



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 02:17 PM JST

PDB ID : 5AWV  
Title : Crystal structure of glycopeptide hexose oxidase DBV29 complexed with te-  
icoplanin  
Authors : Liu, Y.C.; Li, T.L.  
Deposited on : 2015-07-09  
Resolution : 1.93 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](mailto: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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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

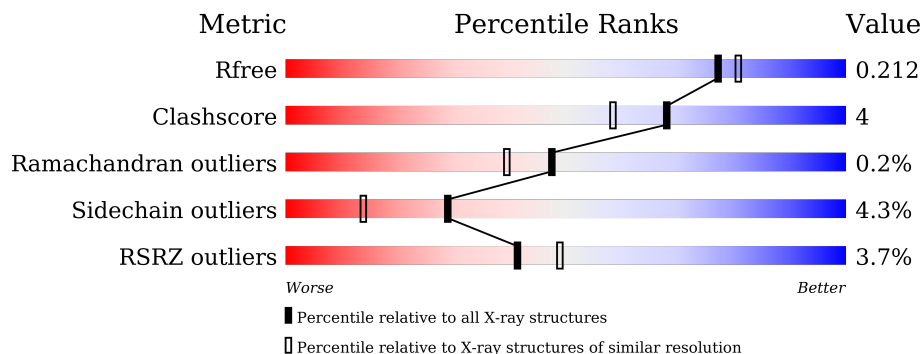
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.93 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.






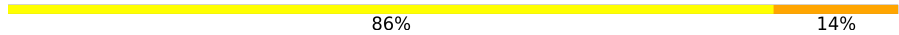
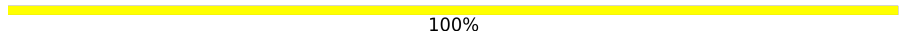
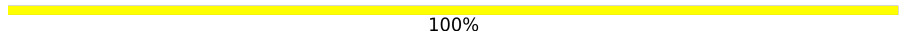
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	523	 2% 84% 10% • 5%
1	B	523	 2% 84% 10% • 5%
1	C	523	 4% 85% 9% • 5%
1	D	523	 7% 85% 10% • 5%
2	I	7	 71% 29%
2	J	7	 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	7	 86% 14%
2	L	7	 43% 57%
2	M	7	 86% 14%
2	N	7	 86% 14%
2	O	7	 100%
2	P	7	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GHP	I	1	-	-	-	X
2	3FG	I	7	-	-	-	X
2	GHP	K	5	-	-	-	X
2	3FG	K	7	-	-	-	X
2	GHP	L	5	-	-	-	X
2	3FG	L	7	-	-	-	X
2	GHP	M	1	-	-	-	X
2	GHP	M	5	-	-	-	X
2	OMY	M	6	-	-	-	X
2	3FG	M	7	-	-	-	X
4	CIT	O	105	-	X	-	-
5	T55	B	602	-	-	-	X
5	T55	N	101	-	-	X	-
5	T55	O	101	-	-	-	X
6	MAN	I	101	-	-	-	X
6	MAN	K	102	-	-	-	X
6	MAN	L	101	-	-	-	X
6	MAN	M	102	-	-	-	X
7	NAG	I	102	-	-	-	X
7	NAG	J	102	-	-	-	X
7	NAG	K	103	-	-	-	X
7	NAG	L	102	-	-	-	X
7	NAG	M	103	-	-	-	X
7	NAG	O	103	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 18119 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.

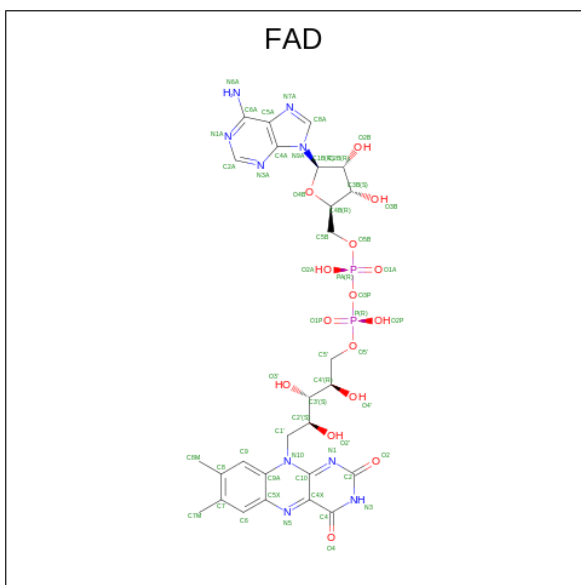
- Molecule 1 is a protein called Putative hexose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	498	3856	2441	685	716	14	0	0	0
1	B	498	3856	2441	685	716	14	0	0	0
1	C	498	3856	2441	685	716	14	0	0	0
1	D	498	3856	2441	685	716	14	0	0	0

- Molecule 2 is a protein called TEICOPLANIN.

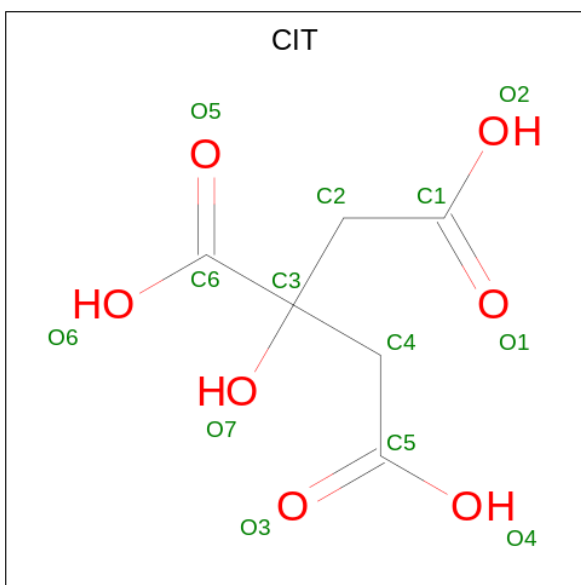
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	Cl	N	O			
2	I	7	85	58	2	7	18	0	0	0
2	J	7	85	58	2	7	18	0	0	0
2	K	7	85	58	2	7	18	0	0	0
2	L	7	85	58	2	7	18	0	0	0
2	M	7	85	58	2	7	18	0	0	0
2	N	7	85	58	2	7	18	0	0	0
2	O	7	85	58	2	7	18	0	0	0
2	P	7	85	58	2	7	18	0	0	0

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



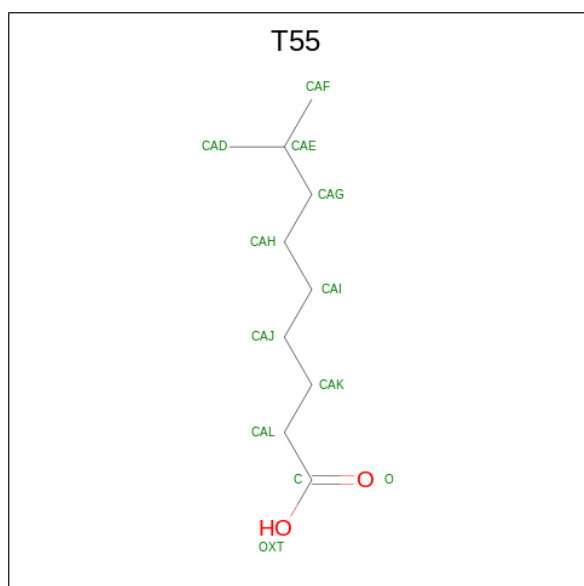
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	A	1	53	27	9	15	2	0	0
3	B	1	53	27	9	15	2	0	0
3	C	1	53	27	9	15	2	0	0
3	D	1	53	27	9	15	2	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



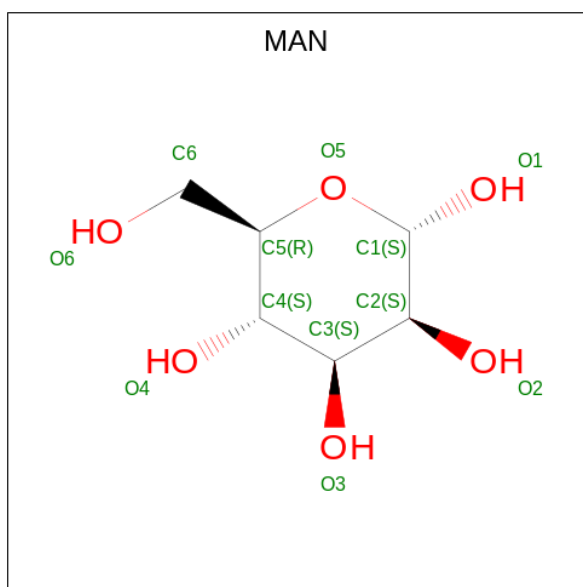
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		
4	O	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is 8-METHYLNONANOIC ACID (three-letter code: T55) (formula: C<sub>10</sub>H<sub>20</sub>O<sub>2</sub>).



