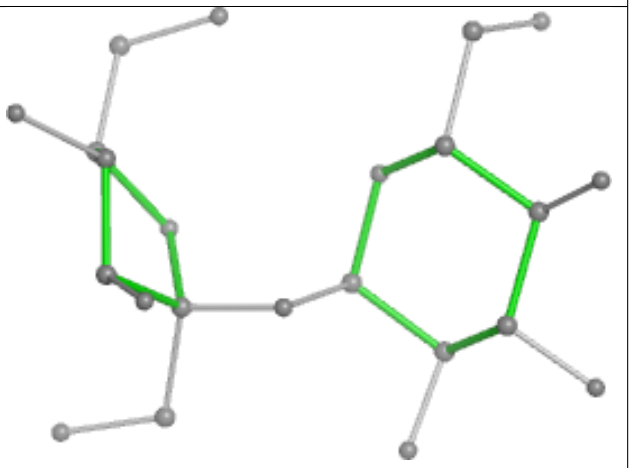
Bond lengths



Bond angles

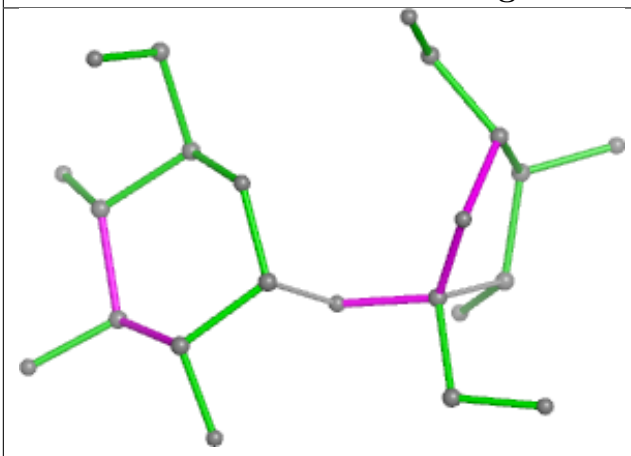


Torsions

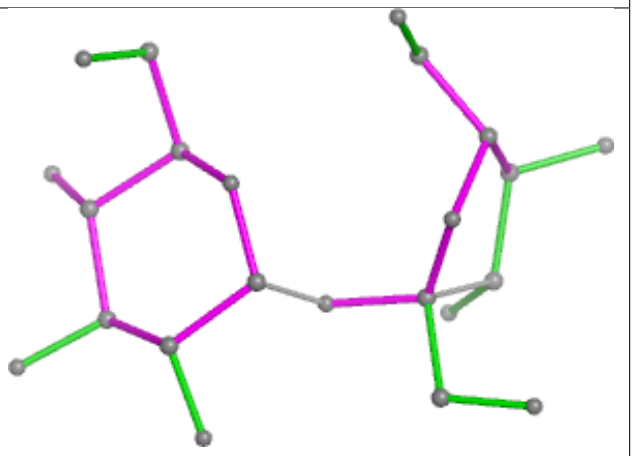


Rings

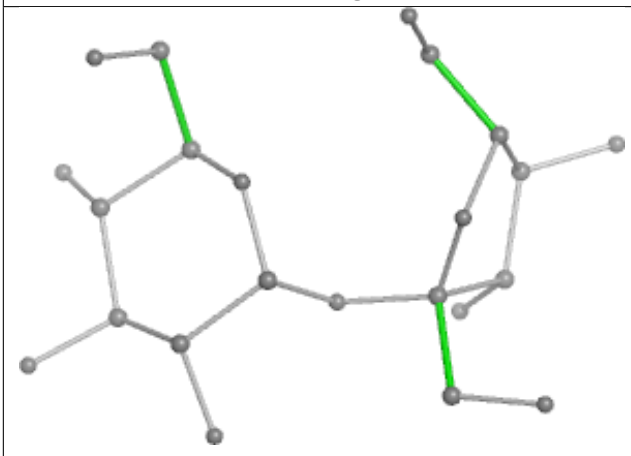
Oligosaccharide Chain J



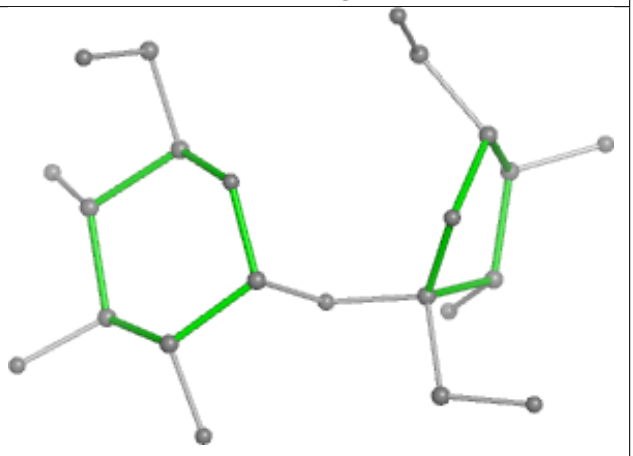
Bond lengths



Bond angles

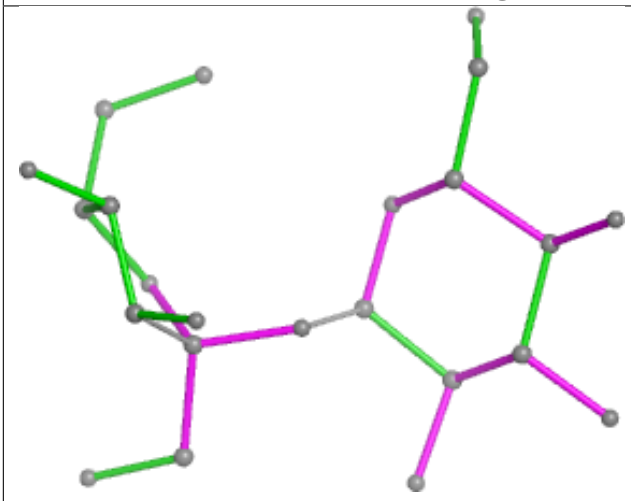


Torsions

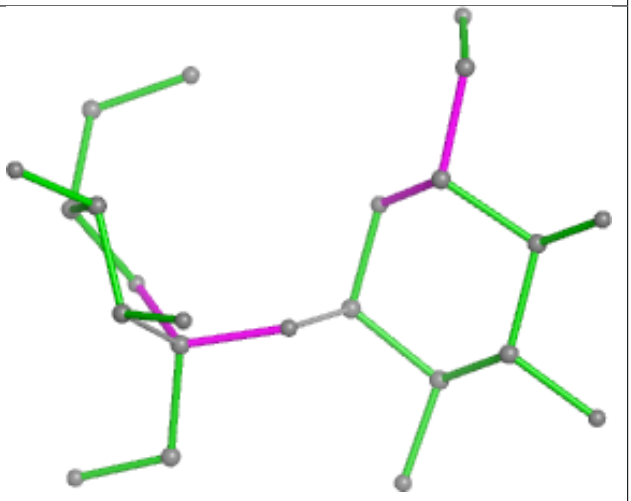


Rings

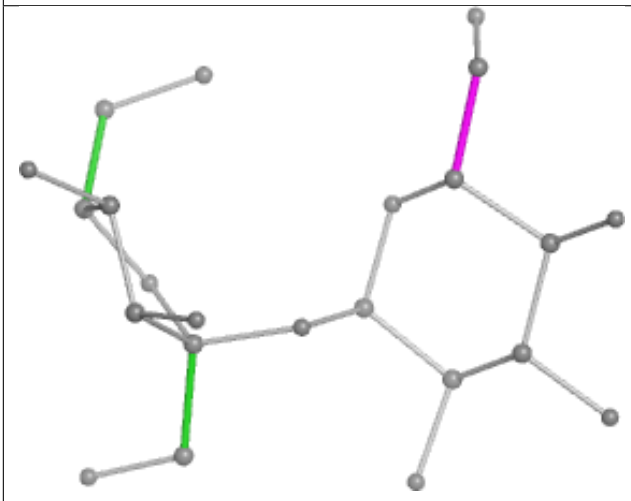
Oligosaccharide Chain K



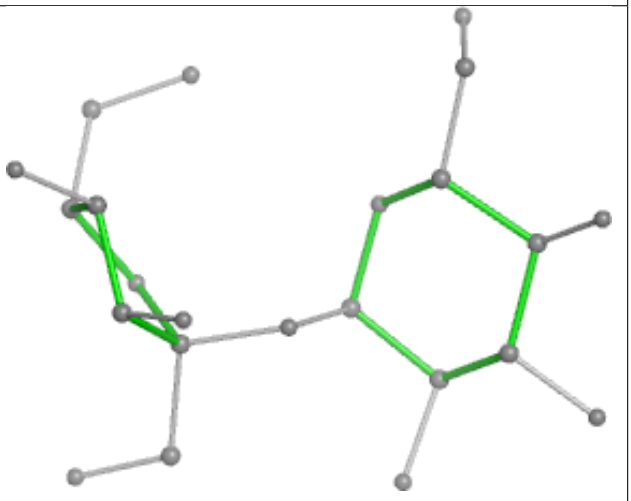
Bond lengths



Bond angles

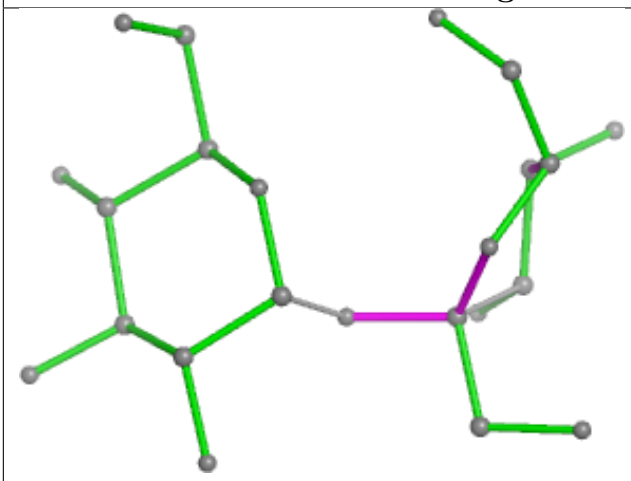


Torsions

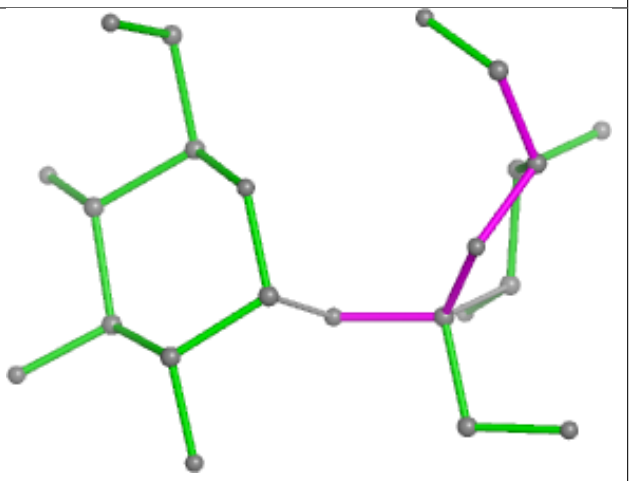


Rings

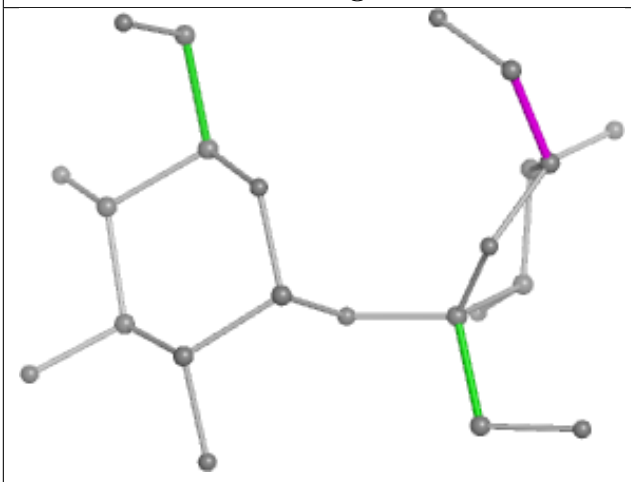
Oligosaccharide Chain L



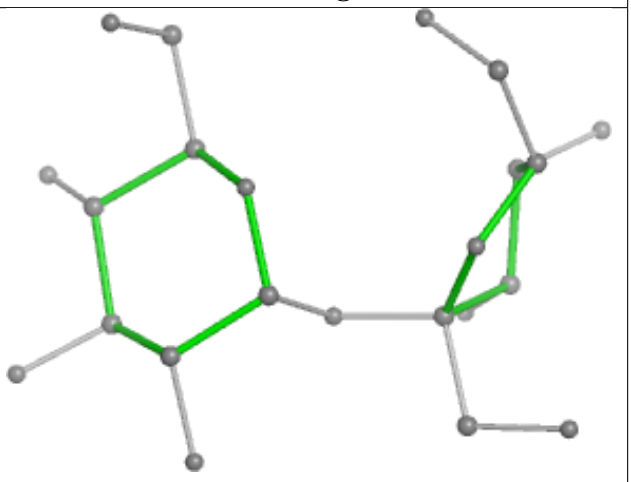
Bond lengths



Bond angles

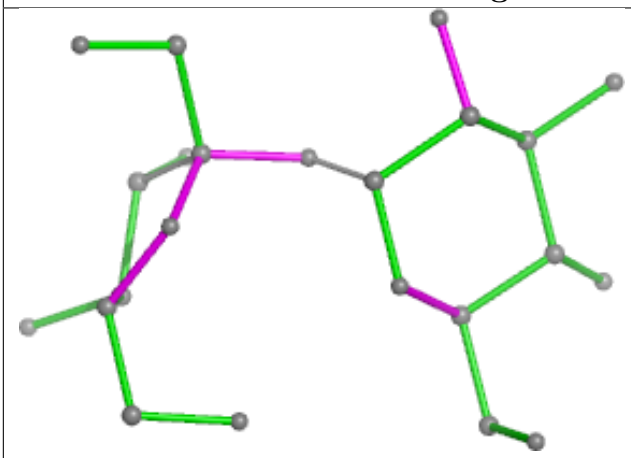


Torsions

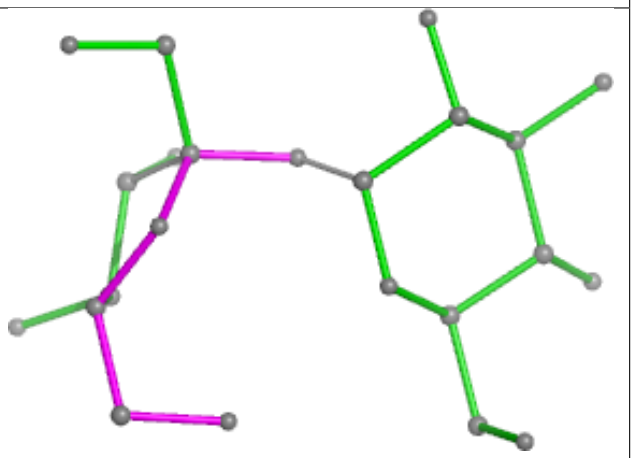


Rings

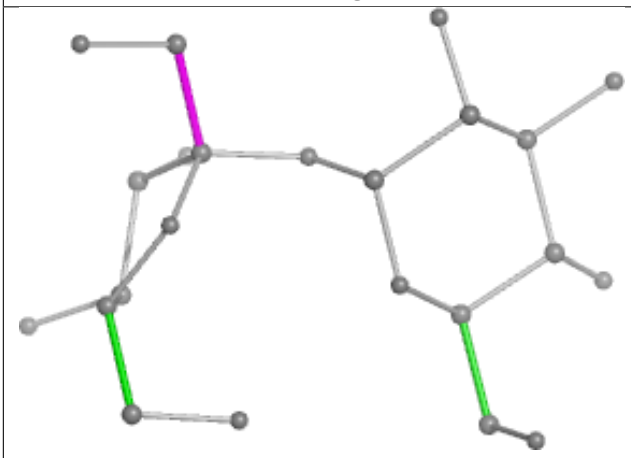
Oligosaccharide Chain M



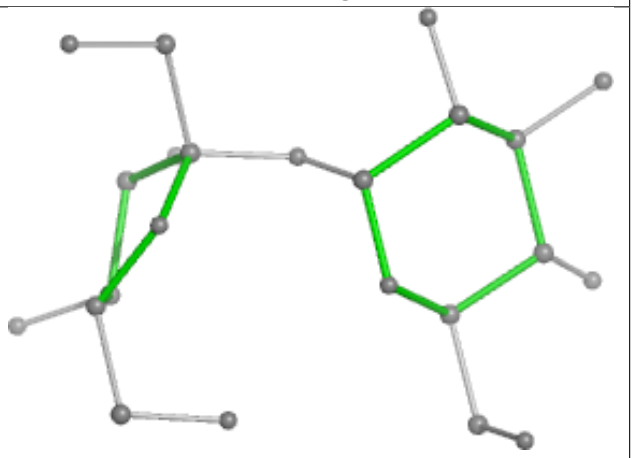
Bond lengths



Bond angles

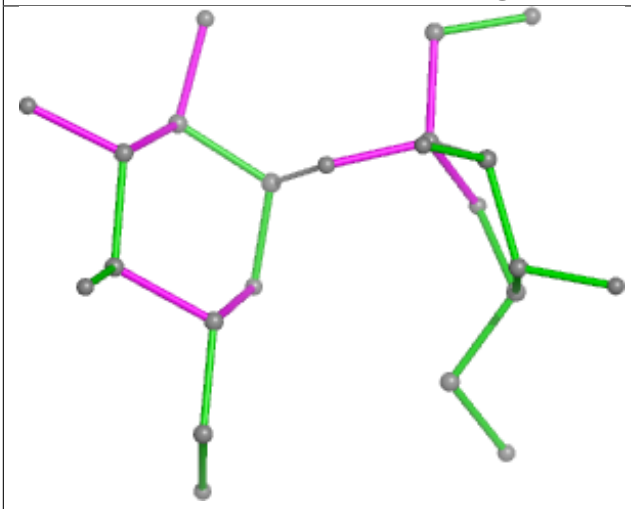


Torsions

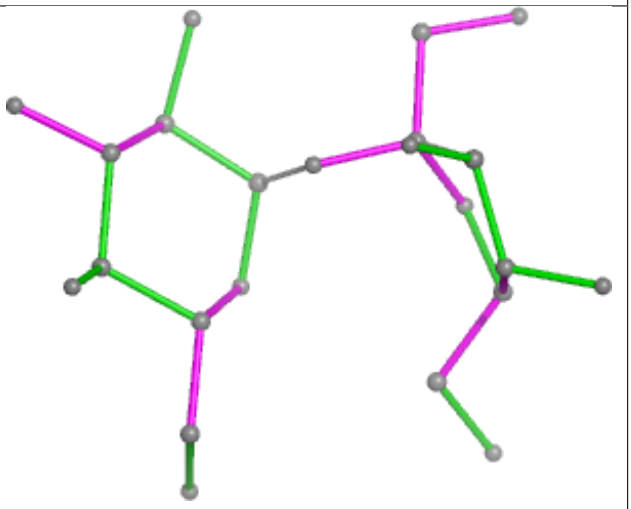


Rings

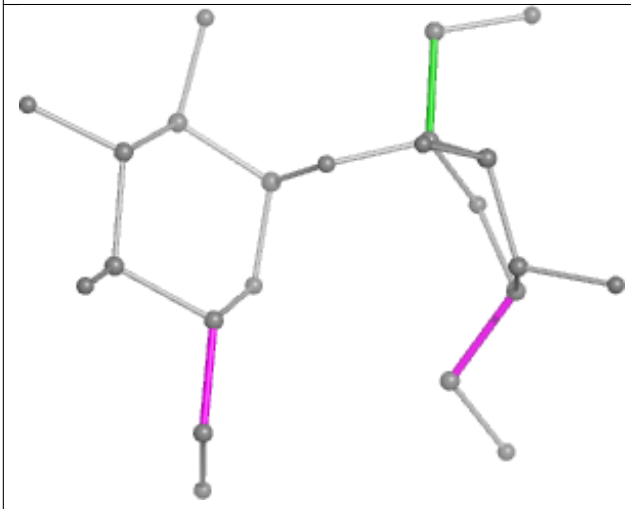
Oligosaccharide Chain N



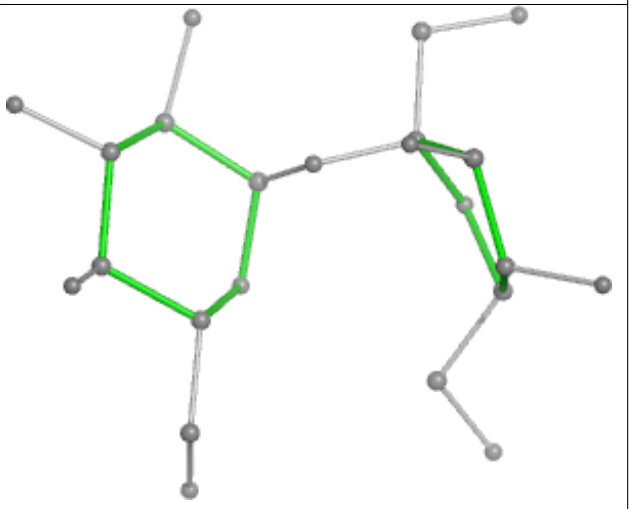
Bond lengths



Bond angles

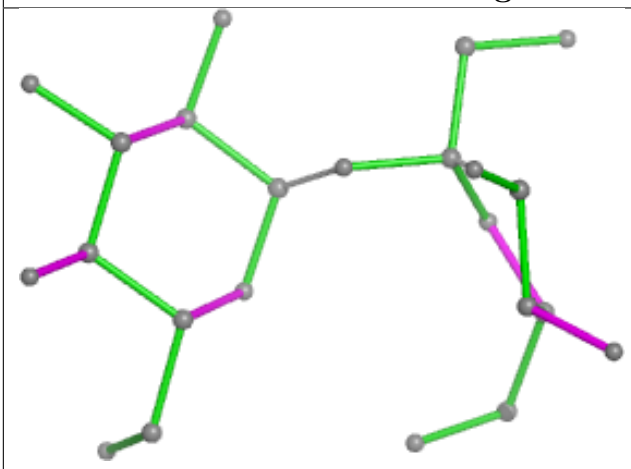


Torsions

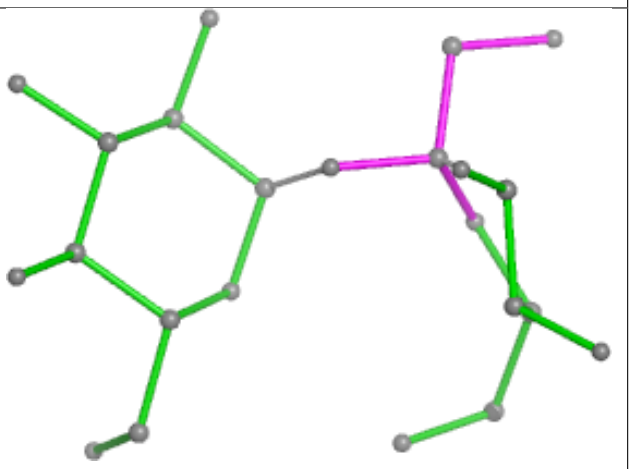


Rings

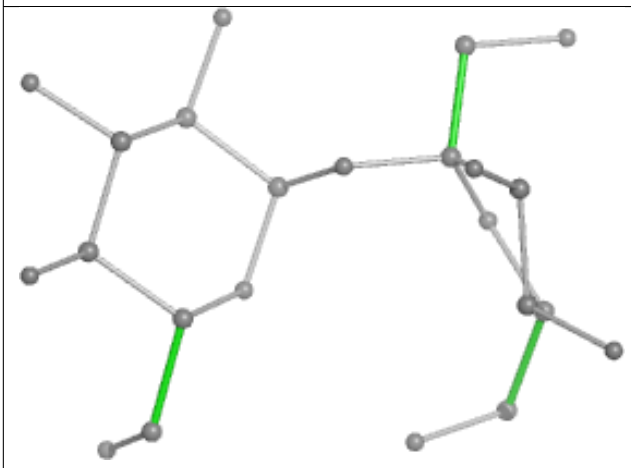
Oligosaccharide Chain O



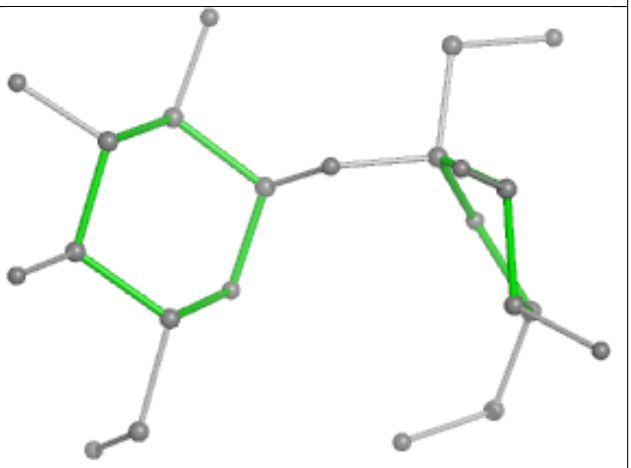
Bond lengths



Bond angles

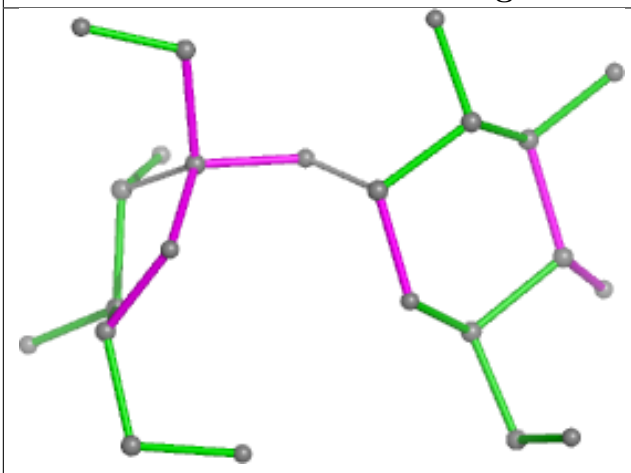


Torsions

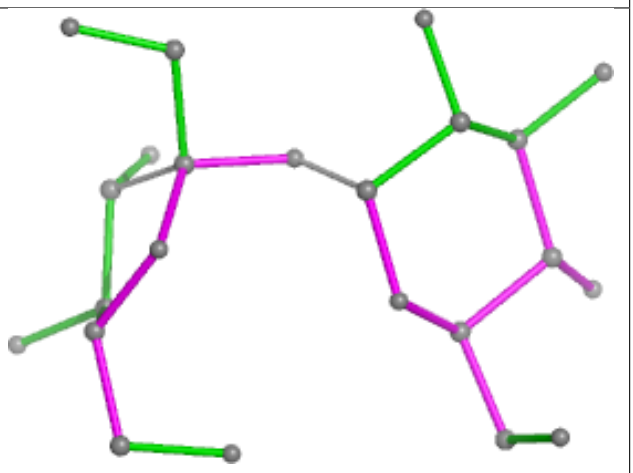


Rings

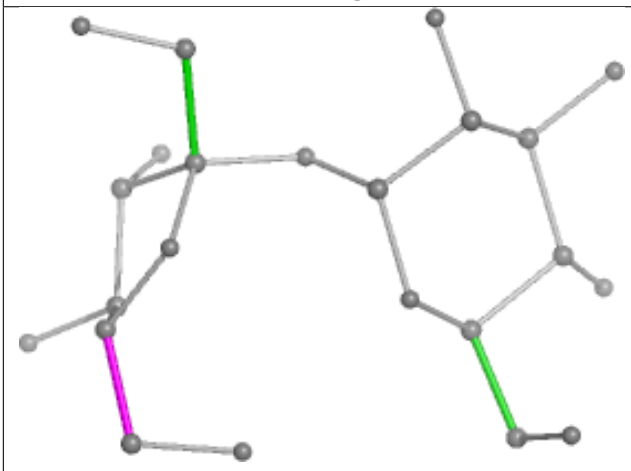
Oligosaccharide Chain P



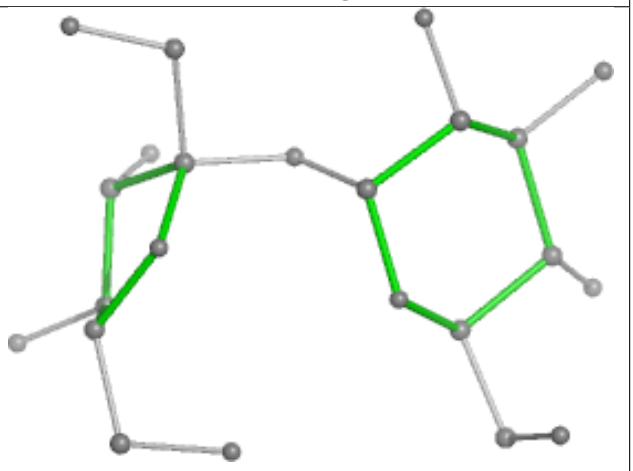
Bond lengths



Bond angles

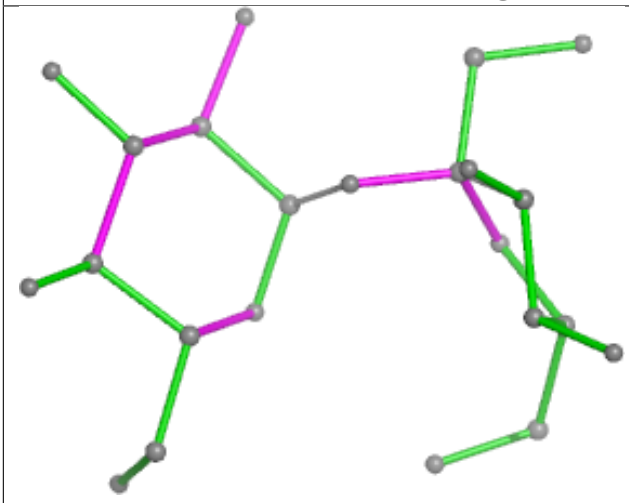


Torsions

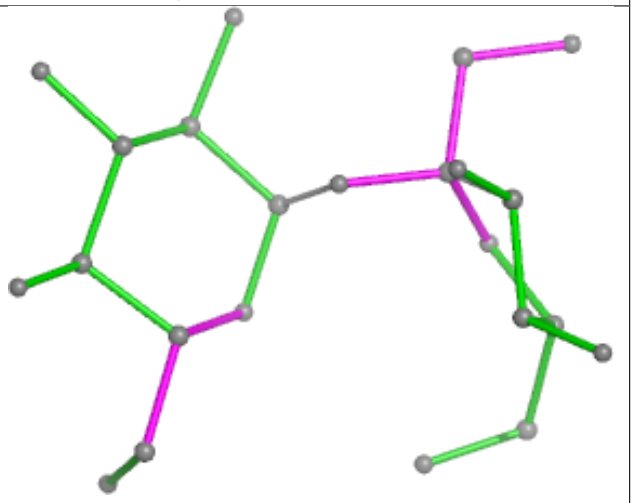


Rings

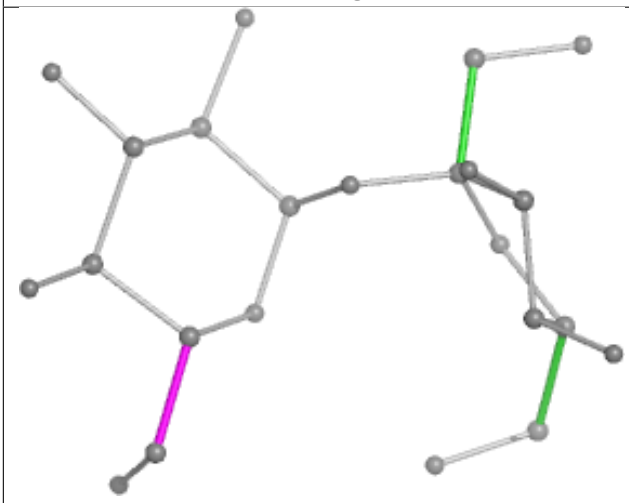
Oligosaccharide Chain Q



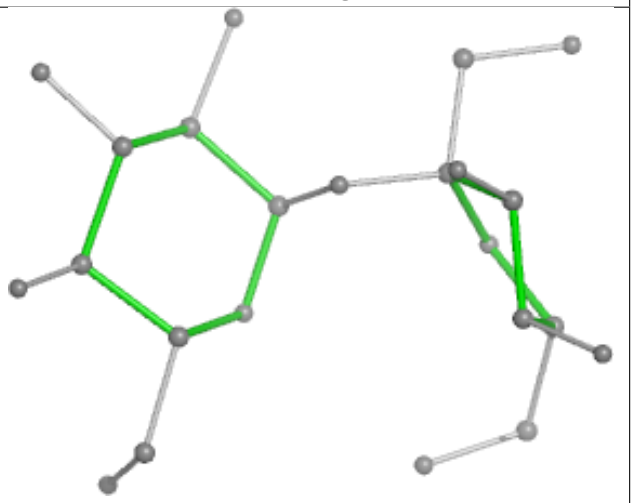
Bond lengths



Bond angles

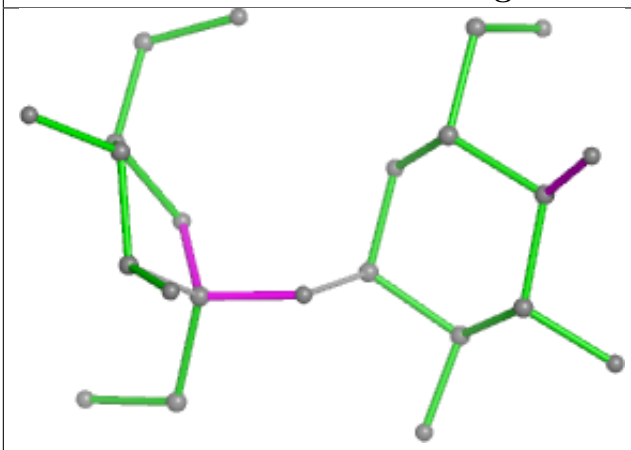


Torsions

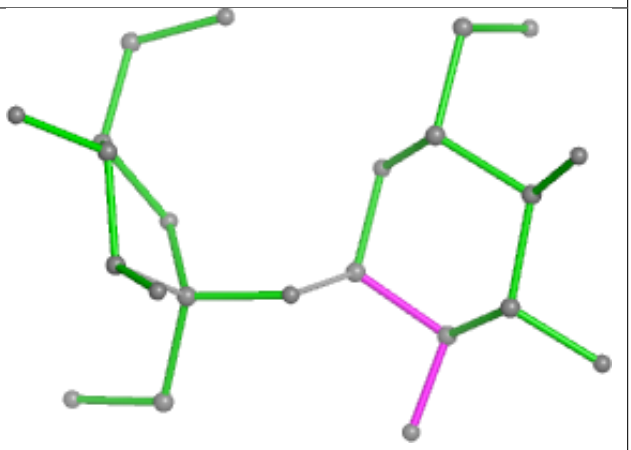


Rings

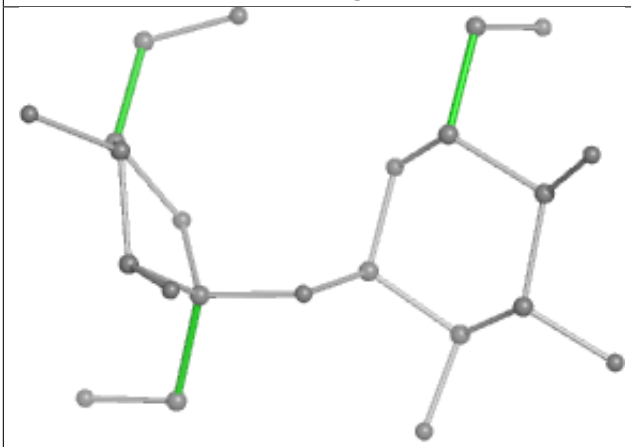
Oligosaccharide Chain R



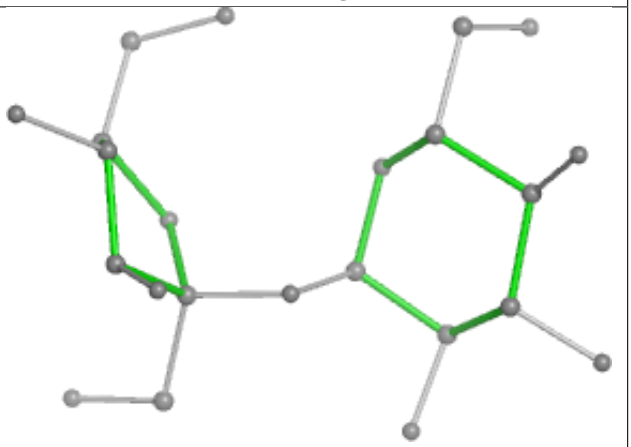
Bond lengths



Bond angles

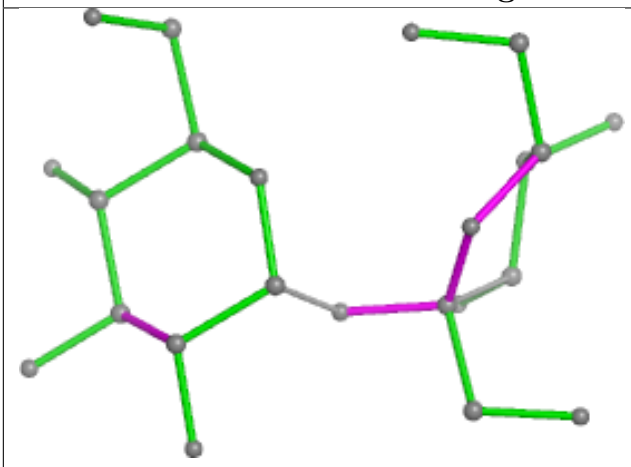


Torsions

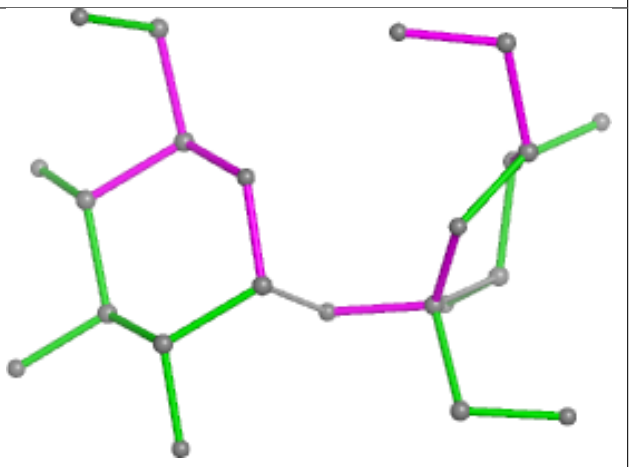


Rings

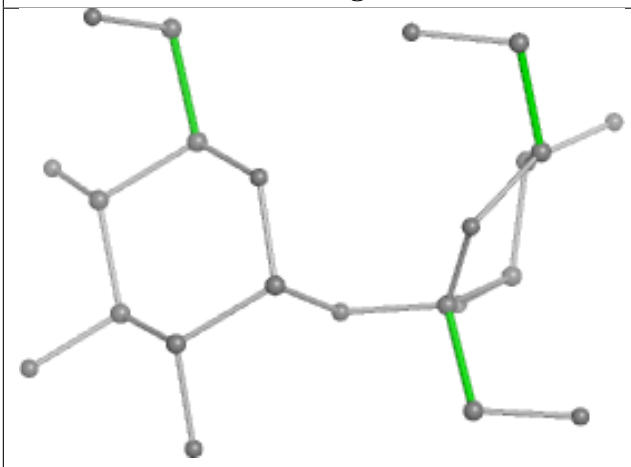
Oligosaccharide Chain S



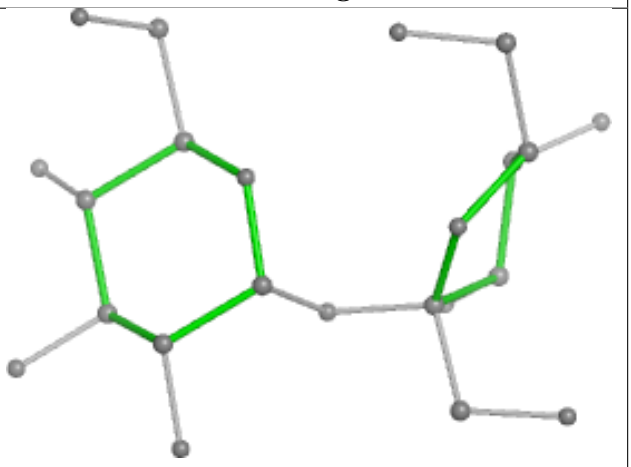
Bond lengths



Bond angles

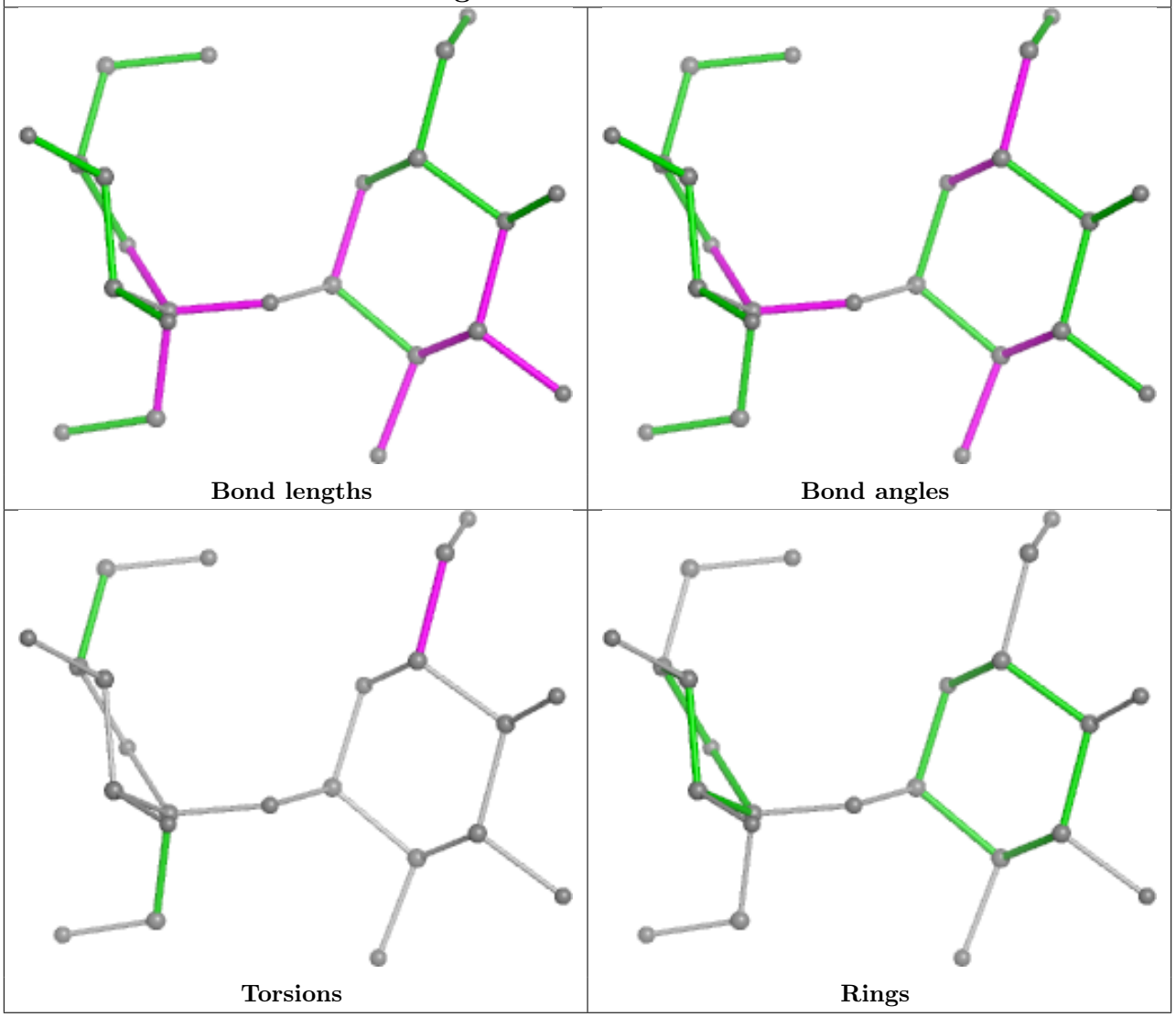


Torsions



Rings

Oligosaccharide Chain T



5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 12 are monoatomic - leaving 27 for Mogul analysis.

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	$\#\|Z\| > 2$