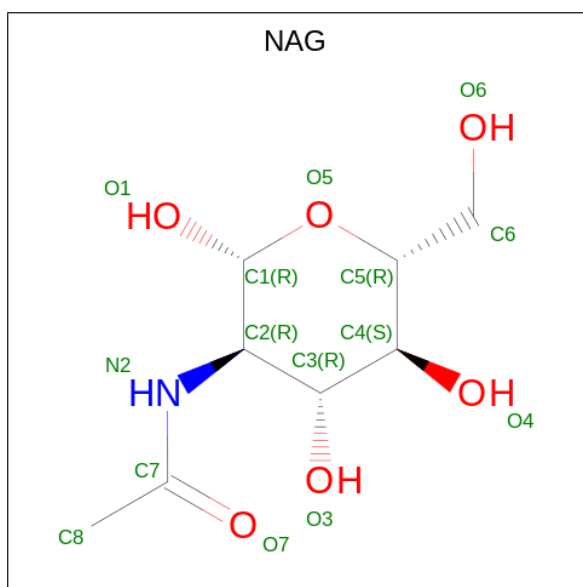
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			11	10	1		
5	K	1	Total	C	O	0	0
			11	10	1		
5	M	1	Total	C	O	0	0
			11	10	1		
5	N	1	Total	C	O	0	0
			11	10	1		
5	O	1	Total	C	O	0	0
			11	10	1		
5	P	1	Total	C	O	0	0
			11	10	1		

- Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total C O 11 6 5	0	0
6	J	1	Total C O 11 6 5	0	0
6	K	1	Total C O 11 6 5	0	0
6	L	1	Total C O 11 6 5	0	0
6	M	1	Total C O 11 6 5	0	0
6	N	1	Total C O 11 6 5	0	0
6	O	1	Total C O 11 6 5	0	0
6	P	1	Total C O 11 6 5	0	0

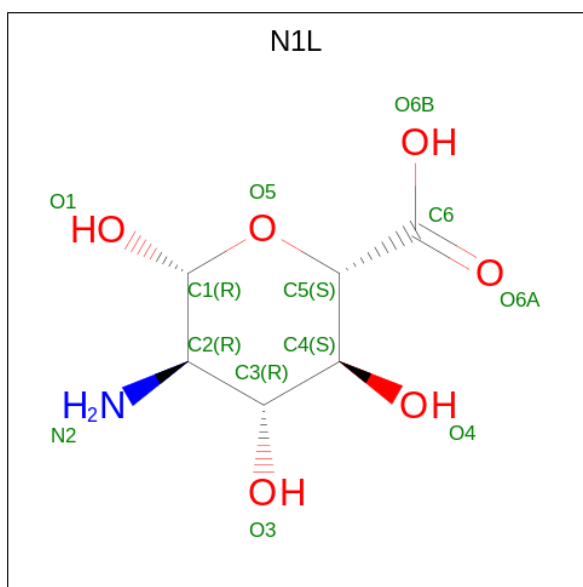
- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	I	1	Total 14	8	1	5	0	0
7	J	1	Total 14	8	1	5	0	0
7	K	1	Total 14	8	1	5	0	0
7	L	1	Total 14	8	1	5	0	0
7	M	1	Total 14	8	1	5	0	0
7	N	1	Total 14	8	1	5	0	0
7	O	1	Total 14	8	1	5	0	0
7	P	1	Total 14	8	1	5	0	0

- Molecule 8 is 2-amino-2-deoxy-beta-D-glucopyranuronic acid (three-letter code: N1L) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>6</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	K	1	12	6	1	5	0	0
8	L	1	12	6	1	5	0	0
8	M	1	12	6	1	5	0	0
8	N	1	12	6	1	5	0	0
8	O	1	12	6	1	5	0	0
8	P	1	12	6	1	5	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	425	425	425	0	0
9	B	379	379	379	0	0
9	C	327	327	327	0	0
9	D	217	217	217	0	0
9	I	6	6	6	0	0
9	J	5	5	5	0	0

*Continued on next page...*

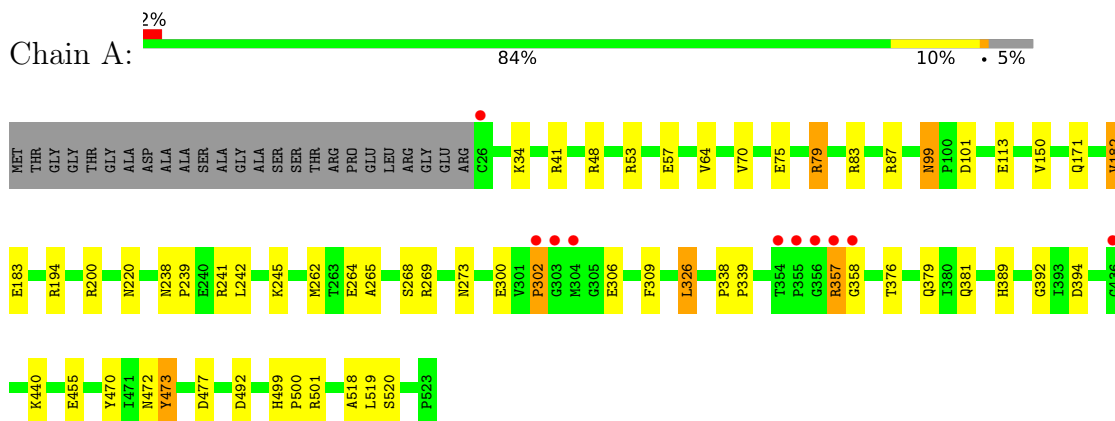
*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	K	3	Total O 3 3	0	0
9	L	1	Total O 1 1	0	0
9	M	1	Total O 1 1	0	0
9	N	12	Total O 12 12	0	0
9	O	16	Total O 16 16	0	0
9	P	8	Total O 8 8	0	0

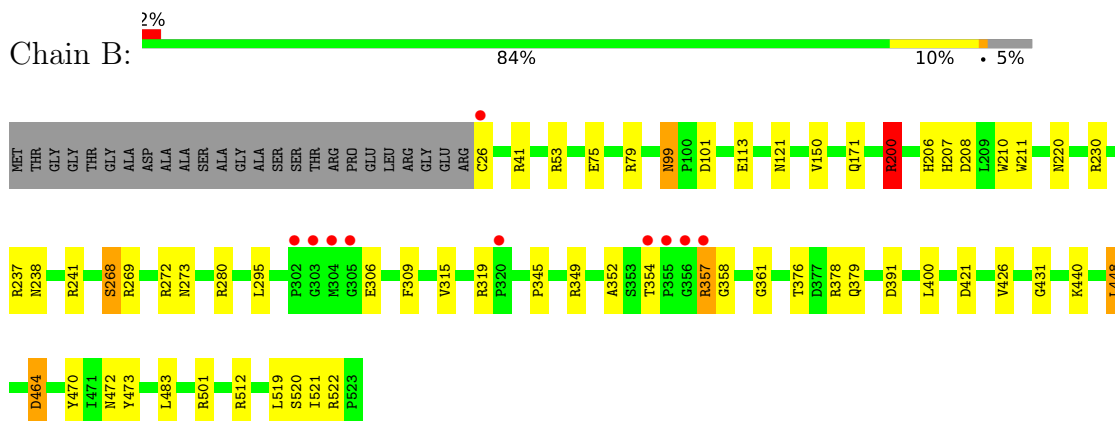
### 3 Residue-property plots [i](#)

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.

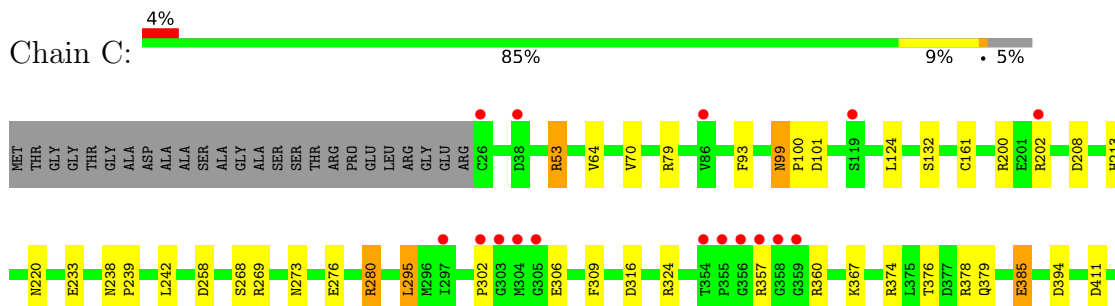
- Molecule 1: Putative hexose oxidase

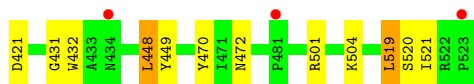


- Molecule 1: Putative hexose oxidase

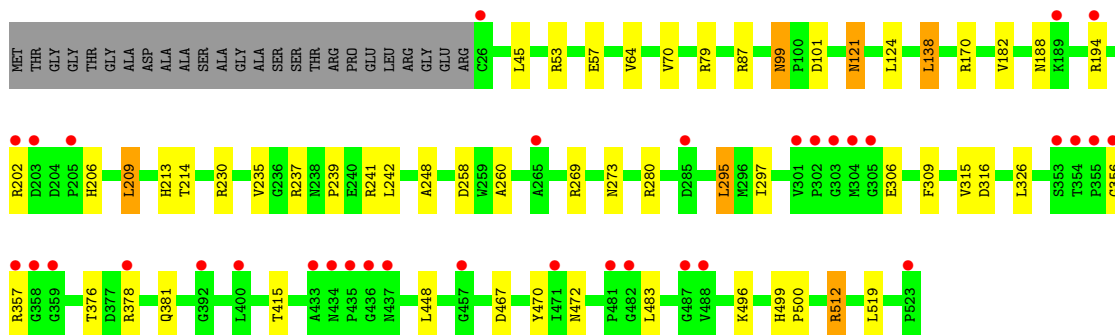
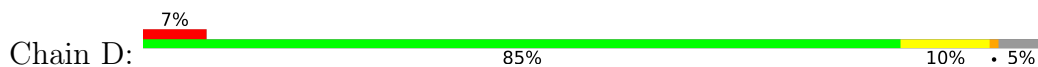


- Molecule 1: Putative hexose oxidase





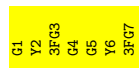
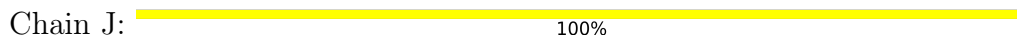
• Molecule 1: Putative hexose oxidase



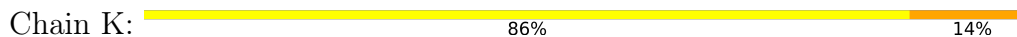
• Molecule 2: TEICOPLANIN



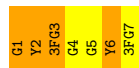
• Molecule 2: TEICOPLANIN



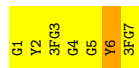
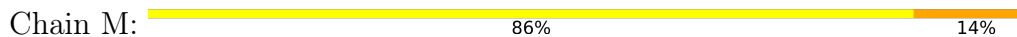
• Molecule 2: TEICOPLANIN




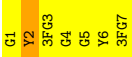
• Molecule 2: TEICOPLANIN



• Molecule 2: TEICOPLANIN





## ● Molecule 2: TEICOPLANIN

Chain N:  86% 14%


G1  
Y2  
3FG3  
G4  
G5  
Y6  
3FG7

## ● Molecule 2: TEICOPLANIN

Chain O:  100%

G1  
Y2  
3FG3  
G4  
G5  
Y6  
3FG7

## ● Molecule 2: TEICOPLANIN

Chain P:  100%

G1  
Y2  
3FG3  
G4  
G5  
Y6  
3FG7

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.79Å 150.78Å 124.85Å 90.00° 98.40° 90.00°	Depositor
Resolution (Å)	29.40 – 1.93 29.49 – 1.93	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.40-1.93) 97.6 (29.49-1.93)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 1.93Å)	Xtrriage
Refinement program	REFMAC 5.8.0124	Depositor
R, $R_{free}$	0.156 , 0.205 0.167 , 0.212	Depositor DCC
$R_{free}$ test set	8214 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtrriage
Anisotropy	0.034	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CIT, N1L, GHP, FAD, 3MY, 3FG, T55, MAN, OMY

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	1.07	3/3966 (0.1%)	1.04	16/5412 (0.3%)
1	B	1.02	1/3966 (0.0%)	1.03	14/5412 (0.3%)
1	C	0.95	0/3966	1.02	16/5412 (0.3%)
1	D	0.85	0/3966	0.94	9/5412 (0.2%)
All	All	0.98	4/15864 (0.0%)	1.01	55/21648 (0.3%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	GLU	CD-OE1	7.79	1.34	1.25
1	A	53	ARG	CZ-NH1	5.67	1.40	1.33
1	A	183	GLU	CD-OE2	-5.50	1.19	1.25
1	A	264	GLU	CD-OE2	5.15	1.31	1.25

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	53	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	A	53	ARG	NE-CZ-NH2	-10.15	115.23	120.30
1	B	53	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	C	53	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	C	448	LEU	CB-CG-CD2	8.79	125.94	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	C	316	ASP	CB-CG-OD1	8.36	125.83	118.30
1	A	41	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	512	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	53	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	A	200	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	B	448	LEU	CB-CG-CD2	7.79	124.24	111.00
1	D	87	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	B	200	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	C	374	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	C	421	ASP	CB-CG-OD1	7.24	124.81	118.30
1	C	324	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	391	ASP	CB-CG-OD1	6.96	124.57	118.30
1	D	87	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	477	ASP	CB-CG-OD1	6.80	124.42	118.30
1	D	53	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	C	200	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	421	ASP	CB-CG-OD1	6.59	124.24	118.30
1	B	391	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	B	512	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	C	200	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	B	230	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	41	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	280	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	326	LEU	CB-CG-CD2	5.92	121.07	111.00
1	D	53	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	87	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	48	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	241	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	280	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	501	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	200	ARG	NE-CZ-NH2	5.57	123.09	120.30
1	D	202	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	519	LEU	CB-CG-CD1	5.48	120.32	111.00
1	D	316	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	492	ASP	CB-CG-OD1	5.45	123.20	118.30
1	C	501	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	378	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	208	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	87	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	182	VAL	CB-CA-C	-5.30	101.33	111.40
1	A	473	TYR	CB-CG-CD2	-5.30	117.82	121.00

*Continued on next page...*



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	448	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	83	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	41	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	295	LEU	CB-CG-CD2	5.17	119.79	111.00
1	C	501	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	D	79	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	138	LEU	CB-CG-CD1	5.06	119.60	111.00
1	D	170	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	357	ARG	Peptide

## 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	3856	0	3743	38	0
1	B	3856	0	3743	29	0
1	C	3856	0	3744	27	0
1	D	3856	0	3744	21	0
2	I	85	0	35	2	0
2	J	85	0	36	0	0
2	K	85	0	32	1	0
2	L	85	0	34	3	0
2	M	85	0	34	1	0
2	N	85	0	34	5	0
2	O	85	0	36	0	0
2	P	85	0	34	0	0
3	A	53	0	29	0	0
3	B	53	0	29	0	0
3	C	53	0	29	0	0
3	D	53	0	29	0	0
4	A	13	0	5	0	0
4	B	13	0	5	0	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	13	0	5	0	0
4	D	13	0	5	0	0
4	O	13	0	5	0	0
5	B	11	0	19	1	0
5	K	11	0	19	1	0
5	M	11	0	19	4	0
5	N	11	0	19	14	0
5	O	11	0	19	0	0
5	P	11	0	19	0	1
6	I	11	0	10	0	0
6	J	11	0	10	0	0
6	K	11	0	10	0	0
6	L	11	0	10	0	0
6	M	11	0	10	0	0
6	N	11	0	10	0	0
6	O	11	0	9	0	0
6	P	11	0	10	0	0
7	I	14	0	13	0	0
7	J	14	0	13	0	0
7	K	14	0	13	0	0
7	L	14	0	13	3	0
7	M	14	0	13	0	0
7	N	14	0	13	0	0
7	O	14	0	13	0	0
7	P	14	0	13	0	0
8	K	12	0	7	1	0
8	L	12	0	7	2	0
8	M	12	0	7	1	0
8	N	12	0	6	0	0
8	O	12	0	7	0	0
8	P	12	0	7	0	0
9	A	425	0	0	10	4
9	B	379	0	0	7	1
9	C	327	0	0	7	1
9	D	217	0	0	5	0
9	I	6	0	0	0	0
9	J	5	0	0	0	0
9	K	3	0	0	0	0
9	L	1	0	0	0	0
9	M	1	0	0	0	0
9	N	12	0	0	0	0
9	O	16	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	P	8	0	0	0	0
All	All	18119	0	15728	123	4