3	FAD	H	551	-	53,58,58	1.59	8 (15%)	68,89,89	1.72	16 (23%)
6	PG4	E	582	-	12,12,12	1.02	0	11,11,11	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FAD	B	551	-	53,58,58	1.77	13 (24%)	68,89,89	1.68	12 (17%)
6	PG4	H	582	-	12,12,12	0.77	0	11,11,11	0.82	0
3	FAD	A	551	-	53,58,58	1.94	12 (22%)	68,89,89	1.80	16 (23%)
3	FAD	F	551	-	53,58,58	1.60	9 (16%)	68,89,89	1.64	12 (17%)
6	PG4	B	582	-	12,12,12	0.91	0	11,11,11	0.80	0
6	PG4	C	582	-	12,12,12	0.87	0	11,11,11	0.90	0
6	PG4	E	583	-	12,12,12	0.99	0	11,11,11	1.21	1 (9%)
6	PG4	C	581	-	12,12,12	0.93	0	11,11,11	1.26	2 (18%)
6	PG4	D	582	-	12,12,12	0.93	0	11,11,11	0.64	0
6	PG4	E	581	-	12,12,12	0.86	0	11,11,11	0.54	0
6	PG4	G	582	-	12,12,12	0.87	0	11,11,11	0.64	0
6	PG4	B	584	-	12,12,12	0.80	0	11,11,11	1.16	1 (9%)
6	PG4	F	582	-	12,12,12	0.91	0	11,11,11	1.09	1 (9%)
6	PG4	A	583	-	12,12,12	0.98	0	11,11,11	1.32	1 (9%)
6	PG4	H	581	-	12,12,12	0.84	0	11,11,11	0.70	0
6	PG4	B	581	-	12,12,12	0.67	0	11,11,11	0.59	0
3	FAD	D	551	-	53,58,58	1.93	12 (22%)	68,89,89	1.71	15 (22%)
3	FAD	E	551	-	53,58,58	1.71	8 (15%)	68,89,89	1.75	18 (26%)
6	PG4	G	581	-	12,12,12	0.74	0	11,11,11	0.59	0
6	PG4	D	581	-	12,12,12	0.96	0	11,11,11	0.66	0
6	PG4	A	582	-	12,12,12	0.91	0	11,11,11	0.64	0
6	PG4	A	581	-	12,12,12	0.98	0	11,11,11	0.77	0
3	FAD	C	551	-	53,58,58	1.89	10 (18%)	68,89,89	1.65	14 (20%)
6	PG4	F	581	-	12,12,12	0.98	1 (8%)	11,11,11	0.52	0
3	FAD	G	551	-	53,58,58	1.79	14 (26%)	68,89,89	1.76	12 (17%)

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
3	FAD	H	551	-	-	6/30/50/50	0/6/6/6
6	PG4	E	582	-	-	5/10/10/10	-
3	FAD	B	551	-	-	6/30/50/50	0/6/6/6
6	PG4	H	582	-	-	4/10/10/10	-
3	FAD	A	551	-	-	5/30/50/50	0/6/6/6
3	FAD	F	551	-	-	2/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PG4	B	582	-	-	6/10/10/10	-
6	PG4	C	582	-	-	7/10/10/10	-
6	PG4	E	583	-	-	4/10/10/10	-
6	PG4	C	581	-	-	7/10/10/10	-
6	PG4	D	582	-	-	5/10/10/10	-
6	PG4	E	581	-	-	6/10/10/10	-
6	PG4	G	582	-	-	5/10/10/10	-
6	PG4	B	584	-	-	6/10/10/10	-
6	PG4	F	582	-	-	7/10/10/10	-
6	PG4	A	583	-	-	3/10/10/10	-
6	PG4	H	581	-	-	6/10/10/10	-
6	PG4	B	581	-	-	5/10/10/10	-
3	FAD	D	551	-	-	4/30/50/50	0/6/6/6
3	FAD	E	551	-	-	3/30/50/50	0/6/6/6
6	PG4	G	581	-	-	5/10/10/10	-
6	PG4	D	581	-	-	7/10/10/10	-
6	PG4	A	582	-	-	8/10/10/10	-
6	PG4	A	581	-	-	7/10/10/10	-
3	FAD	C	551	-	-	8/30/50/50	0/6/6/6
6	PG4	F	581	-	-	5/10/10/10	-
3	FAD	G	551	-	-	10/30/50/50	0/6/6/6

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	551	FAD	C2A-N3A	7.10	1.43	1.32
3	C	551	FAD	C2A-N3A	6.43	1.42	1.32
3	A	551	FAD	C2A-N3A	6.24	1.42	1.32
3	C	551	FAD	C7M-C7	-5.74	1.39	1.51
3	E	551	FAD	C7M-C7	-5.53	1.40	1.51
3	G	551	FAD	C8M-C8	-5.43	1.40	1.51
3	F	551	FAD	C8M-C8	-5.41	1.40	1.51
3	D	551	FAD	C7M-C7	-5.39	1.40	1.51
3	A	551	FAD	C8M-C8	-5.00	1.41	1.51
3	E	551	FAD	C2A-N3A	5.00	1.40	1.32
3	C	551	FAD	C8M-C8	-4.90	1.41	1.51