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 4.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ALA:HA	5:N:101:T55:CAD	1.84	1.06
1:A:265:ALA:HA	5:N:101:T55:HAD1	1.51	0.92
1:D:269:ARG:HE	1:D:273:ASN:HD21	1.23	0.86
1:C:269:ARG:HE	1:C:273:ASN:HD21	1.23	0.86
1:A:519:LEU:N	9:A:701:HOH:O	1.59	0.81
1:C:93:PHE:CZ	8:M:104:N1L:O4	2.33	0.80
1:D:512:ARG:NH1	9:D:701:HOH:O	2.14	0.79
1:C:411:ASP:OD1	9:C:701:HOH:O	2.03	0.76
1:A:265:ALA:HA	5:N:101:T55:HAD2	1.65	0.76
1:A:265:ALA:CA	5:N:101:T55:HAD2	2.17	0.75
1:A:265:ALA:CA	5:N:101:T55:CAD	2.65	0.75
1:B:400:LEU:HD23	1:B:426:VAL:HG22	1.71	0.73
1:A:376:THR:H	1:A:379:GLN:HE21	1.37	0.72
1:B:519:LEU:N	9:B:701:HOH:O	1.62	0.71
1:A:57:GLU:OE1	9:A:702:HOH:O	2.09	0.69
1:C:208:ASP:HB2	9:C:731:HOH:O	1.92	0.69
2:N:2:3MY:HB2C	5:N:101:T55:HAG1	1.75	0.68
1:B:376:THR:H	1:B:379:GLN:HE21	1.42	0.67
1:C:376:THR:H	1:C:379:GLN:HE21	1.40	0.67
1:A:265:ALA:CB	5:N:101:T55:HAD2	2.26	0.66
2:N:2:3MY:OBD	5:N:101:T55:O	2.13	0.66
1:B:280:ARG:HD2	9:B:993:HOH:O	1.97	0.65
1:C:269:ARG:HE	1:C:273:ASN:ND2	1.96	0.63
1:B:361:GLY:HA2	7:L:102:NAG:H3	1.80	0.62
1:C:233:GLU:OE2	9:C:702:HOH:O	2.16	0.62
1:A:381:GLN:HG2	9:O:206:HOH:O	2.00	0.61
1:A:99:ASN:HD22	1:A:101:ASP:H	1.49	0.60
1:A:171:GLN:HG3	9:A:889:HOH:O	2.01	0.60
1:A:470:TYR:CZ	1:A:472:ASN:HB2	2.36	0.60
1:A:220:ASN:HD21	1:A:520:SER:HA	1.67	0.59
1:D:57:GLU:HG3	9:D:716:HOH:O	2.03	0.59
1:A:518:ALA:CA	9:A:701:HOH:O	2.48	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:GLU:O	1:C:280:ARG:HD3	2.02	0.58
1:A:455:GLU:OE1	9:A:703:HOH:O	2.17	0.58
1:C:239:PRO:HA	1:C:242:LEU:HD12	1.84	0.58
1:B:269:ARG:HE	1:B:273:ASN:HD21	1.51	0.58
1:B:473:TYR:CZ	8:L:103:N1L:O6A	2.57	0.57
1:B:473:TYR:OH	8:L:103:N1L:O6A	2.23	0.57
1:B:470:TYR:CZ	1:B:472:ASN:HB2	2.40	0.57
1:A:518:ALA:N	9:A:701:HOH:O	2.39	0.55
1:D:121:ASN:HD21	1:D:237:ARG:HA	1.71	0.55
1:D:188:ASN:O	1:D:512:ARG:HD2	2.08	0.54
1:A:389:HIS:CE1	9:A:887:HOH:O	2.60	0.54
1:B:99:ASN:HD22	1:B:101:ASP:H	1.56	0.54
1:C:504:LYS:HD2	9:C:703:HOH:O	2.08	0.54
1:A:150:VAL:HB	2:K:2:3MY:CL	2.45	0.54
1:D:470:TYR:CZ	1:D:472:ASN:HB2	2.43	0.54
1:C:470:TYR:CZ	1:C:472:ASN:HB2	2.43	0.53
1:D:280:ARG:NH1	9:D:707:HOH:O	2.42	0.52
1:A:357:ARG:HG3	1:A:358:GLY:HA3	1.91	0.52
1:B:522:ARG:O	9:B:702:HOH:O	2.19	0.51
1:B:268:SER:OG	1:B:272:ARG:NH1	2.44	0.51
1:A:357:ARG:HG2	9:A:916:HOH:O	2.10	0.51
1:D:295:LEU:HD13	1:D:297:ILE:HD11	1.93	0.51
1:D:99:ASN:HD22	1:D:101:ASP:H	1.59	0.50
1:A:241:ARG:NH1	9:A:707:HOH:O	2.44	0.50
1:A:269:ARG:HE	1:A:273:ASN:HD21	1.60	0.50
1:B:200:ARG:HB3	1:B:210:TRP:CE2	2.46	0.50
1:C:208:ASP:OD2	9:C:703:HOH:O	2.20	0.48
1:B:171:GLN:HG3	9:B:884:HOH:O	2.12	0.48
2:N:2:3MY:CB	5:N:101:T55:HAG1	2.43	0.48
1:D:258:ASP:OD2	1:D:260:ALA:HB3	2.13	0.48
1:B:207:HIS:CE1	2:I:3:3FG:HG1	2.49	0.48
1:B:431:GLY:C	5:B:602:T55:HAD2	2.33	0.48
1:C:394:ASP:HB2	5:M:101:T55:HAD1	1.94	0.48
1:B:220:ASN:HD21	1:B:520:SER:HA	1.79	0.48
1:A:392:GLY:HA3	1:A:440:LYS:HE2	1.97	0.47
1:C:64:VAL:HG21	1:C:70:VAL:HG22	1.97	0.47
1:D:235:VAL:O	1:D:235:VAL:HG12	2.14	0.47
1:A:262:MET:CE	1:A:339:PRO:HG2	2.45	0.47
1:A:245:LYS:HB2	1:A:245:LYS:HE2	1.83	0.46
1:C:220:ASN:HD21	1:C:520:SER:HA	1.81	0.46
1:B:357:ARG:NH2	2:L:6:OMY:O	2.49	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:TYR:CZ	8:K:104:N1L:O6A	2.68	0.46
1:C:53:ARG:NH2	9:C:706:HOH:O	2.42	0.46
1:A:239:PRO:HA	1:A:242:LEU:HD12	1.97	0.45
1:A:265:ALA:CA	5:N:101:T55:HAD1	2.36	0.45
1:C:99:ASN:HD22	1:C:101:ASP:H	1.63	0.45
1:C:431:GLY:C	5:M:101:T55:HAD2	2.37	0.45
2:M:6:OMY:CL	5:M:101:T55:O	2.72	0.45
1:B:349:ARG:HB2	1:B:352:ALA:HB2	1.99	0.45
1:B:464:ASP:HB2	9:B:933:HOH:O	2.16	0.45
1:D:214:THR:HB	1:D:415:THR:HB	1.98	0.45
1:D:248:ALA:HA	9:D:871:HOH:O	2.17	0.45
1:B:79:ARG:HD2	9:B:1052:HOH:O	2.17	0.45
1:B:358:GLY:C	7:L:102:NAG:H81	2.37	0.45
1:A:99:ASN:HD22	1:A:101:ASP:N	2.14	0.45
1:B:357:ARG:NH2	7:L:102:NAG:H83	2.31	0.44
1:A:268:SER:HB3	5:N:101:T55:HAD3	1.98	0.44
1:D:499:HIS:HB3	1:D:500:PRO:HD3	2.00	0.44
1:B:206:HIS:HD2	9:B:742:HOH:O	2.00	0.44
1:B:400:LEU:HD23	1:B:426:VAL:CG2	2.45	0.44
1:B:220:ASN:ND2	1:B:521:ILE:H	2.16	0.44
2:L:1:GHP:C2	2:L:3:3FG:CG2	2.94	0.43
1:A:79:ARG:NE	9:A:714:HOH:O	2.51	0.43
1:A:394:ASP:HB3	5:K:101:T55:HAD1	2.00	0.43
1:B:150:VAL:HB	2:L:2:3MY:CL	2.56	0.43
1:D:239:PRO:HA	1:D:242:LEU:HD12	2.00	0.43
1:C:269:ARG:NE	1:C:273:ASN:HD21	2.03	0.42
1:D:64:VAL:HG21	1:D:70:VAL:HG22	2.00	0.42
2:I:1:GHP:C2	2:I:3:3FG:HG2	2.49	0.42
1:C:394:ASP:CB	5:M:101:T55:HAD1	2.49	0.42
1:D:188:ASN:OD1	1:D:188:ASN:C	2.58	0.42
1:D:209:LEU:HD22	1:D:213:HIS:CE1	2.54	0.42
2:N:2:3MY:CG	5:N:101:T55:HAI1	2.50	0.42
2:N:2:3MY:CZ	5:N:101:T55:HAK1	2.50	0.42
1:C:53:ARG:HD2	1:C:432:TRP:CZ2	2.54	0.41
1:A:338:PRO:N	1:A:339:PRO:CD	2.84	0.41
1:C:385:GLU:HG2	9:C:954:HOH:O	2.18	0.41
1:D:99:ASN:HD21	1:D:101:ASP:HB2	1.85	0.41
1:B:121:ASN:HD21	1:B:237:ARG:HA	1.86	0.41
1:C:161:CYS:HA	1:C:213:HIS:O	2.20	0.41
1:C:99:ASN:HB2	1:C:100:PRO:HD2	2.01	0.41
1:A:64:VAL:HG21	1:A:70:VAL:HG22	2.03	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:TRP:CZ3	1:B:501:ARG:HG2	2.56	0.40
1:C:367:LYS:HE3	1:C:449:TYR:CD2	2.56	0.40
1:D:467:ASP:OD1	1:D:496:LYS:NZ	2.36	0.40
1:A:265:ALA:HB1	5:N:101:T55:HAD2	1.99	0.40
1:C:53:ARG:HD2	1:C:432:TRP:HZ2	1.87	0.40
1:A:499:HIS:N	1:A:500:PRO:CD	2.85	0.40
1:A:499:HIS:HB3	1:A:500:PRO:HD3	2.02	0.40
1:C:220:ASN:ND2	1:C:521:ILE:H	2.19	0.40
1:D:206:HIS:HD2	9:D:727:HOH:O	2.04	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:722:HOH:O	9:A:890:HOH:O[1_455]	2.02	0.18
9:A:800:HOH:O	9:C:948:HOH:O[1_655]	2.02	0.18
5:P:101:T55:CAD	9:A:724:HOH:O[2_7413]	2.16	0.04
9:A:886:HOH:O	9:B:983:HOH:O[2_7513]	2.19	0.01