3	H	551	FAD	C7M-C7	-4.83	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	551	FAD	C2A-N3A	4.52	1.39	1.32
3	B	551	FAD	C2A-N1A	4.51	1.42	1.33
3	A	551	FAD	C7M-C7	-4.45	1.42	1.51
3	E	551	FAD	C8M-C8	-4.44	1.42	1.51
3	G	551	FAD	C7M-C7	-4.43	1.42	1.51
3	F	551	FAD	C7M-C7	-4.40	1.42	1.51
3	B	551	FAD	C7M-C7	-4.32	1.42	1.51
3	D	551	FAD	C8M-C8	-4.27	1.42	1.51
3	B	551	FAD	C8M-C8	-4.09	1.42	1.51
3	B	551	FAD	C2A-N3A	4.02	1.38	1.32
3	C	551	FAD	C2A-N1A	3.99	1.41	1.33
3	F	551	FAD	C2A-N3A	3.85	1.38	1.32
3	A	551	FAD	C4X-N5	3.72	1.38	1.30
3	G	551	FAD	C2A-N3A	3.71	1.38	1.32
3	H	551	FAD	C2B-C1B	3.59	1.59	1.53
3	B	551	FAD	C5'-C4'	3.52	1.56	1.51
3	A	551	FAD	C2A-N1A	3.52	1.40	1.33
3	G	551	FAD	C2A-N1A	3.50	1.40	1.33
3	H	551	FAD	C8M-C8	-3.46	1.44	1.51
3	E	551	FAD	C2A-N1A	3.37	1.40	1.33
3	H	551	FAD	C5A-C4A	-3.30	1.32	1.40
3	G	551	FAD	C9A-N10	-3.29	1.35	1.41
3	A	551	FAD	C1'-N10	3.29	1.56	1.48
3	G	551	FAD	C2B-C1B	3.21	1.58	1.53
3	F	551	FAD	C10-N1	3.21	1.39	1.33
3	D	551	FAD	C2A-N1A	3.16	1.39	1.33
3	C	551	FAD	O4B-C1B	3.00	1.45	1.41
3	A	551	FAD	C5A-C4A	-2.99	1.33	1.40
3	D	551	FAD	O4B-C4B	2.87	1.51	1.45
3	G	551	FAD	C4X-N5	2.86	1.36	1.30
3	D	551	FAD	C10-N1	2.61	1.38	1.33
3	D	551	FAD	C9A-N10	-2.59	1.36	1.41
3	D	551	FAD	C9-C9A	2.55	1.43	1.39
3	F	551	FAD	C5A-C4A	-2.54	1.34	1.40
3	F	551	FAD	P-O2P	-2.48	1.43	1.55
3	B	551	FAD	C4X-N5	2.47	1.35	1.30
3	D	551	FAD	O4B-C1B	2.47	1.44	1.41
3	G	551	FAD	C2-N1	2.46	1.42	1.36
3	C	551	FAD	C1'-C2'	2.43	1.56	1.52
3	B	551	FAD	C4'-C3'	-2.43	1.48	1.53
3	E	551	FAD	C5X-N5	-2.43	1.34	1.39
3	D	551	FAD	C4X-N5	2.43	1.35	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	551	FAD	C1'-N10	2.38	1.54	1.48
3	D	551	FAD	C5A-C4A	-2.37	1.34	1.40
3	C	551	FAD	O4B-C4B	2.36	1.50	1.45
3	C	551	FAD	O3B-C3B	2.30	1.48	1.43
3	A	551	FAD	O4B-C1B	2.29	1.44	1.41
3	A	551	FAD	C4'-C3'	-2.29	1.49	1.53
3	E	551	FAD	C5A-C4A	-2.29	1.34	1.40
3	F	551	FAD	C9A-N10	-2.26	1.37	1.41
3	B	551	FAD	C6A-C5A	-2.25	1.34	1.43
3	E	551	FAD	C4X-N5	2.24	1.35	1.30
3	H	551	FAD	C6A-C5A	-2.22	1.35	1.43
3	D	551	FAD	C2B-C1B	2.22	1.57	1.53
3	F	551	FAD	C6A-C5A	-2.22	1.35	1.43
3	E	551	FAD	C4'-C3'	-2.19	1.49	1.53
3	G	551	FAD	C5X-N5	-2.17	1.35	1.39
3	G	551	FAD	C6A-C5A	-2.15	1.35	1.43
3	G	551	FAD	C2'-C3'	2.14	1.57	1.53
3	A	551	FAD	C6-C7	2.13	1.42	1.39
3	B	551	FAD	P-O2P	-2.12	1.45	1.55
3	B	551	FAD	C4A-N3A	-2.11	1.32	1.35
3	F	551	FAD	C1'-C2'	2.11	1.55	1.52
3	G	551	FAD	C5A-N7A	-2.10	1.32	1.39
3	A	551	FAD	C6A-C5A	-2.10	1.35	1.43
3	C	551	FAD	C10-N1	2.08	1.37	1.33
3	B	551	FAD	PA-O1A	-2.07	1.43	1.50
3	B	551	FAD	PA-O5B	-2.07	1.50	1.59
3	A	551	FAD	C10-N1	2.06	1.37	1.33
3	G	551	FAD	C10-N1	2.06	1.37	1.33
3	C	551	FAD	C9A-N10	-2.05	1.37	1.41
3	B	551	FAD	C5A-C4A	-2.04	1.35	1.40
6	F	581	PG4	O2-C2	2.04	1.50	1.42
3	H	551	FAD	C1'-N10	2.03	1.53	1.48
3	H	551	FAD	C4X-N5	2.00	1.34	1.30

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	551	FAD	N3A-C2A-N1A	-7.16	117.48	128.68
3	E	551	FAD	N3A-C2A-N1A	-6.96	117.79	128.68
3	B	551	FAD	N3A-C2A-N1A	-6.82	118.01	128.68
3	D	551	FAD	N3A-C2A-N1A	-6.67	118.26	128.68
3	A	551	FAD	N3A-C2A-N1A	-6.57	118.41	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	551	FAD	N3A-C2A-N1A	-5.63	119.87	128.68
3	G	551	FAD	N3A-C2A-N1A	-5.40	120.23	128.68
3	C	551	FAD	N3A-C2A-N1A	-5.29	120.41	128.68
3	G	551	FAD	C4'-C3'-C2'	-4.70	103.58	113.36
3	G	551	FAD	O4B-C1B-C2B	-4.27	100.68	106.93
3	E	551	FAD	C1B-N9A-C4A	-4.15	119.36	126.64
3	G	551	FAD	C4X-C10-N10	4.12	122.50	116.48
3	D	551	FAD	C4X-C10-N10	4.10	122.48	116.48
3	H	551	FAD	C1B-N9A-C4A	-4.08	119.47	126.64
3	C	551	FAD	C4'-C3'-C2'	-4.03	104.98	113.36
3	G	551	FAD	C10-C4X-N5	-3.88	116.62	124.86
3	B	551	FAD	C4'-C3'-C2'	-3.78	105.50	113.36
3	H	551	FAD	C4X-C10-N10	3.69	121.87	116.48
3	F	551	FAD	C4'-C3'-C2'	-3.67	105.72	113.36
3	A	551	FAD	C1B-N9A-C4A	-3.53	120.43	126.64
3	F	551	FAD	C1B-N9A-C4A	-3.48	120.52	126.64
3	G	551	FAD	C4-C4X-N5	3.48	123.19	118.23
3	C	551	FAD	C4X-C10-N10	3.47	121.55	116.48
3	G	551	FAD	C4-N3-C2	-3.45	119.27	125.64
3	B	551	FAD	C4X-C10-N10	3.43	121.50	116.48
3	F	551	FAD	C4X-C10-N10	3.39	121.43	116.48
3	D	551	FAD	C1B-N9A-C4A	-3.34	120.78	126.64
3	E	551	FAD	C4'-C3'-C2'	-3.27	106.56	113.36
3	B	551	FAD	C1B-N9A-C4A	-3.26	120.92	126.64
3	A	551	FAD	C4-C4X-N5	3.20	122.79	118.23
3	C	551	FAD	C4-N3-C2	-3.17	119.79	125.64
3	D	551	FAD	C4'-C3'-C2'	-3.14	106.83	113.36
3	E	551	FAD	C4X-C10-N10	3.14	121.07	116.48
3	A	551	FAD	C4'-C3'-C2'	-3.12	106.88	113.36
6	A	583	PG4	C3-O2-C2	2.97	126.16	113.29
3	H	551	FAD	C4'-C3'-C2'	-2.96	107.20	113.36
3	A	551	FAD	O2'-C2'-C1'	2.96	116.95	109.80
3	C	551	FAD	C10-C4X-N5	-2.94	118.61	124.86
3	A	551	FAD	C9A-C5X-N5	-2.94	119.24	122.43
3	B	551	FAD	C10-C4X-N5	-2.91	118.69	124.86
3	A	551	FAD	C4X-C10-N10	2.89	120.71	116.48
3	G	551	FAD	O4-C4-N3	-2.89	114.57	120.12
3	A	551	FAD	C5A-C6A-N6A	-2.85	116.02	120.35
3	G	551	FAD	C4X-C4-N3	2.76	120.20	113.19
3	H	551	FAD	C10-N1-C2	2.76	122.42	116.90
3	E	551	FAD	C10-C4X-N5	-2.75	119.02	124.86
3	H	551	FAD	C4-N3-C2	-2.74	120.58	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	584	PG4	C5-O3-C4	2.73	125.14	113.29
3	A	551	FAD	C4X-C4-N3	2.72	120.09	113.19
3	E	551	FAD	C9A-C5X-N5	-2.72	119.48	122.43
3	D	551	FAD	C10-C4X-N5	-2.71	119.11	124.86
3	D	551	FAD	O2P-P-O1P	2.70	125.57	112.24
3	C	551	FAD	C4X-C4-N3	2.69	120.02	113.19
3	A	551	FAD	C10-C4X-N5	-2.68	119.17	124.86
3	F	551	FAD	O3'-C3'-C2'	2.68	115.28	108.81
3	H	551	FAD	C9A-N10-C10	-2.66	116.62	120.77
3	C	551	FAD	O2-C2-N1	-2.66	117.43	121.83
3	D	551	FAD	P-O3P-PA	-2.62	123.84	132.83
3	E	551	FAD	C4-N3-C2	-2.60	120.83	125.64
3	F	551	FAD	C10-C4X-N5	-2.60	119.35	124.86
3	D	551	FAD	O2-C2-N1	-2.59	117.54	121.83
3	H	551	FAD	O2-C2-N1	-2.50	117.69	121.83
3	A	551	FAD	C10-N1-C2	2.48	121.86	116.90
3	E	551	FAD	C6-C5X-C9A	2.48	122.44	118.94
3	H	551	FAD	C4X-C4-N3	2.46	119.43	113.19
3	B	551	FAD	P-O3P-PA	-2.46	124.40	132.83
3	A	551	FAD	O4B-C4B-C5B	-2.45	101.31	109.37
3	C	551	FAD	C4-C4X-N5	2.44	121.70	118.23
3	F	551	FAD	C4X-C4-N3	2.43	119.36	113.19
3	H	551	FAD	O2-C2-N3	2.42	123.36	118.65
3	D	551	FAD	C4X-C10-N1	-2.40	119.17	124.73
3	A	551	FAD	O2P-P-O1P	2.39	124.04	112.24
3	E	551	FAD	C10-N1-C2	2.39	121.67	116.90
3	A	551	FAD	O4B-C1B-C2B	-2.38	103.44	106.93
3	D	551	FAD	O2-C2-N3	2.38	123.28	118.65
3	B	551	FAD	C4-C4X-N5	2.38	121.61	118.23
3	H	551	FAD	C5A-C6A-N6A	-2.38	116.74	120.35
3	G	551	FAD	C4X-C10-N1	-2.37	119.22	124.73
3	B	551	FAD	C4X-C10-N1	-2.37	119.23	124.73
3	E	551	FAD	C4X-C10-N1	-2.34	119.30	124.73
3	C	551	FAD	C10-N1-C2	2.33	121.56	116.90
3	C	551	FAD	O2-C2-N3	2.32	123.17	118.65
3	D	551	FAD	C5A-C6A-N6A	-2.32	116.83	120.35
3	F	551	FAD	C4-N3-C2	-2.31	121.38	125.64
6	E	583	PG4	C3-O2-C2	2.30	123.27	113.29
3	H	551	FAD	O2P-P-O1P	2.30	123.62	112.24
3	E	551	FAD	C5X-C9A-N10	2.29	120.32	117.95
3	F	551	FAD	C9A-C9-C8	2.29	123.92	119.30
3	E	551	FAD	C4X-C4-N3	2.28	118.97	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	551	FAD	C4X-C10-N1	-2.26	119.49	124.73
3	B	551	FAD	C10-N1-C2	2.25	121.40	116.90
6	C	581	PG4	C3-O2-C2	2.24	123.00	113.29
3	C	551	FAD	C4A-C5A-N7A	-2.24	107.06	109.40
3	G	551	FAD	O2-C2-N1	-2.23	118.14	121.83
3	H	551	FAD	C10-C4X-N5	-2.22	120.14	124.86
3	C	551	FAD	C4X-C10-N1	-2.21	119.61	124.73
3	C	551	FAD	C9A-C5X-N5	-2.21	120.03	122.43
3	E	551	FAD	C9A-N10-C10	-2.19	117.35	120.77
3	D	551	FAD	C4-N3-C2	-2.19	121.59	125.64
3	D	551	FAD	C10-N1-C2	2.18	121.27	116.90
3	D	551	FAD	C4X-C4-N3	2.18	118.72	113.19
6	F	582	PG4	C3-O2-C2	2.17	122.68	113.29
3	E	551	FAD	O2-C2-N1	-2.16	118.25	121.83
3	B	551	FAD	O4B-C1B-C2B	-2.15	103.79	106.93
3	E	551	FAD	C1'-C2'-C3'	2.14	115.78	109.79
3	F	551	FAD	C10-N1-C2	2.14	121.18	116.90
3	E	551	FAD	O3'-C3'-C2'	2.13	113.96	108.81
3	H	551	FAD	C4-C4X-N5	2.13	121.26	118.23
3	B	551	FAD	C4-N3-C2	-2.12	121.73	125.64
3	F	551	FAD	C9A-N10-C10	-2.12	117.47	120.77
3	H	551	FAD	C4X-C10-N1	-2.10	119.86	124.73
3	H	551	FAD	O3B-C3B-C4B	-2.10	104.98	111.05
3	B	551	FAD	C4X-C4-N3	2.08	118.48	113.19
3	A	551	FAD	C4-N3-C2	-2.08	121.80	125.64
3	E	551	FAD	C4A-C5A-N7A	-2.08	107.23	109.40
3	G	551	FAD	O2A-PA-O1A	2.08	122.50	112.24
6	C	581	PG4	O2-C2-C1	2.05	119.06	110.07
3	E	551	FAD	O5'-P-O1P	-2.03	101.14	109.07
3	C	551	FAD	O4B-C1B-C2B	-2.02	103.97	106.93
3	A	551	FAD	C4A-C5A-N7A	-2.01	107.30	109.40
3	D	551	FAD	C9A-N10-C10	-2.00	117.65	120.77

There are no chirality outliers.

All (152) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	551	FAD	C1'-C2'-C3'-C4'
3	C	551	FAD	C1'-C2'-C3'-C4'
3	G	551	FAD	C1'-C2'-C3'-C4'
6	A	582	PG4	C3-C4-O3-C5
6	B	582	PG4	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
6	B	584	PG4	C6-C5-O3-C4
6	C	581	PG4	C1-C2-O2-C3
6	D	582	PG4	O3-C5-C6-O4
6	E	581	PG4	O2-C3-C4-O3
6	E	582	PG4	O3-C5-C6-O4
6	F	581	PG4	O2-C3-C4-O3
6	A	582	PG4	O3-C5-C6-O4
6	D	582	PG4	O2-C3-C4-O3
6	H	581	PG4	O3-C5-C6-O4
6	A	581	PG4	O3-C5-C6-O4
6	E	583	PG4	O2-C3-C4-O3
6	H	581	PG4	O2-C3-C4-O3
6	G	582	PG4	O2-C3-C4-O3
6	B	581	PG4	O3-C5-C6-O4
6	F	582	PG4	O3-C5-C6-O4
6	G	581	PG4	O3-C5-C6-O4
6	C	581	PG4	C8-C7-O4-C6
6	D	581	PG4	O3-C5-C6-O4
6	A	581	PG4	O1-C1-C2-O2
6	A	582	PG4	O4-C7-C8-O5
6	B	582	PG4	O1-C1-C2-O2
6	B	582	PG4	O4-C7-C8-O5
6	D	581	PG4	O4-C7-C8-O5
6	F	581	PG4	O1-C1-C2-O2
6	B	581	PG4	O2-C3-C4-O3
6	E	581	PG4	O3-C5-C6-O4
6	A	581	PG4	O4-C7-C8-O5
6	C	582	PG4	O4-C7-C8-O5
6	D	581	PG4	O1-C1-C2-O2
6	E	582	PG4	O4-C7-C8-O5
6	F	582	PG4	O1-C1-C2-O2
6	H	582	PG4	O1-C1-C2-O2
6	C	582	PG4	O2-C3-C4-O3
6	B	582	PG4	O3-C5-C6-O4
6	C	582	PG4	O1-C1-C2-O2
6	G	582	PG4	O1-C1-C2-O2
3	A	551	FAD	C3B-C4B-C5B-O5B
3	G	551	FAD	O2'-C2'-C3'-C4'
6	G	582	PG4	O3-C5-C6-O4
6	F	582	PG4	O2-C3-C4-O3
6	C	582	PG4	C1-C2-O2-C3
6	B	581	PG4	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	B	584	PG4	O1-C1-C2-O2
6	D	582	PG4	O4-C7-C8-O5
6	F	582	PG4	C4-C3-O2-C2
3	A	551	FAD	O4B-C4B-C5B-O5B
3	H	551	FAD	O4B-C4B-C5B-O5B
6	D	582	PG4	O1-C1-C2-O2
3	A	551	FAD	P-O3P-PA-O1A
3	G	551	FAD	P-O3P-PA-O1A
6	G	581	PG4	O2-C3-C4-O3
3	B	551	FAD	O4B-C4B-C5B-O5B
3	C	551	FAD	O4B-C4B-C5B-O5B
6	C	581	PG4	O1-C1-C2-O2
6	A	582	PG4	O2-C3-C4-O3
3	D	551	FAD	PA-O3P-P-O5'
3	G	551	FAD	PA-O3P-P-O5'
6	E	581	PG4	O1-C1-C2-O2
6	B	582	PG4	C5-C6-O4-C7
6	G	582	PG4	C4-C3-O2-C2
6	H	581	PG4	C8-C7-O4-C6
6	B	581	PG4	C3-C4-O3-C5
6	C	581	PG4	C5-C6-O4-C7
6	E	582	PG4	C4-C3-O2-C2
6	C	581	PG4	C4-C3-O2-C2
6	A	582	PG4	C1-C2-O2-C3
6	G	581	PG4	C3-C4-O3-C5
6	B	581	PG4	C1-C2-O2-C3
6	A	583	PG4	C5-C6-O4-C7
6	C	582	PG4	O3-C5-C6-O4
6	F	582	PG4	C8-C7-O4-C6
6	G	581	PG4	C4-C3-O2-C2
6	A	581	PG4	C1-C2-O2-C3
6	A	582	PG4	C5-C6-O4-C7
6	D	581	PG4	C3-C4-O3-C5
6	H	581	PG4	C6-C5-O3-C4
6	C	582	PG4	C3-C4-O3-C5
3	F	551	FAD	O4B-C4B-C5B-O5B
6	B	584	PG4	C5-C6-O4-C7
6	F	581	PG4	C1-C2-O2-C3
6	H	581	PG4	C3-C4-O3-C5
6	E	581	PG4	C6-C5-O3-C4
6	E	583	PG4	C6-C5-O3-C4
6	G	582	PG4	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
6	D	581	PG4	O2-C3-C4-O3
6	H	581	PG4	C4-C3-O2-C2
3	H	551	FAD	O4'-C4'-C5'-O5'
6	F	581	PG4	C8-C7-O4-C6
6	B	584	PG4	C3-C4-O3-C5
6	C	581	PG4	O4-C7-C8-O5
3	B	551	FAD	O2'-C2'-C3'-C4'
6	C	581	PG4	O3-C5-C6-O4
6	E	581	PG4	C4-C3-O2-C2
6	F	582	PG4	O4-C7-C8-O5
3	E	551	FAD	O4B-C4B-C5B-O5B
3	G	551	FAD	O4B-C4B-C5B-O5B
6	F	582	PG4	C5-C6-O4-C7
6	A	582	PG4	C4-C3-O2-C2
6	A	582	PG4	C6-C5-O3-C4
6	A	583	PG4	O1-C1-C2-O2
6	E	582	PG4	O1-C1-C2-O2
6	H	582	PG4	O4-C7-C8-O5
6	E	583	PG4	C5-C6-O4-C7
6	E	582	PG4	C8-C7-O4-C6
6	D	581	PG4	C1-C2-O2-C3
3	D	551	FAD	O4B-C4B-C5B-O5B
3	H	551	FAD	C3B-C4B-C5B-O5B
6	B	582	PG4	C1-C2-O2-C3
6	A	581	PG4	C3-C4-O3-C5
6	D	582	PG4	C1-C2-O2-C3
3	B	551	FAD	C3B-C4B-C5B-O5B
6	A	581	PG4	C6-C5-O3-C4
6	H	582	PG4	C5-C6-O4-C7
6	F	581	PG4	C4-C3-O2-C2
6	A	581	PG4	C8-C7-O4-C6
6	G	581	PG4	C8-C7-O4-C6
3	A	551	FAD	P-O3P-PA-O2A
3	C	551	FAD	P-O3P-PA-O1A
3	H	551	FAD	P-O3P-PA-O1A
6	A	583	PG4	C1-C2-O2-C3
6	E	583	PG4	C4-C3-O2-C2
3	C	551	FAD	C3B-C4B-C5B-O5B
3	C	551	FAD	PA-O3P-P-O5'
3	D	551	FAD	C3B-C4B-C5B-O5B
6	E	581	PG4	C8-C7-O4-C6
6	H	582	PG4	C8-C7-O4-C6

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Mol	Chain	Res	Type	Atoms
3	G	551	FAD	O4'-C4'-C5'-O5'
3	G	551	FAD	C3B-C4B-C5B-O5B
3	E	551	FAD	C3B-C4B-C5B-O5B
3	F	551	FAD	C3B-C4B-C5B-O5B
3	D	551	FAD	P-O3P-PA-O2A
3	G	551	FAD	P-O3P-PA-O2A
3	H	551	FAD	P-O3P-PA-O2A
6	D	581	PG4	C8-C7-O4-C6
3	B	551	FAD	O2'-C2'-C3'-O3'
3	G	551	FAD	O2'-C2'-C3'-O3'
3	C	551	FAD	O2'-C2'-C3'-C4'
6	B	584	PG4	O2-C3-C4-O3
3	C	551	FAD	C5'-O5'-P-O1P
3	A	551	FAD	C1'-C2'-C3'-O3'
3	B	551	FAD	C1'-C2'-C3'-O3'
3	C	551	FAD	C1'-C2'-C3'-O3'
3	E	551	FAD	C1'-C2'-C3'-O3'
3	G	551	FAD	C1'-C2'-C3'-O3'
3	H	551	FAD	C1'-C2'-C3'-O3'
6	C	582	PG4	C5-C6-O4-C7
6	B	584	PG4	C8-C7-O4-C6

There are no ring outliers.

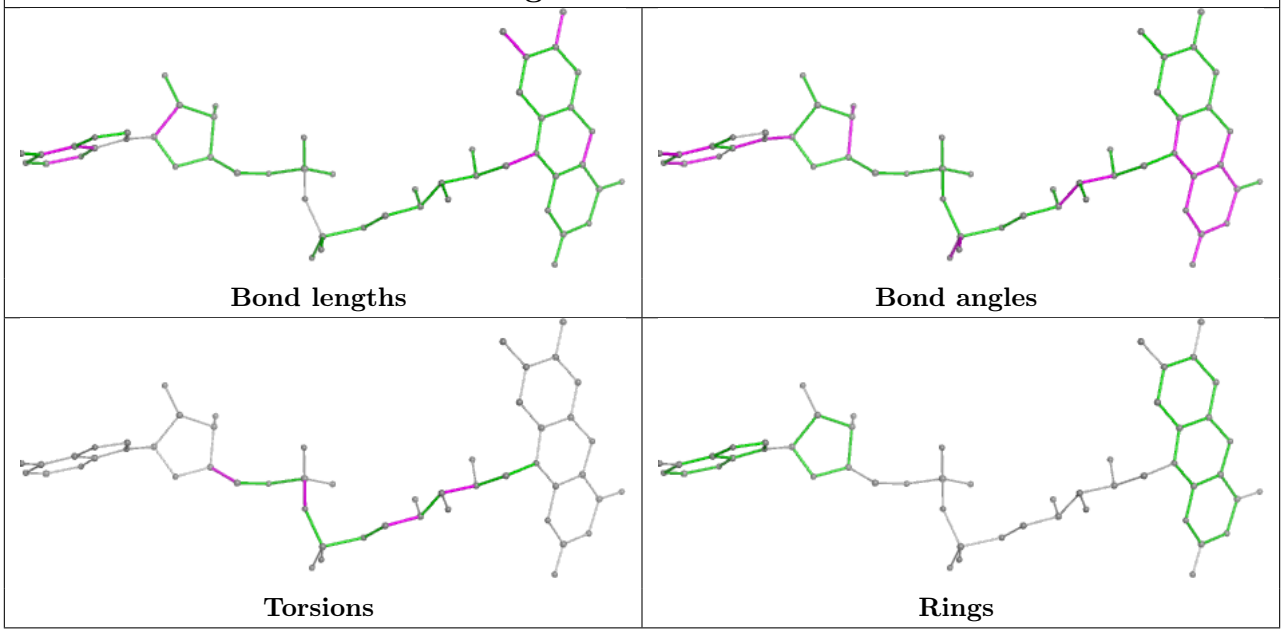
13 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	551	FAD	1	0
6	B	582	PG4	2	0
6	C	582	PG4	1	0
6	C	581	PG4	2	0
6	E	581	PG4	4	0
6	G	582	PG4	2	0
6	F	582	PG4	3	0
3	D	551	FAD	3	0
3	E	551	FAD	2	0
6	D	581	PG4	4	0
6	A	581	PG4	1	0
3	C	551	FAD	1	0
3	G	551	FAD	2	0

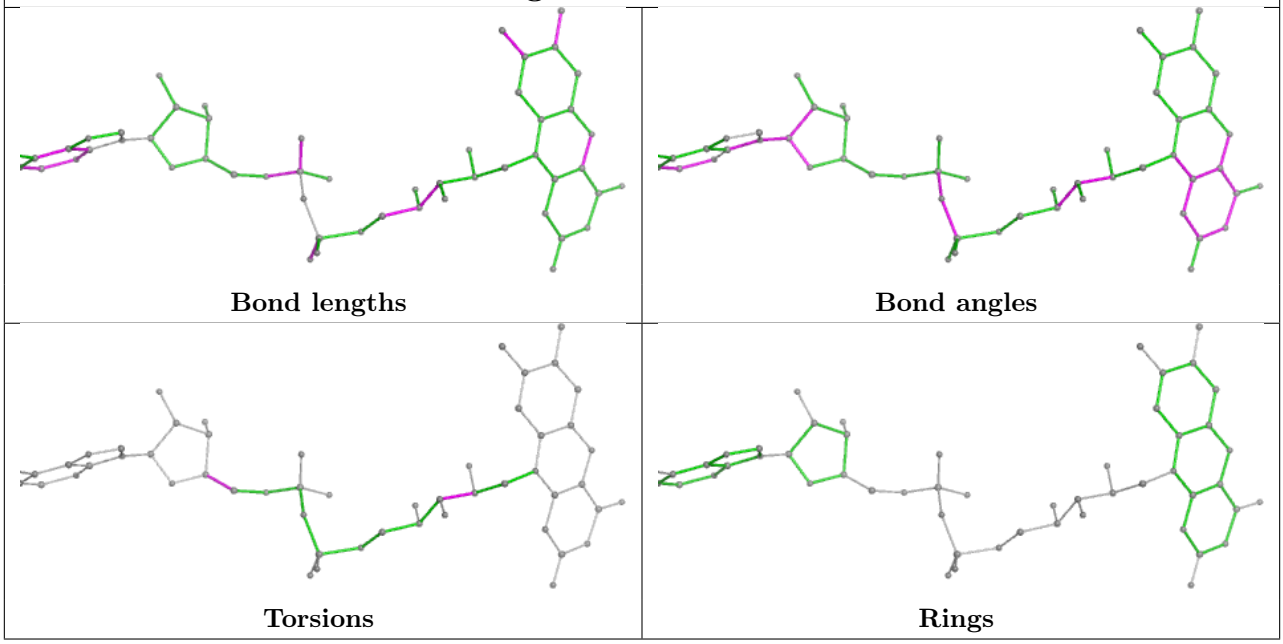
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