## 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	496/523 (95%)	479 (97%)	16 (3%)	1 (0%)	47	39
1	B	496/523 (95%)	478 (96%)	18 (4%)	0	100	100
1	C	496/523 (95%)	478 (96%)	17 (3%)	1 (0%)	47	39
1	D	496/523 (95%)	473 (95%)	21 (4%)	2 (0%)	34	24
All	All	1984/2092 (95%)	1908 (96%)	72 (4%)	4 (0%)	47	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	PRO
1	D	356	GLY
1	D	376	THR
1	C	302	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/419 (96%)	390 (96%)	14 (4%)	36	21
1	B	404/419 (96%)	386 (96%)	18 (4%)	27	12
1	C	404/419 (96%)	387 (96%)	17 (4%)	30	14
1	D	404/419 (96%)	383 (95%)	21 (5%)	23	9
All	All	1616/1676 (96%)	1546 (96%)	70 (4%)	29	14

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	75	GLU
1	A	79	ARG
1	A	99	ASN
1	A	113	GLU
1	A	182	VAL
1	A	194	ARG
1	A	238	ASN
1	A	300	GLU
1	A	302	PRO
1	A	306	GLU
1	A	309	PHE
1	A	326	LEU
1	A	357	ARG
1	B	26	CYS
1	B	99	ASN
1	B	113	GLU
1	B	200	ARG

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	238	ASN
1	B	268	SER
1	B	295	LEU
1	B	306	GLU
1	B	309	PHE
1	B	315	VAL
1	B	319	ARG
1	B	345	PRO
1	B	354	THR
1	B	357	ARG
1	B	440	LYS
1	B	448	LEU
1	B	464	ASP
1	B	483	LEU
1	C	79	ARG
1	C	99	ASN
1	C	124	LEU
1	C	132	SER
1	C	202	ARG
1	C	238	ASN
1	C	258	ASP
1	C	268	SER
1	C	295	LEU
1	C	306	GLU
1	C	309	PHE
1	C	357	ARG
1	C	360	ARG
1	C	378	ARG
1	C	385	GLU
1	C	448	LEU
1	C	519	LEU
1	D	45	LEU
1	D	99	ASN
1	D	121	ASN
1	D	124	LEU
1	D	138	LEU
1	D	182	VAL
1	D	194	ARG
1	D	209	LEU
1	D	230	ARG
1	D	241	ARG
1	D	295	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	306	GLU
1	D	309	PHE
1	D	315	VAL
1	D	326	LEU
1	D	378	ARG
1	D	381	GLN
1	D	448	LEU
1	D	483	LEU
1	D	512	ARG
1	D	519	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	99	ASN
1	A	121	ASN
1	A	207	HIS
1	A	220	ASN
1	A	238	ASN
1	A	273	ASN
1	A	348	GLN
1	A	379	GLN
1	A	437	ASN
1	A	513	ASN
1	B	99	ASN
1	B	121	ASN
1	B	207	HIS
1	B	220	ASN
1	B	238	ASN
1	B	273	ASN
1	B	379	GLN
1	B	437	ASN
1	B	513	ASN
1	C	55	ASN
1	C	99	ASN
1	C	121	ASN
1	C	220	ASN
1	C	238	ASN
1	C	273	ASN
1	C	379	GLN
1	C	513	ASN

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
1	D	55	ASN
1	D	99	ASN
1	D	121	ASN
1	D	190	GLN
1	D	207	HIS
1	D	220	ASN
1	D	273	ASN
1	D	348	GLN
1	D	379	GLN
1	D	381	GLN
1	D	513	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

56 non-standard protein/DNA/RNA residues 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	GHP	J	4	2	10,11,12	3.24	5 (50%)	11,14,16	1.19	1 (9%)
2	GHP	I	1	2	10,11,12	3.15	2 (20%)	11,14,16	0.86	0
2	3MY	K	2	2	12,13,14	3.36	3 (25%)	14,17,19	2.10	3 (21%)
2	3MY	N	2	2	12,13,14	2.76	2 (16%)	14,17,19	2.61	7 (50%)
2	OMY	L	6	7,2	12,14,15	2.62	4 (33%)	17,19,21	2.12	6 (35%)
2	GHP	N	4	2,8	10,11,12	3.73	2 (20%)	11,14,16	0.94	0
2	GHP	L	5	2	10,11,12	3.21	2 (20%)	11,14,16	2.64	5 (45%)
2	OMY	P	6	7,2	12,14,15	2.11	2 (16%)	17,19,21	2.37	4 (23%)
2	GHP	L	4	2,8	10,11,12	3.17	4 (40%)	11,14,16	1.11	1 (9%)
2	GHP	P	5	2	10,11,12	3.39	3 (30%)	11,14,16	2.72	5 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	3FG	J	7	6,2	12,13,13	3.11	7 (58%)	14,18,18	1.37	2 (14%)
2	3FG	M	7	6,2	12,13,13	2.58	4 (33%)	14,18,18	1.61	2 (14%)
2	3FG	L	3	2	11,12,13	3.43	5 (45%)	13,16,18	1.63	3 (23%)
2	3MY	I	2	2	12,13,14	2.20	3 (25%)	14,17,19	2.42	5 (35%)
2	3MY	O	2	2	12,13,14	2.05	3 (25%)	14,17,19	1.96	5 (35%)
2	3FG	P	3	2	11,12,13	2.30	4 (36%)	13,16,18	1.65	3 (23%)
2	3FG	K	7	6,2	12,13,13	2.60	4 (33%)	14,18,18	1.27	2 (14%)
2	3FG	O	7	6,2	12,13,13	2.60	4 (33%)	14,18,18	1.51	2 (14%)
2	3FG	P	7	6,2	12,13,13	2.91	4 (33%)	14,18,18	1.39	3 (21%)
2	GHP	K	5	2	10,11,12	3.82	2 (20%)	11,14,16	1.68	3 (27%)
2	3FG	I	7	6,2	12,13,13	2.81	4 (33%)	14,18,18	1.41	3 (21%)
2	GHP	O	4	2,8	10,11,12	3.03	3 (30%)	11,14,16	1.15	1 (9%)
2	GHP	M	1	2	10,11,12	3.31	3 (30%)	11,14,16	1.21	1 (9%)
2	3MY	L	2	2	12,13,14	2.64	4 (33%)	14,17,19	2.18	4 (28%)
2	GHP	K	1	2	10,11,12	3.34	2 (20%)	11,14,16	0.95	1 (9%)
2	GHP	J	5	2	10,11,12	2.61	2 (20%)	11,14,16	2.57	4 (36%)
2	GHP	M	5	2	10,11,12	3.56	3 (30%)	11,14,16	2.25	5 (45%)
2	GHP	P	4	2,8	10,11,12	2.10	3 (30%)	11,14,16	1.86	4 (36%)
2	OMY	J	6	7,2	12,14,15	2.81	7 (58%)	17,19,21	2.61	5 (29%)
2	OMY	M	6	7,2	12,14,15	2.62	4 (33%)	17,19,21	2.24	5 (29%)
2	GHP	O	1	2	10,11,12	3.14	2 (20%)	11,14,16	0.84	0
2	3FG	L	7	6,2	12,13,13	2.92	3 (25%)	14,18,18	1.60	3 (21%)
2	OMY	N	6	7,2	12,14,15	2.37	7 (58%)	17,19,21	1.97	5 (29%)
2	OMY	I	6	7,2	12,14,15	2.94	7 (58%)	17,19,21	2.48	5 (29%)
2	GHP	J	1	2	10,11,12	2.87	3 (30%)	11,14,16	1.44	2 (18%)
2	3FG	K	3	2	11,12,13	3.06	2 (18%)	13,16,18	1.81	3 (23%)
2	OMY	K	6	7,2	12,14,15	2.42	5 (41%)	17,19,21	1.64	4 (23%)
2	GHP	N	5	2	10,11,12	3.05	2 (20%)	11,14,16	2.20	3 (27%)
2	GHP	M	4	2,8	10,11,12	2.94	3 (30%)	11,14,16	1.01	0
2	GHP	O	5	2	10,11,12	3.16	6 (60%)	11,14,16	1.74	2 (18%)
2	OMY	O	6	7,2	12,14,15	2.40	5 (41%)	17,19,21	1.63	2 (11%)
2	3FG	J	3	2	11,12,13	2.53	6 (54%)	13,16,18	2.40	3 (23%)
2	GHP	P	1	2	10,11,12	3.62	7 (70%)	11,14,16	1.06	1 (9%)
2	3MY	P	2	2	12,13,14	2.05	6 (50%)	14,17,19	1.92	3 (21%)
2	3FG	M	3	2	11,12,13	3.25	3 (27%)	13,16,18	1.47	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	3FG	N	3	2	11,12,13	2.43	3 (27%)	13,16,18	2.13	3 (23%)
2	GHP	K	4	2,8	10,11,12	2.14	3 (30%)	11,14,16	1.02	0
2	3FG	N	7	6,2	12,13,13	2.71	5 (41%)	14,18,18	1.32	2 (14%)
2	GHP	N	1	2	10,11,12	2.42	5 (50%)	11,14,16	1.16	0
2	GHP	I	4	2	10,11,12	2.74	3 (30%)	11,14,16	1.13	1 (9%)
2	3MY	J	2	2	12,13,14	2.90	3 (25%)	14,17,19	1.90	6 (42%)
2	GHP	I	5	2	10,11,12	3.25	3 (30%)	11,14,16	2.18	4 (36%)
2	3MY	M	2	2	12,13,14	2.87	2 (16%)	14,17,19	2.77	3 (21%)
2	GHP	L	1	2	10,11,12	3.07	3 (30%)	11,14,16	0.62	0
2	3FG	O	3	2	11,12,13	1.73	3 (27%)	13,16,18	1.75	4 (30%)
2	3FG	I	3	2	11,12,13	3.43	2 (18%)	13,16,18	1.77	4 (30%)

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	GHP	J	4	2	-	2/4/6/8	0/1/1/1
2	GHP	I	1	2	-	2/4/6/8	0/1/1/1
2	3MY	K	2	2	-	1/5/6/8	0/1/1/1
2	3MY	N	2	2	-	0/5/6/8	0/1/1/1
2	OMY	L	6	7,2	-	2/9/10/12	0/1/1/1
2	GHP	N	4	2,8	-	2/4/6/8	0/1/1/1
2	GHP	L	5	2	-	0/4/6/8	0/1/1/1
2	OMY	P	6	7,2	-	1/9/10/12	0/1/1/1
2	GHP	L	4	2,8	-	2/4/6/8	0/1/1/1
2	GHP	P	5	2	-	0/4/6/8	0/1/1/1
2	3FG	J	7	6,2	-	2/8/8/8	0/1/1/1
2	3FG	M	7	6,2	-	4/8/8/8	0/1/1/1
2	3FG	L	3	2	-	0/4/6/8	0/1/1/1
2	3MY	I	2	2	-	1/5/6/8	0/1/1/1
2	3MY	O	2	2	-	1/5/6/8	0/1/1/1
2	3FG	P	3	2	-	2/4/6/8	0/1/1/1
2	3FG	K	7	6,2	-	5/8/8/8	0/1/1/1
2	3FG	O	7	6,2	-	2/8/8/8	0/1/1/1
2	3FG	P	7	6,2	-	5/8/8/8	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GHP	K	5	2	-	0/4/6/8	0/1/1/1
2	3FG	I	7	6,2	-	1/8/8/8	0/1/1/1
2	GHP	O	4	2,8	-	2/4/6/8	0/1/1/1
2	GHP	M	1	2	-	4/4/6/8	0/1/1/1
2	3MY	L	2	2	-	0/5/6/8	0/1/1/1
2	GHP	K	1	2	-	4/4/6/8	0/1/1/1
2	GHP	J	5	2	-	0/4/6/8	0/1/1/1
2	GHP	M	5	2	-	0/4/6/8	0/1/1/1
2	GHP	P	4	2,8	-	1/4/6/8	0/1/1/1
2	OMY	J	6	7,2	-	1/9/10/12	0/1/1/1
2	OMY	M	6	7,2	-	0/9/10/12	0/1/1/1
2	GHP	O	1	2	-	2/4/6/8	0/1/1/1
2	3FG	L	7	6,2	-	2/8/8/8	0/1/1/1
2	OMY	N	6	7,2	-	1/9/10/12	0/1/1/1
2	OMY	I	6	7,2	-	1/9/10/12	0/1/1/1
2	GHP	J	1	2	-	1/4/6/8	0/1/1/1
2	3FG	K	3	2	-	0/4/6/8	0/1/1/1
2	OMY	K	6	7,2	-	3/9/10/12	0/1/1/1
2	GHP	N	5	2	-	0/4/6/8	0/1/1/1
2	GHP	M	4	2,8	-	0/4/6/8	0/1/1/1
2	GHP	O	5	2	-	0/4/6/8	0/1/1/1
2	OMY	O	6	7,2	-	1/9/10/12	0/1/1/1
2	3FG	J	3	2	-	0/4/6/8	0/1/1/1
2	GHP	P	1	2	-	0/4/6/8	0/1/1/1
2	3MY	P	2	2	-	0/5/6/8	0/1/1/1
2	3FG	M	3	2	-	0/4/6/8	0/1/1/1
2	3FG	N	3	2	-	0/4/6/8	0/1/1/1
2	GHP	K	4	2,8	-	1/4/6/8	0/1/1/1
2	3FG	N	7	6,2	-	2/8/8/8	0/1/1/1
2	GHP	N	1	2	-	1/4/6/8	0/1/1/1
2	GHP	I	4	2	-	3/4/6/8	0/1/1/1
2	3MY	J	2	2	-	0/5/6/8	0/1/1/1
2	GHP	I	5	2	-	0/4/6/8	0/1/1/1
2	3MY	M	2	2	-	1/5/6/8	0/1/1/1
2	GHP	L	1	2	-	4/4/6/8	0/1/1/1
2	3FG	O	3	2	-	0/4/6/8	0/1/1/1
2	3FG	I	3	2	-	0/4/6/8	0/1/1/1