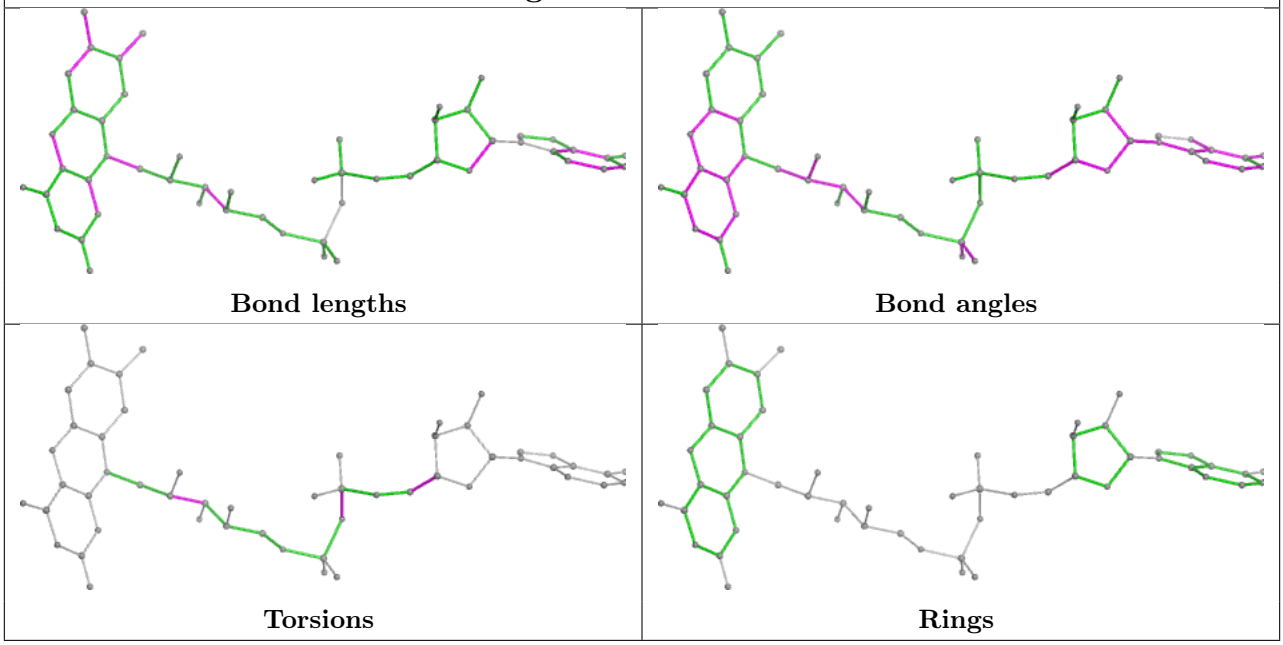
Ligand FAD H 551



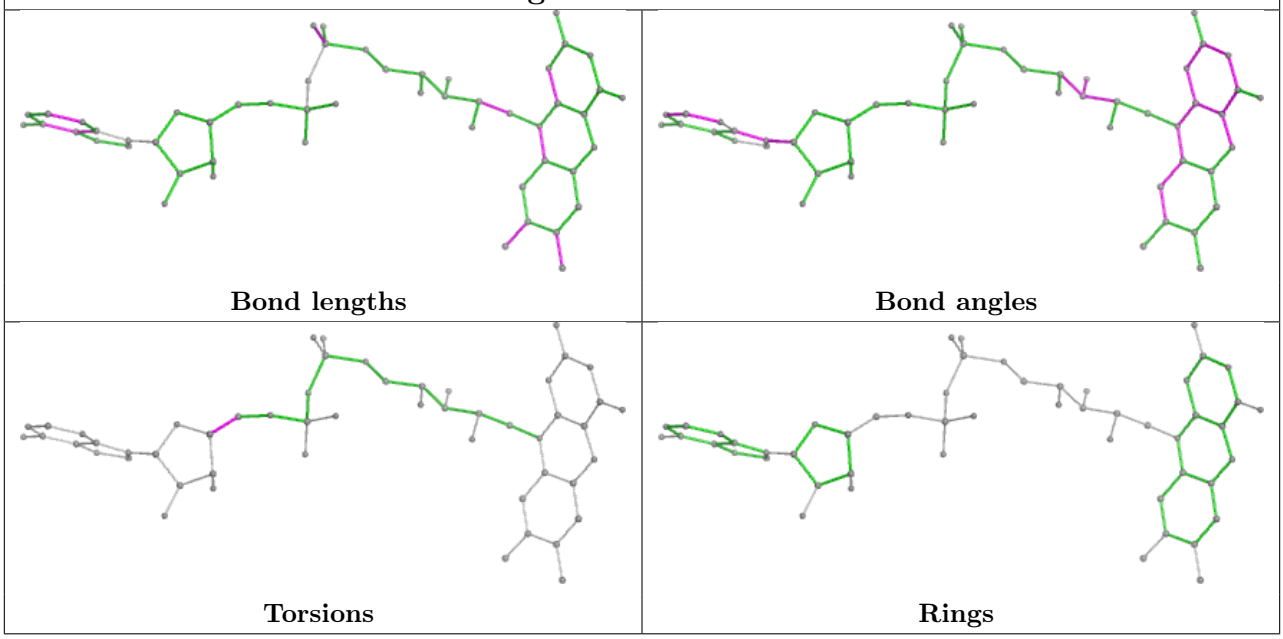
Ligand FAD B 551



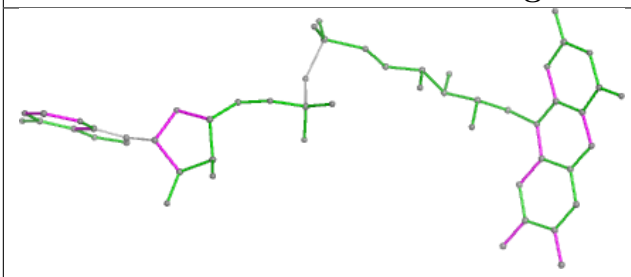
Ligand FAD A 551



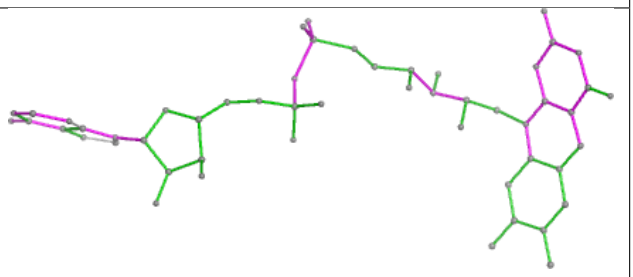
Ligand FAD F 551



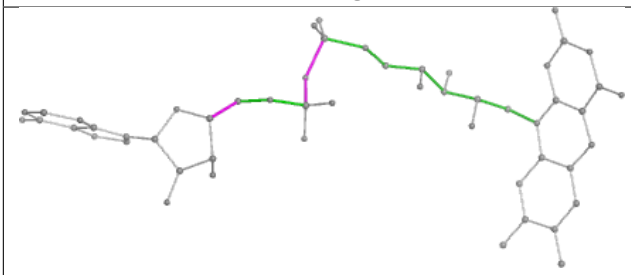
Ligand FAD D 551



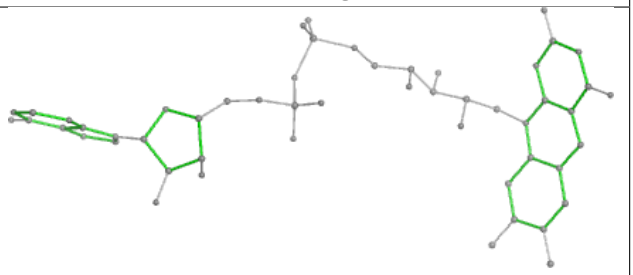
Bond lengths



Bond angles

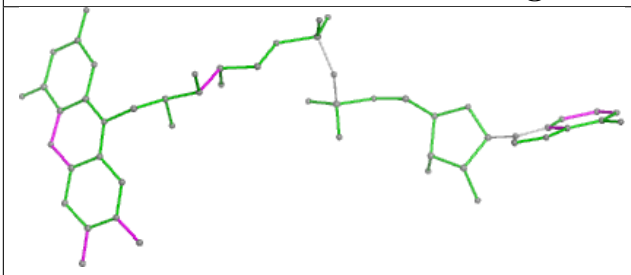


Torsions

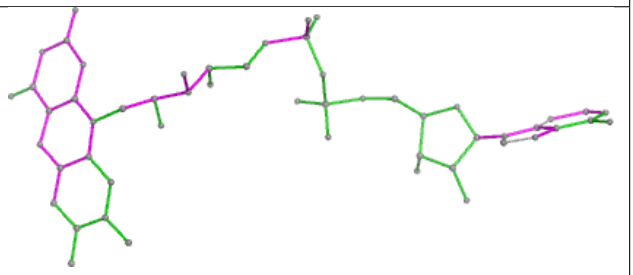


Rings

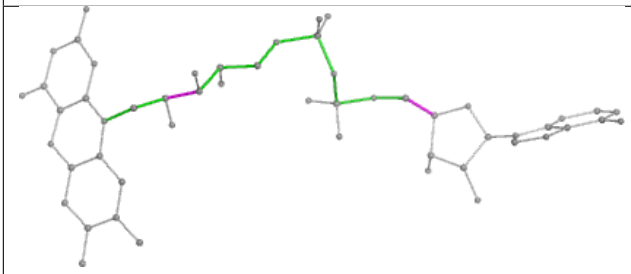
Ligand FAD E 551



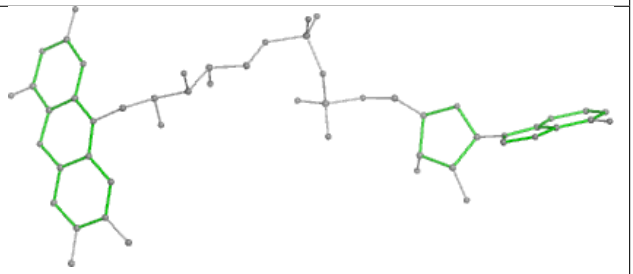
Bond lengths



Bond angles

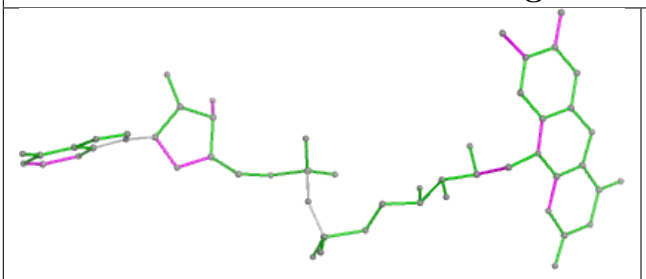


Torsions

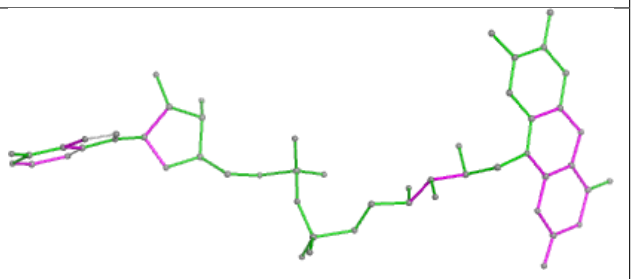


Rings

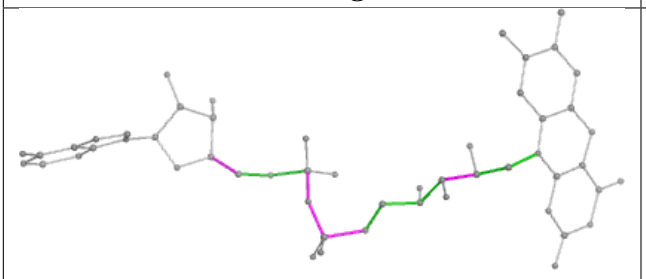
Ligand FAD C 551



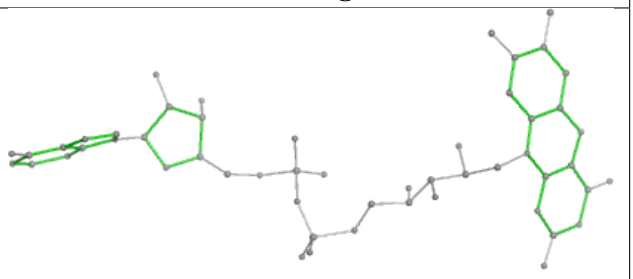
Bond lengths



Bond angles

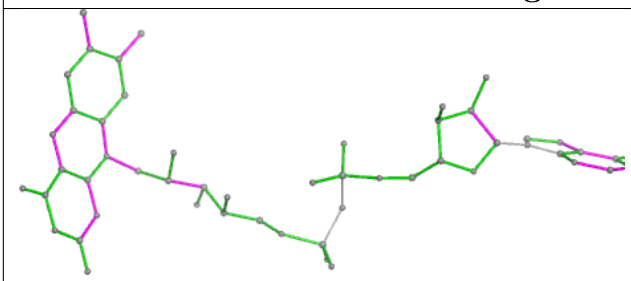


Torsions

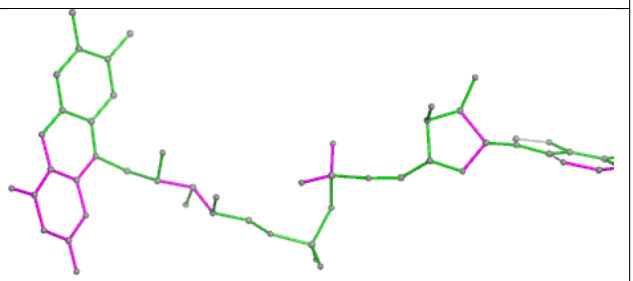


Rings

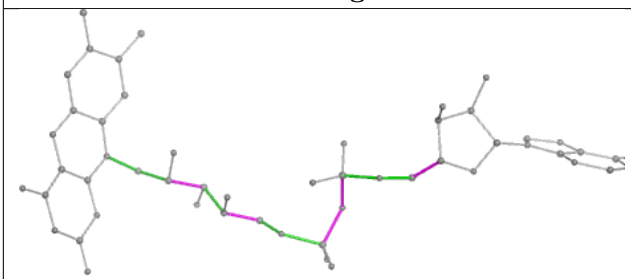
Ligand FAD G 551



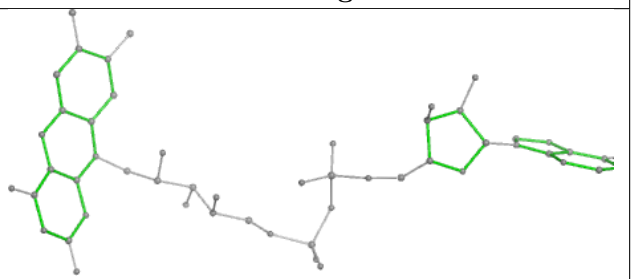
Bond lengths



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	508/530 (95%)	-0.07	9 (1%)	68	66	19, 26, 43, 74	0
1	B	505/530 (95%)	-0.15	9 (1%)	68	66	19, 28, 47, 67	0
1	C	505/530 (95%)	0.07	19 (3%)	40	39	21, 33, 52, 81	0
1	D	508/530 (95%)	0.09	15 (2%)	50	49	21, 32, 52, 77	0
1	E	508/530 (95%)	-0.01	15 (2%)	50	49	19, 30, 51, 77	0
1	F	505/530 (95%)	0.04	19 (3%)	40	39	18, 33, 53, 84	0
1	G	505/530 (95%)	-0.16	7 (1%)	75	74	18, 27, 44, 68	0
1	H	508/530 (95%)	0.02	17 (3%)	46	45	20, 28, 49, 96	0
All	All	4052/4240 (95%)	-0.02	110 (2%)	54	53	18, 30, 50, 96	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	214	GLY	7.2
1	H	331	ASN	5.7
1	C	420	PRO	5.3
1	A	213	GLY	5.0
1	G	213	GLY	4.7
1	E	3	ASP	4.6
1	H	213	GLY	4.6
1	F	332	GLY	4.4
1	D	202	ASP	4.1
1	F	331	ASN	4.1
1	C	213	GLY	4.0
1	C	3	ASP	4.0
1	B	375	GLU	3.8
1	D	214	GLY	3.7
1	C	400	LYS	3.7
1	E	4	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	5	THR	3.7
1	F	215	GLU	3.6
1	E	401	LEU	3.5
1	C	424	GLY	3.5
1	C	4	TRP	3.5
1	G	420	PRO	3.4
1	D	215	GLU	3.4
1	F	420	PRO	3.3
1	G	3	ASP	3.3
1	G	214	GLY	3.3
1	F	424	GLY	3.3
1	H	389	ARG	3.2
1	E	215	GLU	3.2
1	F	3	ASP	3.1
1	H	400	LYS	3.1
1	A	3	ASP	3.1
1	C	215	GLU	3.1
1	C	434	ASN	3.0
1	F	425	ALA	3.0
1	F	386	ASP	3.0
1	D	400	LYS	3.0
1	H	214	GLY	3.0
1	D	389	ARG	3.0
1	C	401	LEU	3.0
1	H	3	ASP	3.0
1	A	215	GLU	3.0
1	D	401	LEU	3.0
1	E	202	ASP	2.9
1	C	425	ALA	2.9
1	B	215	GLU	2.8
1	B	425	ALA	2.8
1	A	422	ASN	2.8
1	H	215	GLU	2.8
1	B	330	ASP	2.8
1	D	331	ASN	2.8
1	D	465	ASP	2.8
1	E	213	GLY	2.8
1	B	332	GLY	2.7
1	G	215	GLU	2.7
1	D	466	GLY	2.7
1	H	332	GLY	2.7
1	H	434	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	399	ALA	2.6
1	D	84	ALA	2.6
1	E	216	THR	2.6
1	B	213	GLY	2.6
1	H	387	ALA	2.6
1	D	397	ASP	2.6
1	A	401	LEU	2.6
1	F	307	ALA	2.6
1	H	401	LEU	2.6
1	H	4	TRP	2.5
1	D	3	ASP	2.5
1	F	4	TRP	2.5
1	E	400	LYS	2.5
1	G	212	SER	2.5
1	A	214	GLY	2.5
1	E	7	GLU	2.5
1	G	425	ALA	2.4
1	F	212	SER	2.3
1	B	214	GLY	2.3
1	H	5	THR	2.3
1	F	330	ASP	2.3
1	D	213	GLY	2.3
1	H	397	ASP	2.2
1	D	464	ALA	2.2
1	A	400	LYS	2.2
1	C	202	ASP	2.2
1	B	420	PRO	2.2
1	E	6	SER	2.2
1	B	3	ASP	2.2
1	H	352	ILE	2.2
1	E	466	GLY	2.2
1	C	7	GLU	2.2
1	A	5	THR	2.2
1	E	83	ASP	2.2
1	F	389	ARG	2.1
1	C	397	ASP	2.1
1	F	203	GLY	2.1
1	D	375	GLU	2.1
1	F	344	ARG	2.1
1	H	212	SER	2.1
1	C	398	ALA	2.1
1	C	203	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	402	GLY	2.1
1	E	214	GLY	2.1
1	C	212	SER	2.0
1	F	213	GLY	2.0
1	F	419	CYS	2.0
1	A	185	GLY	2.0
1	F	218	ARG	2.0
1	E	217	GLN	2.0
1	H	6	SER	2.0
1	F	400	LYS	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FRU	J	2	12/12	0.70	0.21	63,73,76,77	0
2	GLC	J	1	11/12	0.74	0.21	52,62,66,68	0
2	FRU	P	2	12/12	0.77	0.23	64,73,76,82	0
2	GLC	P	1	11/12	0.81	0.19	44,60,64,68	0
2	GLC	L	1	11/12	0.81	0.20	45,61,66,70	0
2	FRU	N	2	12/12	0.82	0.23	46,52,57,57	0
2	FRU	K	2	12/12	0.82	0.29	52,56,61,62	0
2	GLC	K	1	11/12	0.82	0.25	49,58,63,67	0
2	FRU	S	2	12/12	0.84	0.20	46,51,56,56	0
2	FRU	L	2	12/12	0.87	0.16	56,68,71,71	0
2	GLC	T	1	11/12	0.87	0.26	43,47,54,56	0
2	GLC	Q	1	11/12	0.88	0.21	35,44,48,49	0
2	FRU	R	2	12/12	0.89	0.17	45,56,61,62	0
2	GLC	N	1	11/12	0.90	0.22	47,54,60,61	0
2	GLC	S	1	11/12	0.90	0.16	37,43,49,49	0
2	FRU	M	2	12/12	0.91	0.21	43,56,65,65	0
2	GLC	R	1	11/12	0.91	0.11	35,41,44,44	0
2	FRU	Q	2	12/12	0.92	0.17	41,44,46,50	0