All (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	5	GHP	C1-CA	-10.81	1.41	1.52
2	M	5	GHP	C1-CA	-9.96	1.42	1.52
2	N	4	GHP	C1-CA	-9.85	1.42	1.52
2	K	1	GHP	C1-CA	-9.62	1.42	1.52
2	I	3	3FG	CB-CA	-9.56	1.42	1.52
2	K	2	3MY	CE2-CL	9.51	1.96	1.73
2	P	5	GHP	C1-CA	-9.47	1.42	1.52
2	P	1	GHP	C1-CA	-9.42	1.42	1.52
2	M	1	GHP	C1-CA	-9.34	1.42	1.52
2	L	3	3FG	CB-CA	-9.26	1.42	1.52
2	I	1	GHP	C1-CA	-9.15	1.42	1.52
2	I	5	GHP	C1-CA	-8.99	1.43	1.52
2	O	1	GHP	C1-CA	-8.80	1.43	1.52
2	K	3	3FG	CB-CA	-8.74	1.43	1.52
2	N	5	GHP	C1-CA	-8.64	1.43	1.52
2	M	3	3FG	CB-CA	-8.61	1.43	1.52
2	O	4	GHP	C1-CA	-8.41	1.43	1.52
2	L	5	GHP	C1-CA	-8.36	1.43	1.52
2	L	1	GHP	C1-CA	-8.34	1.43	1.52
2	J	4	GHP	C1-CA	-8.06	1.44	1.52
2	M	2	3MY	CE2-CL	7.79	1.92	1.73
2	L	4	GHP	C1-CA	-7.76	1.44	1.52
2	N	2	3MY	CE2-CL	7.71	1.91	1.73
2	P	7	3FG	CB-CA	-7.65	1.43	1.52
2	J	1	GHP	C1-CA	-7.64	1.44	1.52
2	M	4	GHP	C1-CA	-7.63	1.44	1.52
2	L	7	3FG	CB-CA	-7.60	1.43	1.52
2	O	5	GHP	C1-CA	-7.36	1.44	1.52
2	J	5	GHP	C1-CA	-6.97	1.45	1.52
2	L	2	3MY	CE2-CL	6.93	1.90	1.73
2	L	6	OMY	CG-CB	-6.55	1.42	1.51
2	M	6	OMY	CG-CB	-6.38	1.42	1.51
2	K	7	3FG	CB-CA	-6.20	1.45	1.52
2	O	7	3FG	CB-CA	-6.20	1.45	1.52
2	J	2	3MY	CE2-CL	6.16	1.88	1.73
2	N	3	3FG	CB-CA	-6.05	1.46	1.52
2	I	4	GHP	C1-CA	-6.02	1.46	1.52
2	K	2	3MY	CB-CG	-5.76	1.37	1.51
2	I	6	OMY	CG-CB	-5.71	1.43	1.51
2	I	7	3FG	CB-CA	-5.55	1.46	1.52
2	N	4	GHP	CA-C	-5.41	1.39	1.51
2	P	6	OMY	CG-CB	-5.38	1.43	1.51
2	J	2	3MY	CZ-CE2	5.33	1.44	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	7	3FG	CB-CA	-5.27	1.46	1.52
2	N	1	GHP	C1-CA	-5.23	1.47	1.52
2	K	6	OMY	CG-CB	-5.18	1.44	1.51
2	K	4	GHP	C1-CA	-5.16	1.47	1.52
2	N	7	3FG	CA-C	-5.13	1.42	1.54
2	I	3	3FG	CA-C	-5.12	1.40	1.51
2	L	3	3FG	CA-C	-5.12	1.40	1.51
2	J	7	3FG	CG1-CB	5.11	1.47	1.39
2	P	3	3FG	CB-CA	-5.09	1.47	1.52
2	M	2	3MY	CB-CG	-5.08	1.39	1.51
2	M	3	3FG	CA-C	-5.04	1.40	1.51
2	L	5	GHP	CA-C	-5.02	1.40	1.51
2	N	7	3FG	CB-CA	-4.88	1.46	1.52
2	J	7	3FG	CG2-CB	4.77	1.46	1.39
2	K	5	GHP	CA-C	-4.76	1.41	1.51
2	O	6	OMY	CG-CB	-4.74	1.44	1.51
2	K	7	3FG	CA-C	-4.69	1.43	1.54
2	N	6	OMY	CG-CB	-4.66	1.44	1.51
2	I	2	3MY	CZ-CE2	4.66	1.44	1.39
2	O	6	OMY	O-C	4.62	1.38	1.19
2	M	7	3FG	CA-C	-4.61	1.43	1.54
2	I	6	OMY	O-C	4.59	1.38	1.19
2	I	7	3FG	CA-C	-4.59	1.43	1.54
2	J	6	OMY	CZ-CE1	4.47	1.43	1.39
2	M	6	OMY	O-C	4.44	1.37	1.19
2	O	2	3MY	CB-CG	-4.43	1.40	1.51
2	J	6	OMY	O-C	4.42	1.37	1.19
2	I	2	3MY	CB-CG	-4.42	1.40	1.51
2	L	6	OMY	O-C	4.38	1.37	1.19
2	L	4	GHP	CA-C	-4.37	1.41	1.51
2	J	7	3FG	CB-CA	-4.34	1.47	1.52
2	M	5	GHP	CA-C	-4.34	1.42	1.51
2	L	7	3FG	CA-C	-4.30	1.44	1.54
2	K	6	OMY	O-C	4.30	1.37	1.19
2	P	4	GHP	CA-C	-4.25	1.42	1.51
2	P	7	3FG	CA-C	-4.24	1.44	1.54
2	L	2	3MY	CB-CG	-4.17	1.41	1.51
2	I	7	3FG	CG1-CD1	4.16	1.45	1.39
2	J	2	3MY	CB-CG	-4.14	1.41	1.51
2	I	7	3FG	CG1-CB	4.06	1.45	1.39
2	I	6	OMY	CE1-CL	4.01	1.83	1.73
2	M	7	3FG	CG1-CB	4.01	1.45	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	6	OMY	O-C	4.00	1.35	1.19
2	J	6	OMY	CE1-CL	3.97	1.83	1.73
2	J	3	3FG	CB-CA	-3.93	1.48	1.52
2	I	4	GHP	CA-C	-3.89	1.42	1.51
2	O	7	3FG	CG1-CB	3.86	1.45	1.39
2	O	5	GHP	C6-C1	3.85	1.45	1.39
2	P	6	OMY	O-C	3.79	1.35	1.19
2	L	7	3FG	CG1-CB	3.76	1.45	1.39
2	N	2	3MY	CB-CG	-3.76	1.42	1.51
2	K	1	GHP	CA-C	-3.72	1.43	1.51
2	J	6	OMY	CG-CB	-3.62	1.46	1.51
2	J	7	3FG	CG1-CD1	3.57	1.44	1.39
2	K	6	OMY	CZ-CE1	3.56	1.42	1.39
2	J	7	3FG	CA-C	-3.53	1.46	1.54
2	P	3	3FG	CA-C	-3.48	1.43	1.51
2	M	4	GHP	CA-C	-3.47	1.43	1.51
2	L	6	OMY	CZ-CE1	3.47	1.42	1.39
2	P	4	GHP	C1-CA	-3.45	1.48	1.52
2	N	3	3FG	CA-C	-3.45	1.43	1.51
2	J	4	GHP	CA-C	-3.40	1.43	1.51
2	J	3	3FG	OD2-CD2	3.34	1.44	1.37
2	M	6	OMY	CE1-CL	3.27	1.81	1.73
2	K	3	3FG	CA-C	-3.26	1.44	1.51
2	N	7	3FG	CG1-CD1	3.26	1.44	1.39
2	O	2	3MY	CE2-CL	3.15	1.81	1.73
2	J	7	3FG	CZ-CD1	3.14	1.43	1.39
2	P	2	3MY	CB-CG	-3.14	1.43	1.51
2	P	1	GHP	CA-C	-3.06	1.44	1.51
2	J	3	3FG	CG2-CB	3.05	1.43	1.39
2	J	3	3FG	CG2-CD2	3.03	1.43	1.39
2	P	7	3FG	CG1-CB	3.02	1.43	1.39
2	K	7	3FG	CG1-CB	3.01	1.43	1.39
2	J	3	3FG	CG1-CD1	3.01	1.43	1.39
2	J	4	GHP	C3-C2	2.96	1.44	1.38
2	O	7	3FG	CA-C	-2.96	1.47	1.54
2	N	7	3FG	CG1-CB	2.93	1.43	1.39
2	I	6	OMY	CZ-CE1	2.87	1.42	1.39
2	O	3	3FG	CG2-CB	2.83	1.43	1.39
2	M	1	GHP	CA-C	-2.82	1.45	1.51
2	J	3	3FG	CA-C	-2.81	1.45	1.51
2	O	4	GHP	CA-C	-2.80	1.45	1.51
2	I	5	GHP	CA-C	-2.69	1.45	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	3	3FG	CA-C	-2.69	1.45	1.51
2	P	2	3MY	CD1-CG	2.67	1.44	1.38
2	O	7	3FG	CG2-CB	2.67	1.43	1.39
2	L	4	GHP	C3-C2	2.65	1.43	1.38
2	I	6	OMY	CD2-CG	2.65	1.43	1.39
2	P	2	3MY	OBD-CZ	2.64	1.41	1.36
2	P	2	3MY	CD1-CE1	2.63	1.43	1.38
2	N	1	GHP	C6-C1	2.59	1.43	1.39
2	M	6	OMY	CZ-CE1	2.58	1.42	1.39
2	P	2	3MY	CE2-CL	2.57	1.79	1.73
2	P	5	GHP	CA-C	-2.57	1.45	1.51
2	I	4	GHP	C3-C4	2.57	1.43	1.38
2	P	1	GHP	C3-C2	2.56	1.43	1.38
2	J	6	OMY	CA-N	2.54	1.55	1.47
2	P	1	GHP	C6-C5	2.54	1.43	1.38
2	N	6	OMY	CE1-CL	-2.53	1.67	1.73
2	L	1	GHP	CA-C	-2.52	1.45	1.51
2	O	6	OMY	OCZ-CZ	2.49	1.41	1.36
2	N	3	3FG	OD2-CD2	2.49	1.42	1.37
2	O	5	GHP	CA-C	-2.48	1.45	1.51
2	K	4	GHP	C6-C5	2.47	1.43	1.38
2	P	3	3FG	CG2-CD2	2.46	1.42	1.39
2	O	3	3FG	CG2-CD2	2.45	1.42	1.39
2	N	7	3FG	CG2-CB	2.45	1.42	1.39
2	O	5	GHP	C6-C5	2.43	1.43	1.38
2	J	4	GHP	C6-C5	2.43	1.43	1.38
2	O	1	GHP	C3-C2	2.41	1.43	1.38
2	N	6	OMY	CZ-CE1	2.41	1.41	1.39
2	N	5	GHP	C3-C2	2.41	1.43	1.38
2	I	5	GHP	C3-C4	2.39	1.43	1.38
2	O	4	GHP	C6-C1	2.39	1.42	1.39
2	N	1	GHP	C2-C1	2.38	1.42	1.39
2	N	1	GHP	CA-C	-2.36	1.46	1.51
2	I	6	OMY	CA-N	2.36	1.55	1.47
2	M	3	3FG	CZ-CD1	2.34	1.42	1.39
2	M	4	GHP	C6-C5	2.33	1.43	1.38
2	O	5	GHP	C5-C4	2.33	1.43	1.38
2	J	6	OMY	OCZ-CZ	2.31	1.41	1.36
2	J	1	GHP	CA-C	-2.28	1.46	1.51
2	I	1	GHP	CA-C	-2.28	1.46	1.51
2	L	1	GHP	C2-C1	2.28	1.42	1.39
2	J	7	3FG	OD2-CD2	-2.28	1.31	1.37