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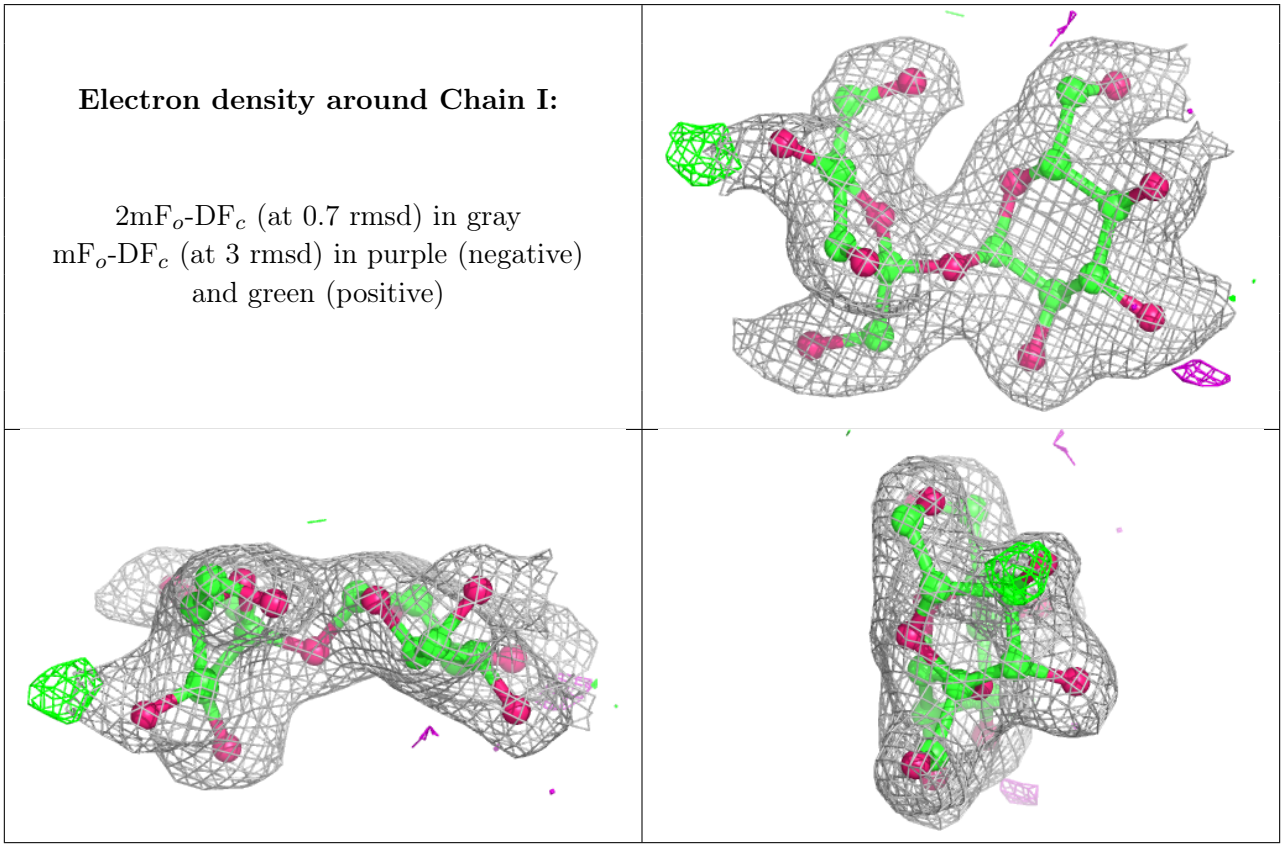
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	M	1	11/12	0.92	0.16	31,35,42,43	0
2	FRU	I	2	12/12	0.94	0.15	39,44,47,48	0
2	FRU	T	2	12/12	0.94	0.25	37,44,46,48	0
2	GLC	I	1	11/12	0.95	0.16	33,34,39,39	0
2	GLC	O	1	11/12	0.96	0.11	26,31,35,38	0
2	FRU	O	2	12/12	0.97	0.12	36,42,47,50	0

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.

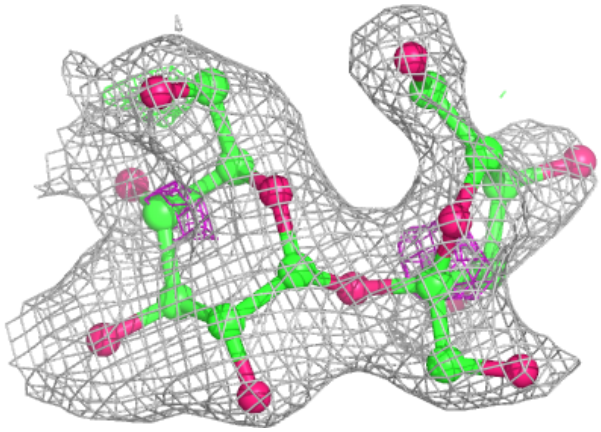
Electron density around Chain I:

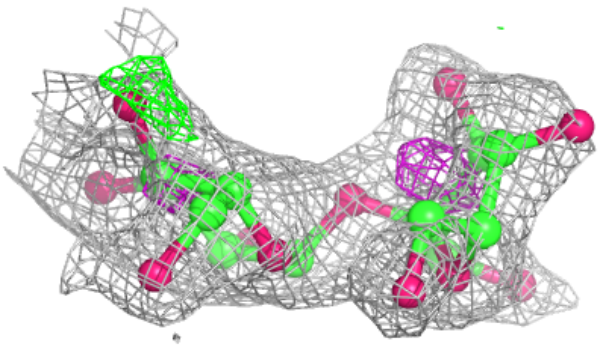
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

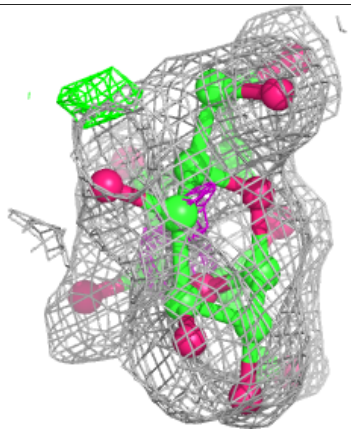


Electron density around Chain J:

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

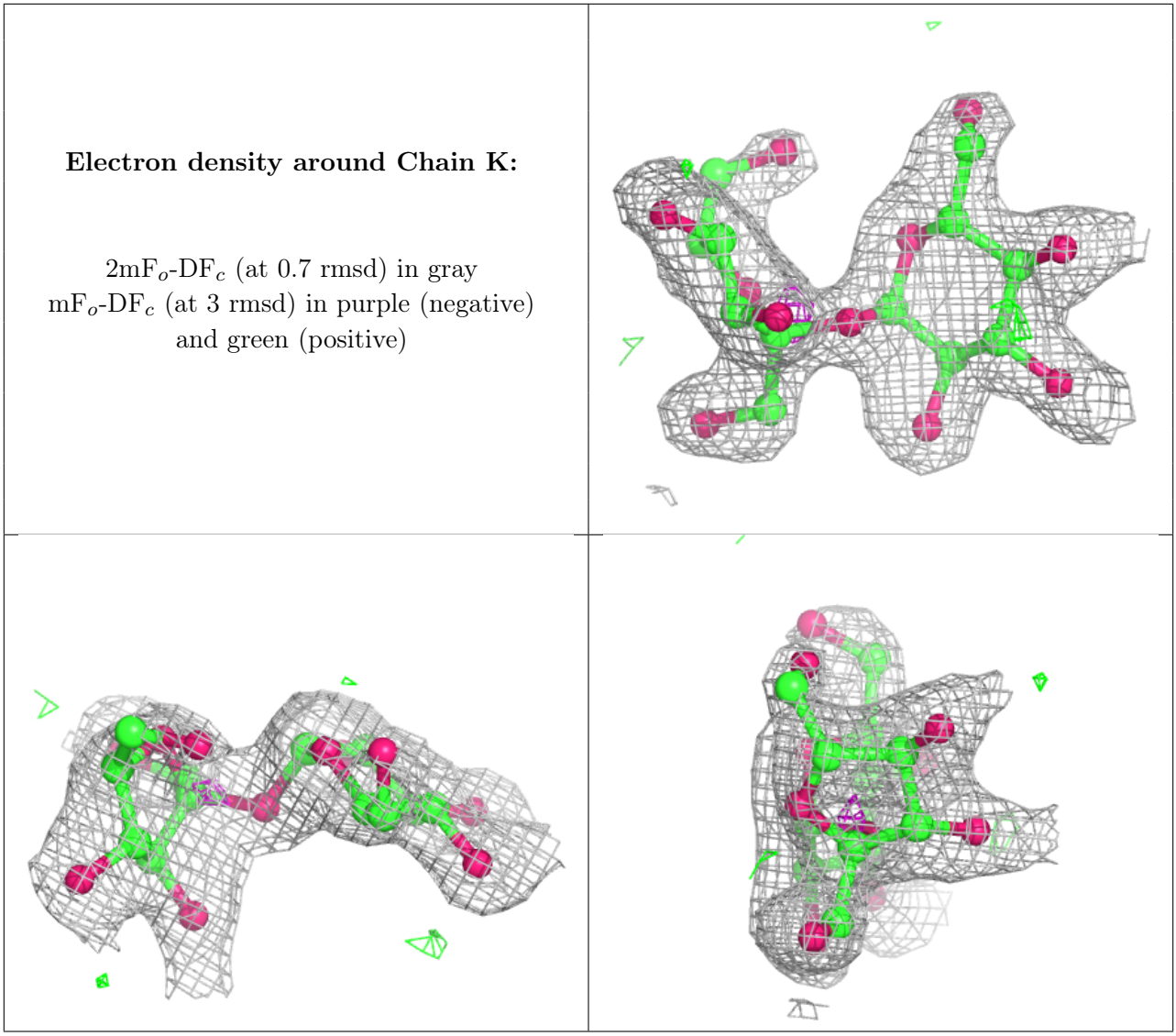






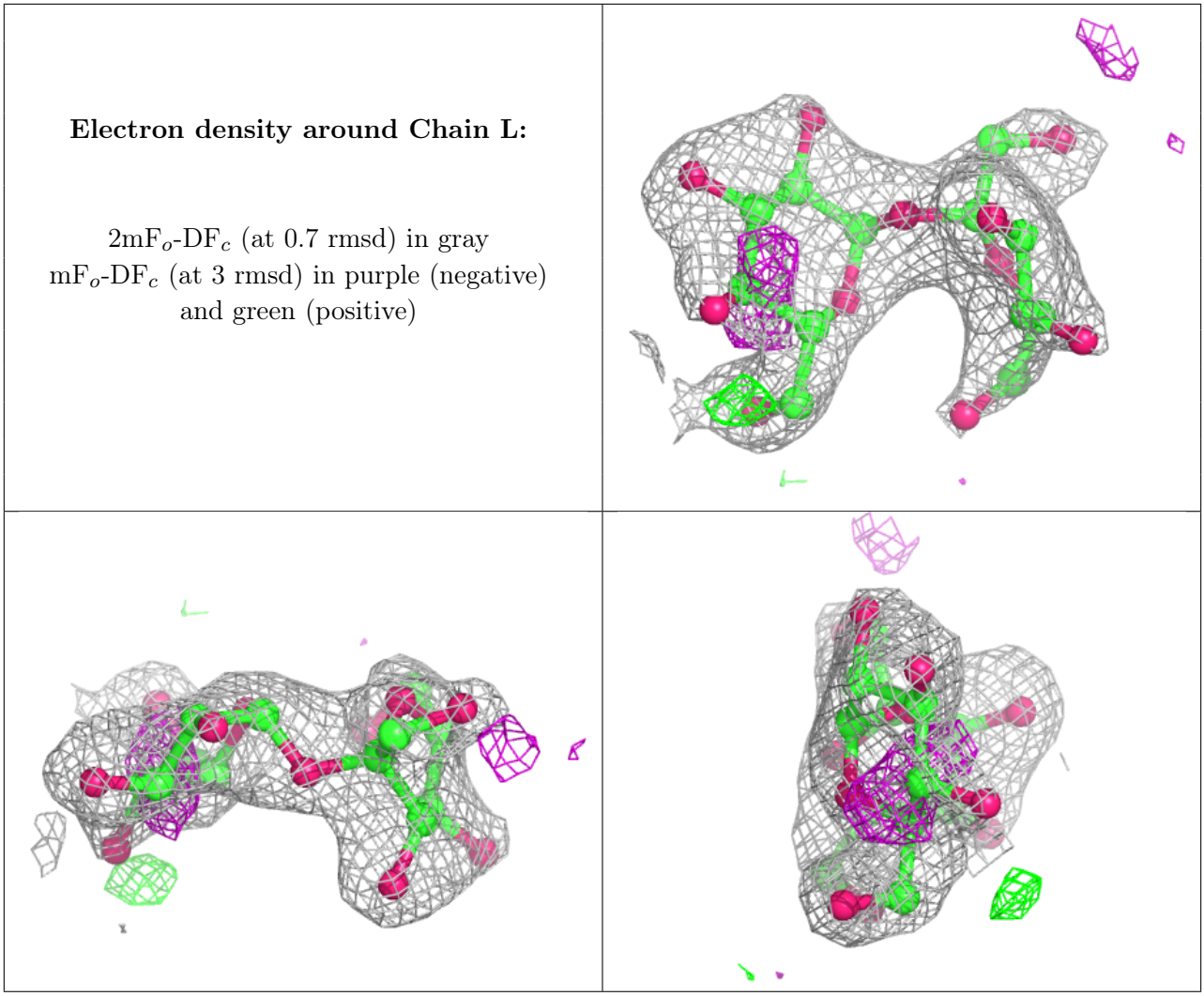
Electron density around Chain K:

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



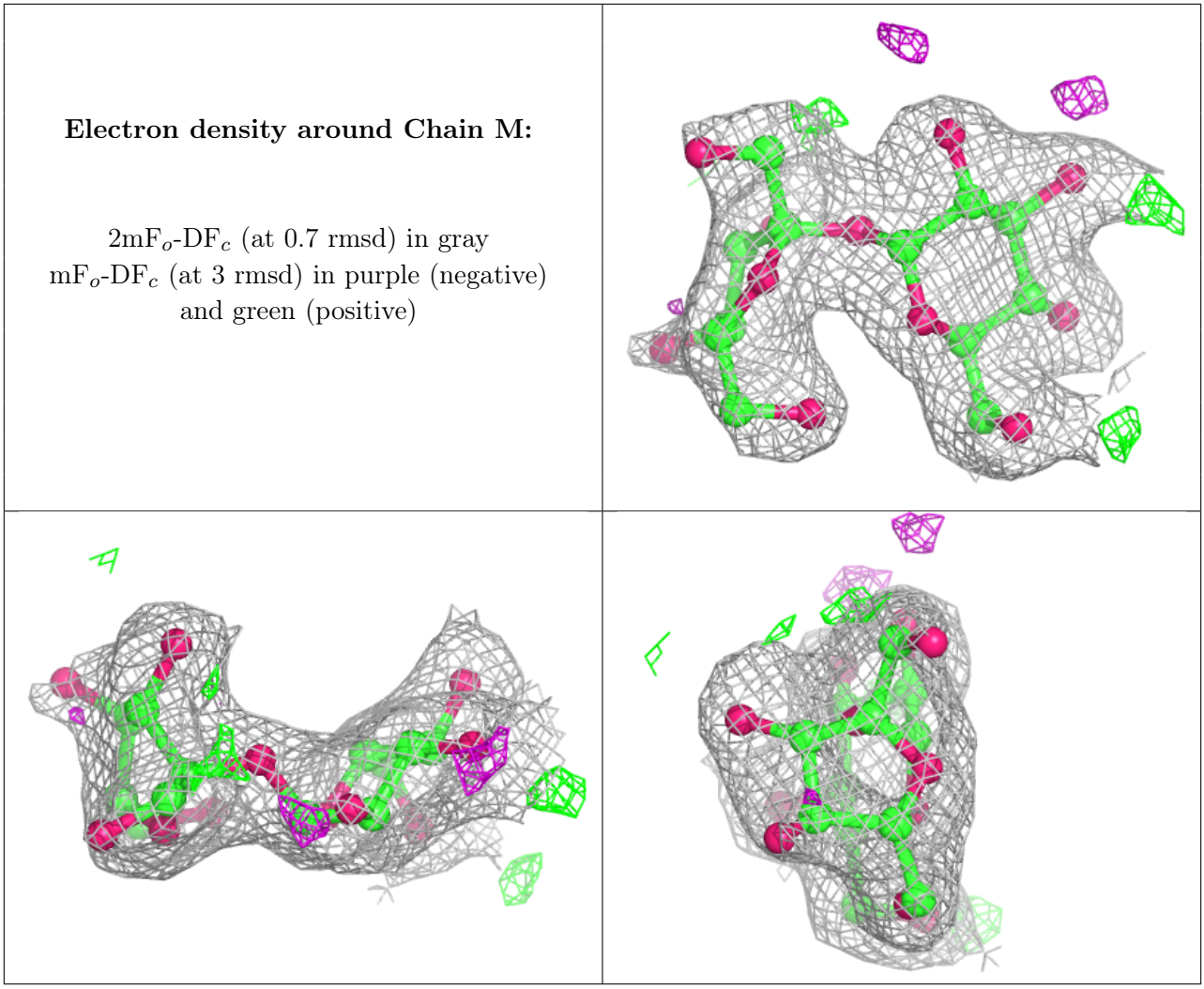
Electron density around Chain L:

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



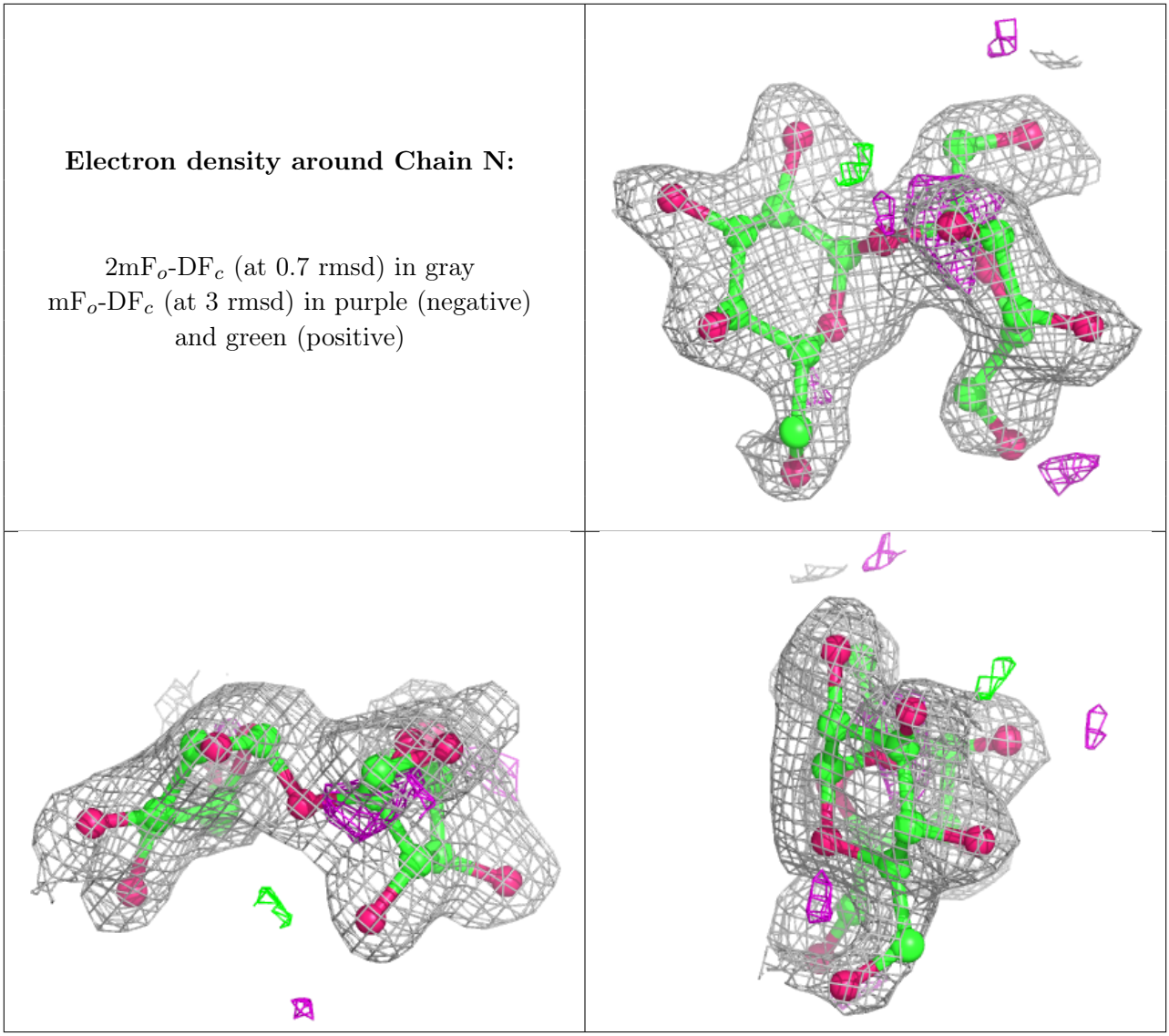
Electron density around Chain M:

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



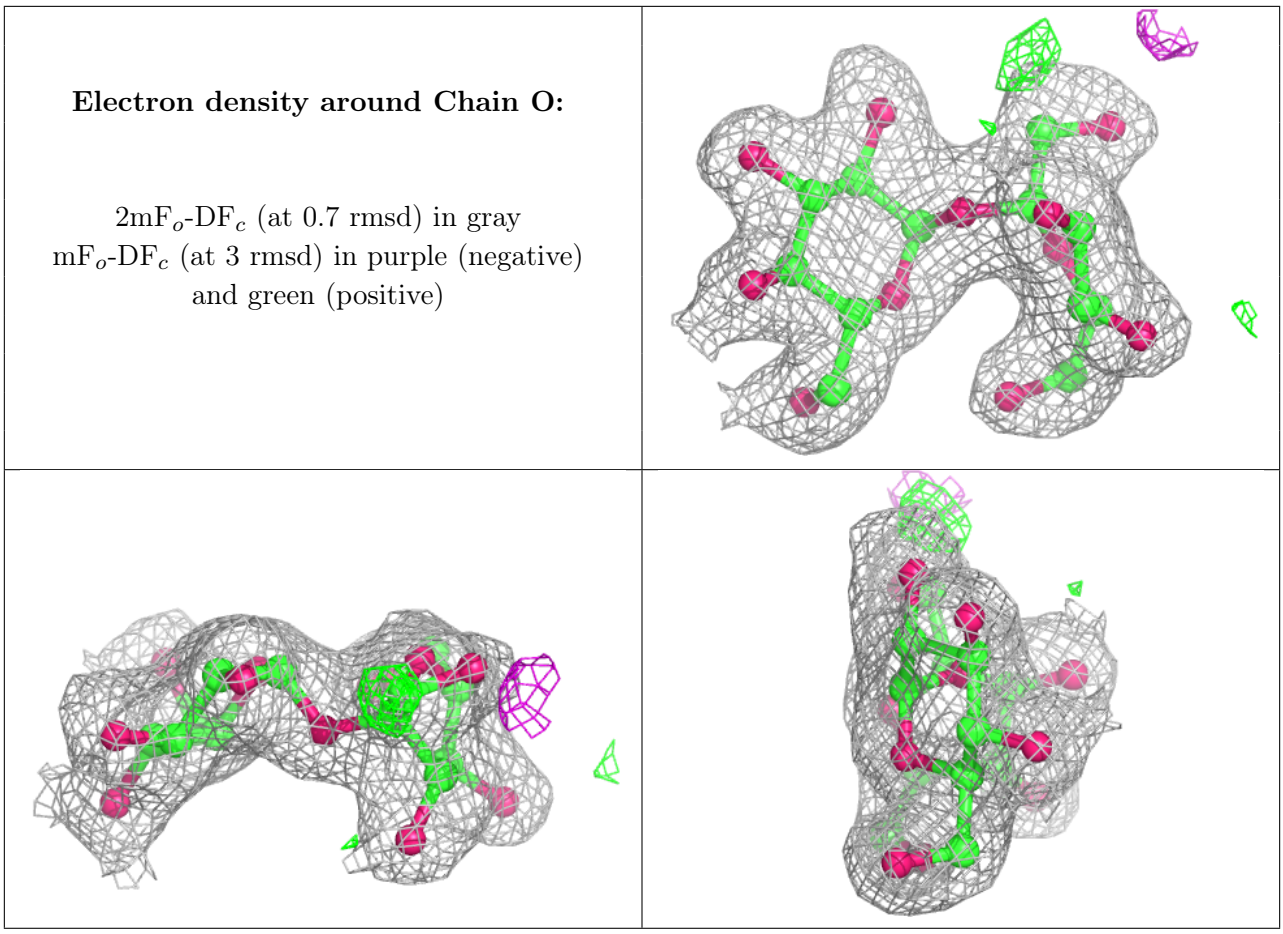
Electron density around Chain N:

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



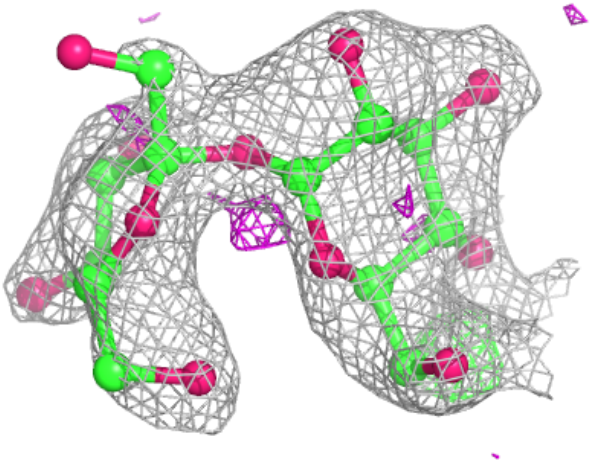
Electron density around Chain O:

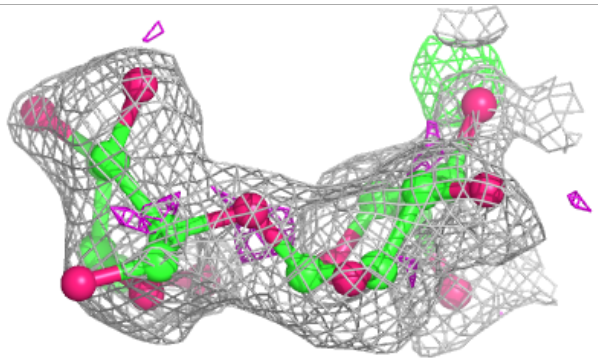
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

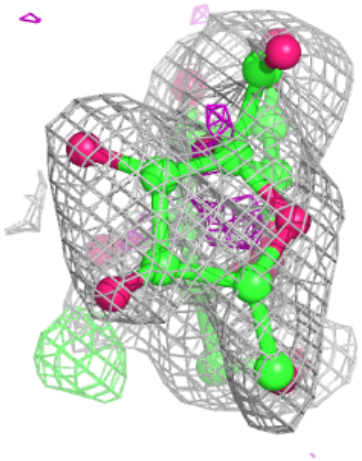


Electron density around Chain P:

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

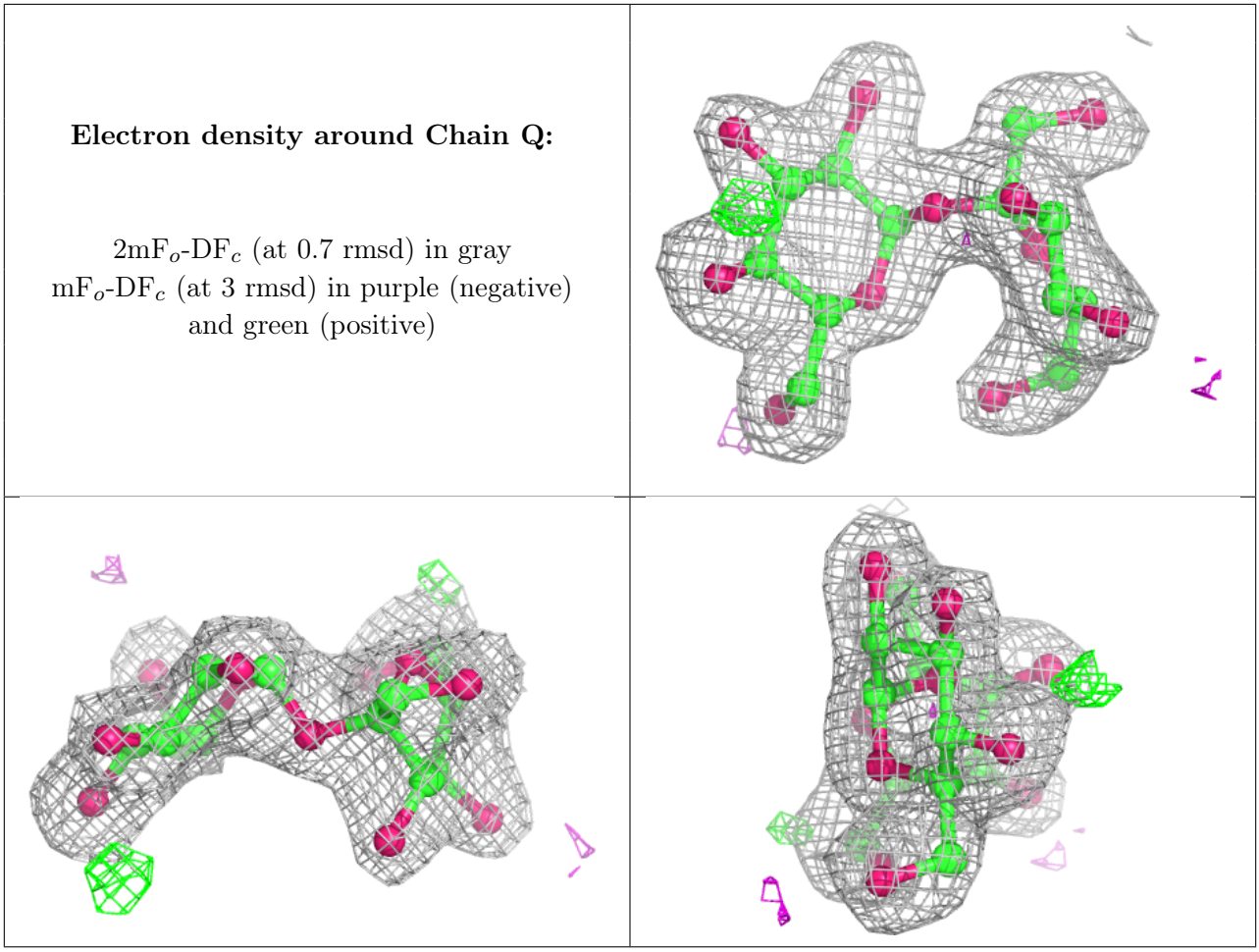






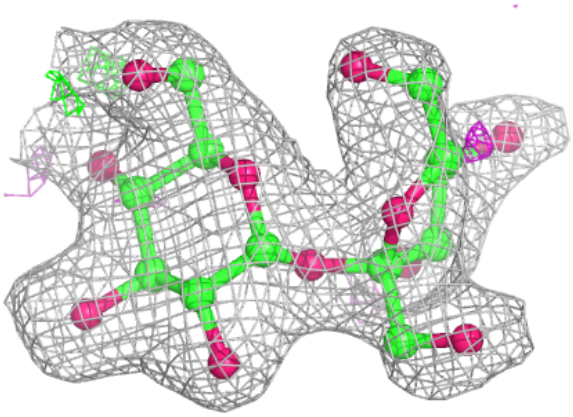
Electron density around Chain Q:

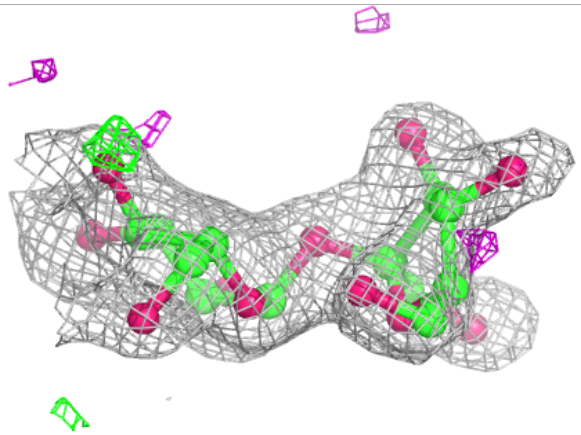
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

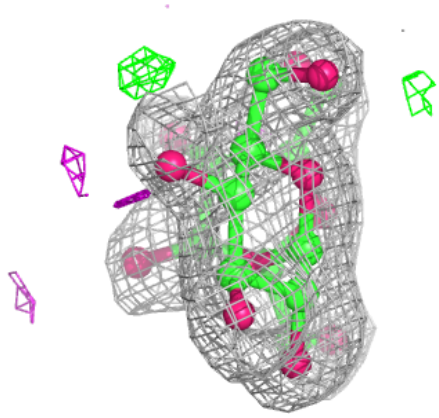


Electron density around Chain R:

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

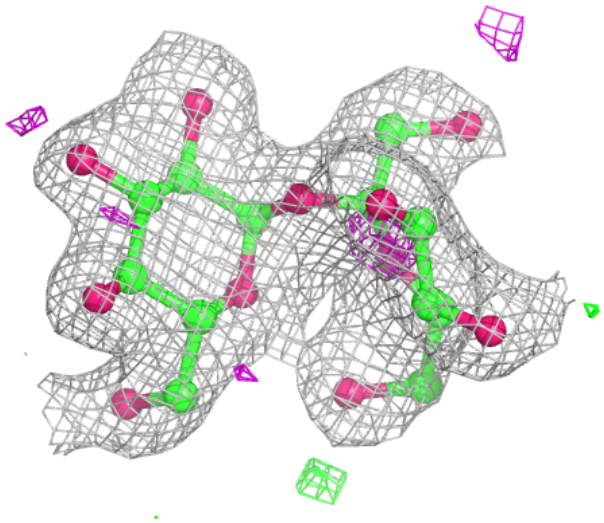


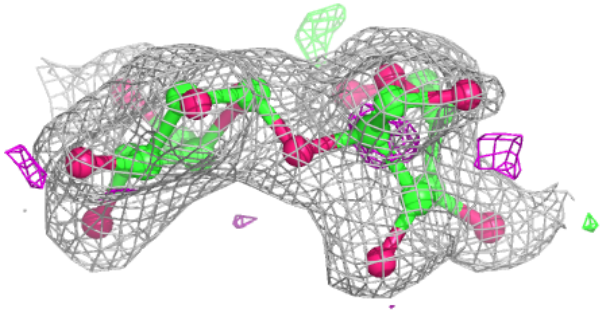


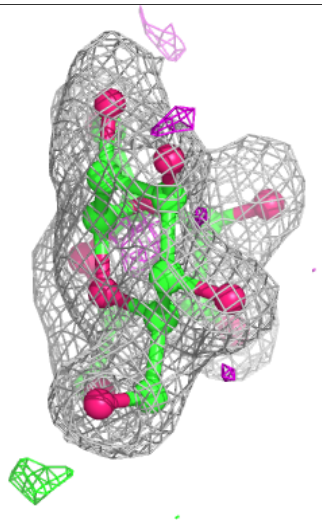


Electron density around Chain S:

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

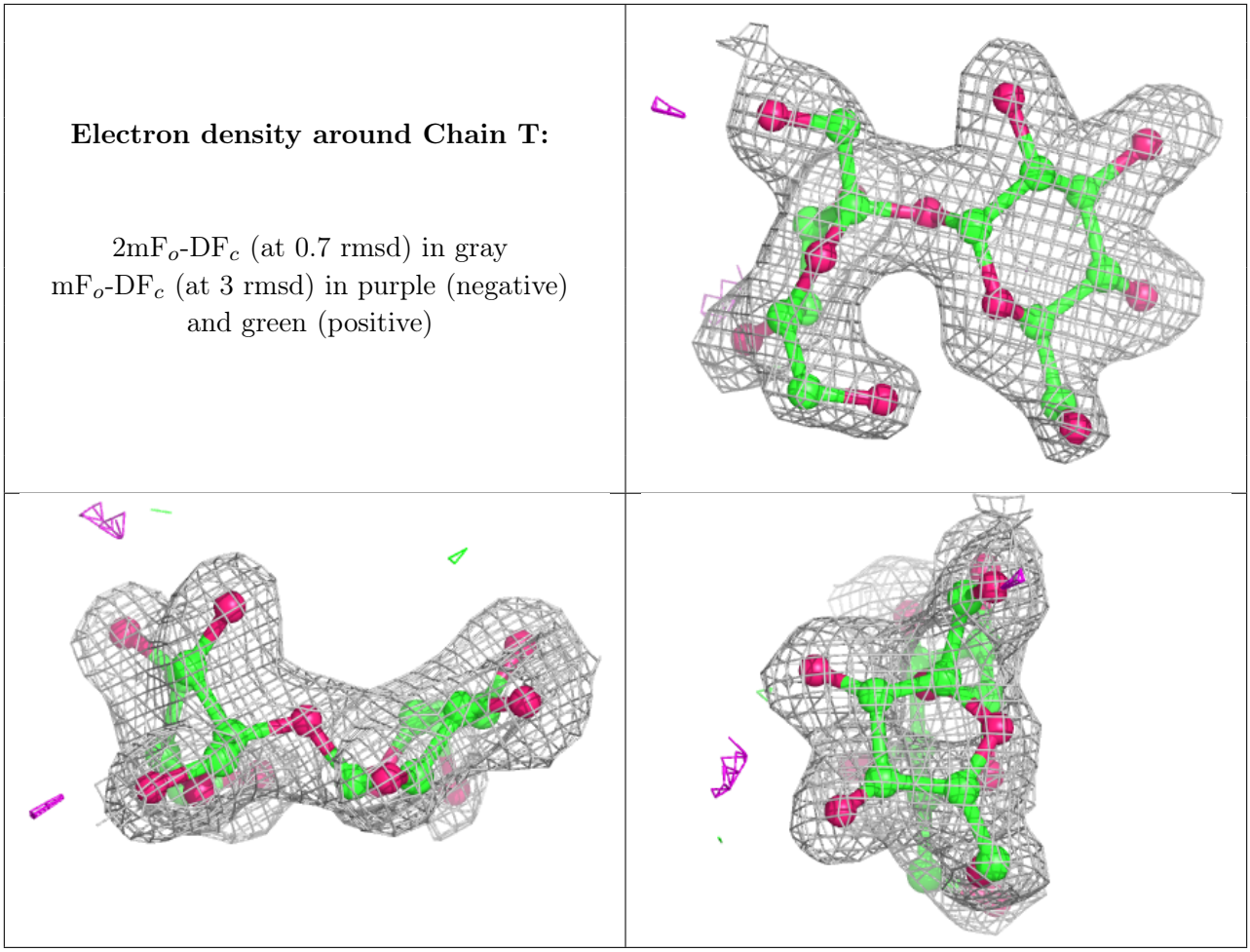






Electron density around Chain T:

$2mF_o$-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
6	PG4	H	582	13/13	0.64	0.47	64,67,76,78	0
6	PG4	E	582	13/13	0.65	0.41	60,68,80,81	0
6	PG4	E	583	13/13	0.69	0.24	53,67,69,71	0
6	PG4	B	584	13/13	0.69	0.28	72,85,90,91	0
6	PG4	G	582	13/13	0.70	0.23	63,69,78,80	0
6	PG4	G	581	13/13	0.75	0.24	67,69,77,78	0
6	PG4	A	582	13/13	0.77	0.34	64,70,76,76	0
6	PG4	F	582	13/13	0.78	0.20	55,60,77,78	0
6	PG4	C	582	13/13	0.78	0.28	56,66,78,79	0
6	PG4	B	582	13/13	0.79	0.24	58,61,64,65	0
6	PG4	D	581	13/13	0.79	0.29	48,56,65,65	0

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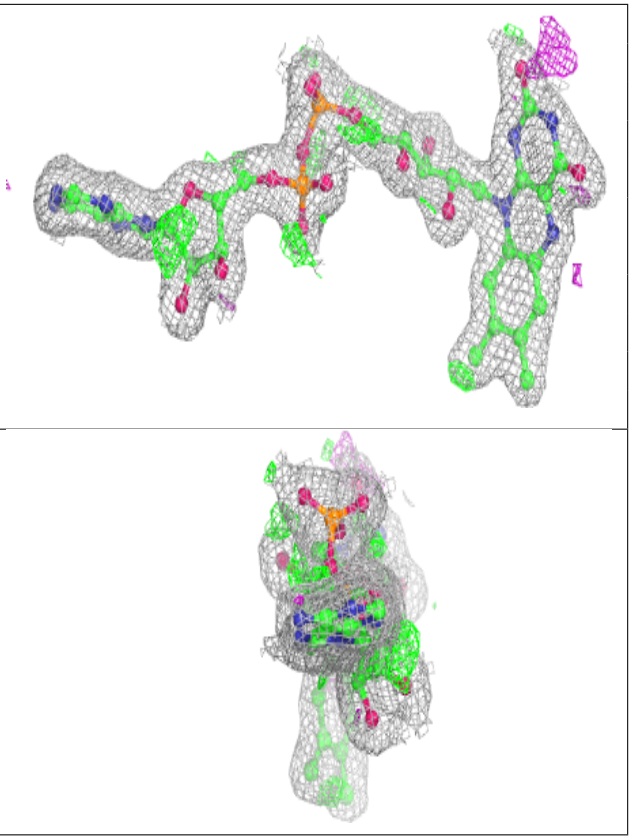
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PG4	E	581	13/13	0.80	0.28	50,59,69,70	0
6	PG4	A	583	13/13	0.80	0.22	48,56,65,67	0
6	PG4	D	582	13/13	0.80	0.33	62,68,78,81	0
6	PG4	F	581	13/13	0.80	0.24	51,60,68,70	0
6	PG4	C	581	13/13	0.81	0.24	47,61,77,79	0
6	PG4	A	581	13/13	0.82	0.36	55,65,71,74	0
6	PG4	B	581	13/13	0.82	0.27	52,68,88,90	0
6	PG4	H	581	13/13	0.83	0.35	55,62,69,72	0
4	NA	G	561	1/1	0.94	0.09	26,26,26,26	0
3	FAD	D	551	53/53	0.97	0.10	22,26,32,35	0
3	FAD	E	551	53/53	0.97	0.10	19,24,33,34	0
3	FAD	H	551	53/53	0.97	0.11	21,23,25,26	0
3	FAD	A	551	53/53	0.97	0.10	20,22,24,28	0
5	CL	C	571	1/1	0.97	0.09	34,34,34,34	0
3	FAD	C	551	53/53	0.97	0.08	23,26,33,38	0
5	CL	D	571	1/1	0.98	0.13	33,33,33,33	0
3	FAD	B	551	53/53	0.98	0.10	19,23,25,29	0
3	FAD	F	551	53/53	0.98	0.10	20,24,28,29	0
5	CL	B	571	1/1	0.98	0.13	33,33,33,33	0
3	FAD	G	551	53/53	0.98	0.09	19,22,25,27	0
4	NA	A	561	1/1	0.99	0.06	23,23,23,23	0
5	CL	E	571	1/1	0.99	0.12	28,28,28,28	0
5	CL	F	571	1/1	0.99	0.10	33,33,33,33	0
5	CL	G	571	1/1	0.99	0.09	27,27,27,27	0
5	CL	H	571	1/1	0.99	0.11	34,34,34,34	0
5	CL	A	571	1/1	0.99	0.10	30,30,30,30	0
4	NA	C	561	1/1	0.99	0.06	22,22,22,22	0
4	NA	E	561	1/1	0.99	0.07	23,23,23,23	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.

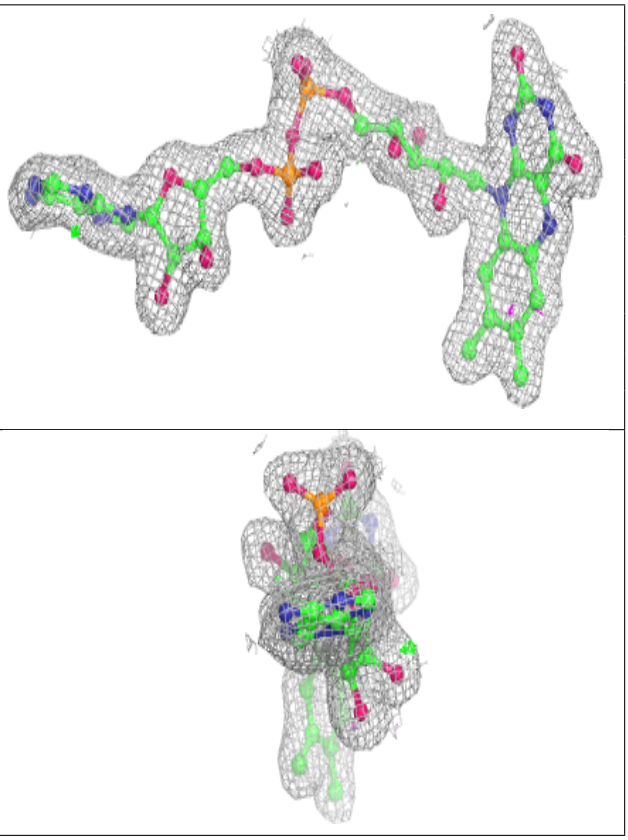
Electron density around FAD D 551:

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



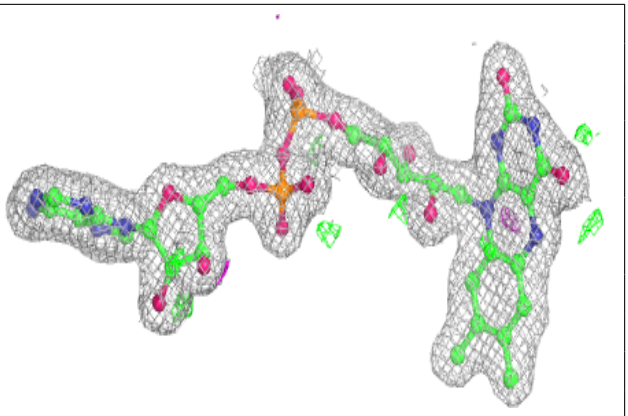
Electron density around FAD E 551:

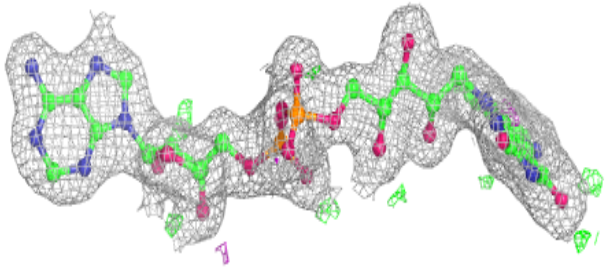
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

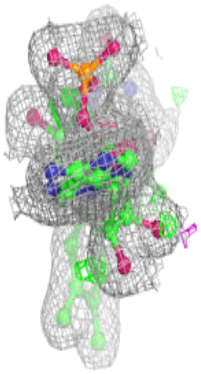


Electron density around FAD H 551:

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

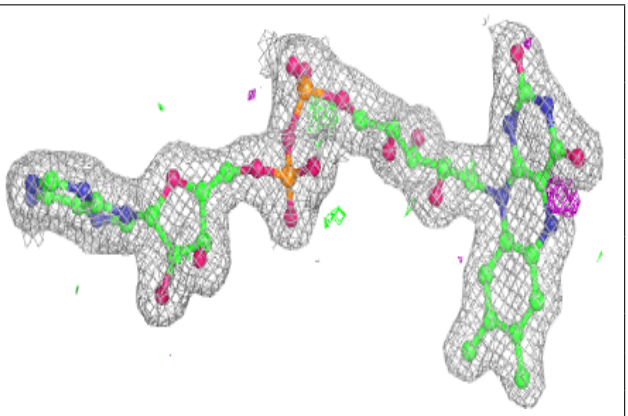


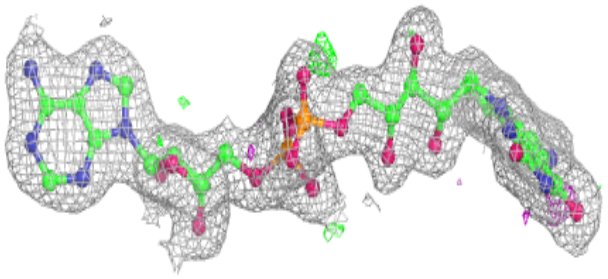


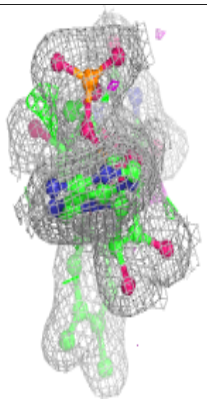


Electron density around FAD A 551:

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

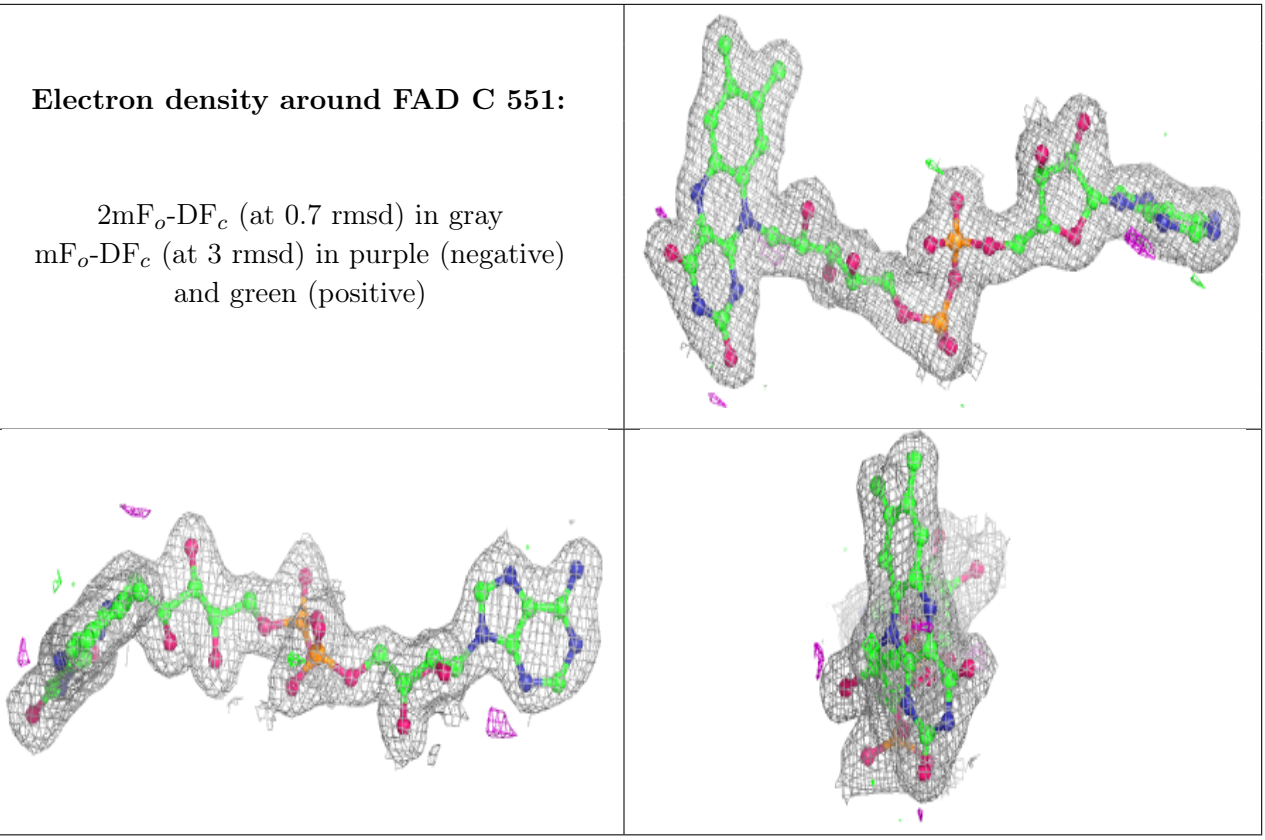






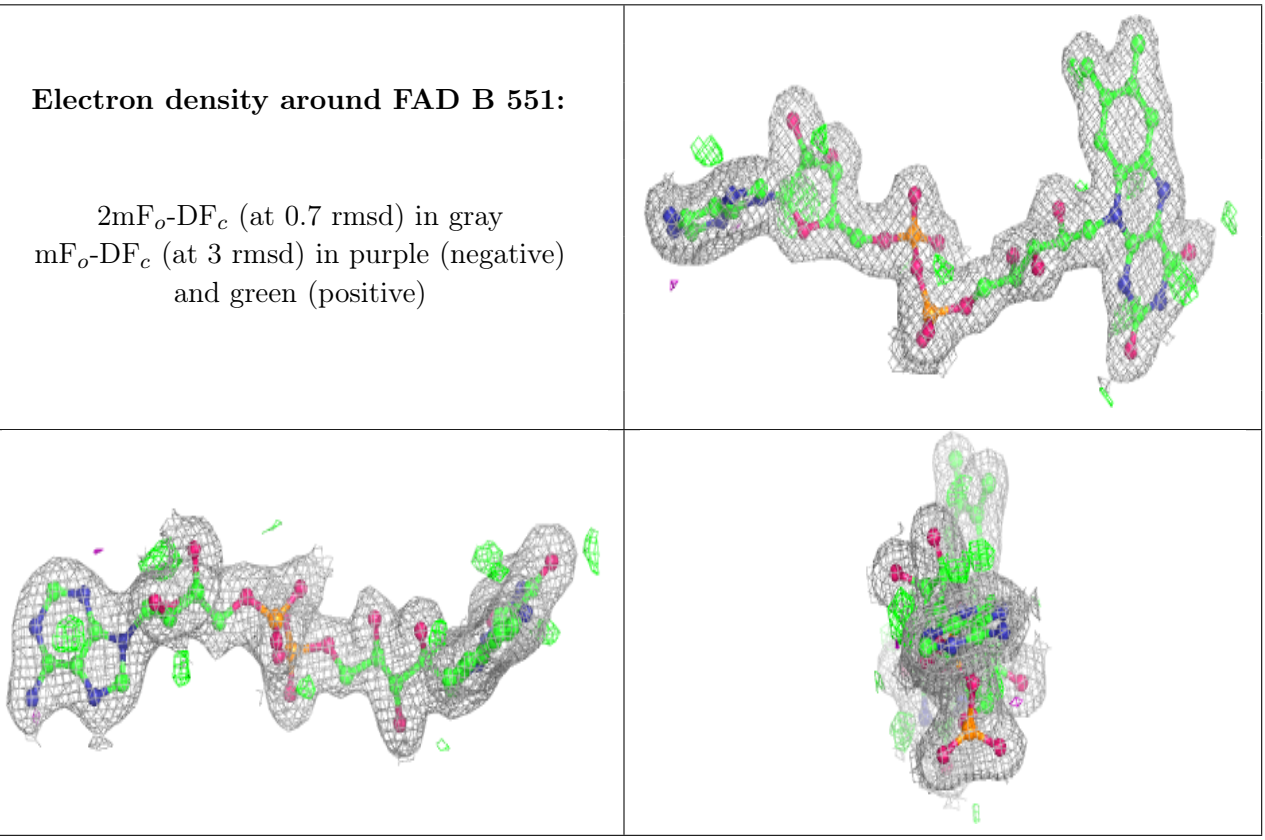
Electron density around FAD C 551:

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



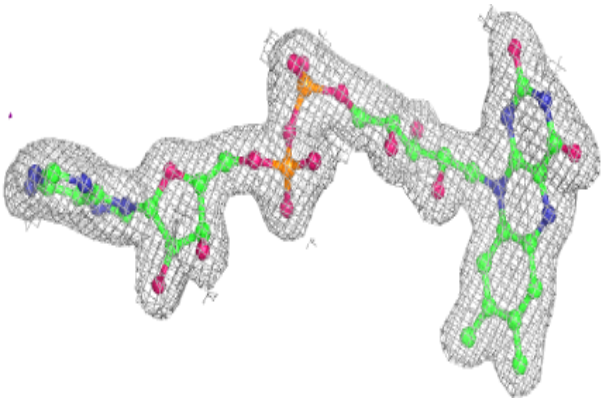
Electron density around FAD B 551:

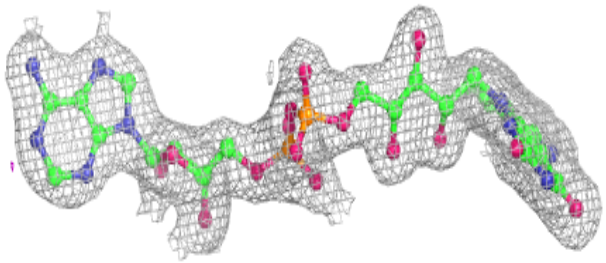
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

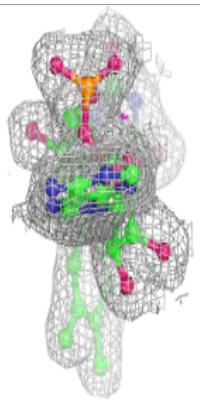


Electron density around FAD F 551:

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

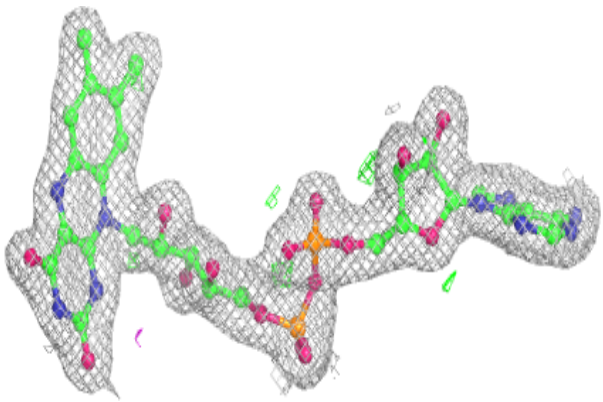


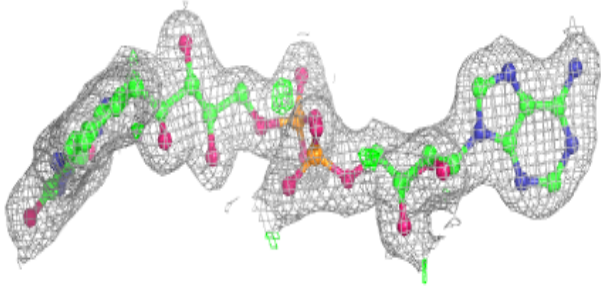


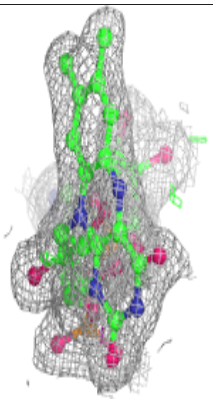


Electron density around FAD G 551:

$2mF_o$-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.