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	6	OMY	CD2-CG	2.28	1.42	1.39
2	J	5	GHP	CA-C	-2.28	1.46	1.51
2	K	2	3MY	CD2-CE2	2.27	1.42	1.38
2	N	6	OMY	ODE-CB	2.27	1.47	1.42
2	P	4	GHP	C3-C2	2.25	1.42	1.38
2	I	2	3MY	OBD-CZ	2.24	1.40	1.36
2	P	2	3MY	CZ-CE2	2.23	1.41	1.39
2	O	5	GHP	C3-C4	2.23	1.43	1.38
2	P	7	3FG	CG1-CD1	2.22	1.42	1.39
2	P	3	3FG	CG2-CB	2.21	1.42	1.39
2	K	4	GHP	CA-C	-2.21	1.46	1.51
2	K	6	OMY	CD2-CG	2.20	1.42	1.39
2	L	4	GHP	C2-C1	2.20	1.42	1.39
2	L	2	3MY	CA-N	2.19	1.54	1.48
2	P	1	GHP	C2-C1	2.19	1.42	1.39
2	P	5	GHP	C3-C2	2.18	1.42	1.38
2	N	6	OMY	CA-N	2.18	1.54	1.47
2	L	3	3FG	CZ-CD1	2.18	1.42	1.39
2	N	1	GHP	C6-C5	2.18	1.42	1.38
2	J	1	GHP	C3-C2	2.17	1.42	1.38
2	J	4	GHP	C2-C1	2.14	1.42	1.39
2	N	6	OMY	CD2-CG	2.13	1.42	1.39
2	O	2	3MY	CA-N	2.12	1.54	1.48
2	M	7	3FG	CG2-CB	2.12	1.42	1.39
2	L	2	3MY	CD2-CE2	2.10	1.42	1.38
2	P	1	GHP	C3-C4	2.10	1.42	1.38
2	L	3	3FG	OD2-CD2	2.10	1.41	1.37
2	O	6	OMY	CD2-CG	2.08	1.42	1.39
2	M	1	GHP	C2-C1	2.06	1.42	1.39
2	K	6	OMY	OCZ-CZ	2.06	1.40	1.36
2	M	5	GHP	C3-C4	2.05	1.42	1.38
2	L	6	OMY	CE1-CL	2.04	1.78	1.73
2	I	6	OMY	OCZ-CZ	2.04	1.40	1.36
2	P	1	GHP	C6-C1	2.03	1.42	1.39
2	L	3	3FG	CG2-CD2	2.03	1.42	1.39
2	K	7	3FG	CG2-CB	2.03	1.42	1.39
2	O	6	OMY	CZ-CE1	2.00	1.41	1.39

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	6	OMY	CG-CB-CA	-7.94	100.86	111.49

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	6	OMY	CG-CB-CA	-7.81	101.03	111.49
2	M	2	3MY	CD2-CE2-CZ	-7.48	116.58	120.91
2	P	6	OMY	CG-CB-CA	-6.92	102.22	111.49
2	M	6	OMY	CG-CB-CA	-6.72	102.49	111.49
2	J	3	3FG	CD2-CG2-CB	6.60	125.77	120.11
2	L	5	GHP	C1-CA-N	6.36	127.63	112.40
2	L	6	OMY	CG-CB-CA	-5.88	103.61	111.49
2	N	3	3FG	CD2-CG2-CB	5.68	124.99	120.11
2	N	6	OMY	CG-CB-CA	-5.56	104.04	111.49
2	K	2	3MY	CD2-CE2-CZ	-5.45	117.75	120.91
2	I	5	GHP	C1-CA-N	5.23	124.93	112.40
2	I	2	3MY	CZ-CE2-CL	5.21	129.32	119.53
2	O	6	OMY	CG-CB-CA	-5.14	104.61	111.49
2	I	2	3MY	CD2-CE2-CL	-5.12	110.23	118.49
2	J	5	GHP	C1-CA-N	5.09	124.59	112.40
2	P	2	3MY	CB-CA-C	5.08	121.00	111.47
2	P	5	GHP	C5-C6-C1	-4.95	116.22	121.20
2	M	7	3FG	CB-CA-C	4.88	121.00	109.96
2	K	6	OMY	CG-CB-CA	-4.87	104.97	111.49
2	M	5	GHP	C1-CA-N	4.78	123.84	112.40
2	N	5	GHP	C1-CA-N	4.52	123.22	112.40
2	N	2	3MY	CG-CB-CA	-4.48	105.03	114.10
2	K	3	3FG	CD2-CG2-CB	4.47	123.95	120.11
2	L	2	3MY	CD2-CE2-CL	4.41	125.61	118.49
2	L	2	3MY	CD2-CE2-CZ	-4.38	118.37	120.91
2	M	2	3MY	CD2-CE2-CL	4.15	125.19	118.49
2	J	5	GHP	C2-C3-C4	-4.10	115.38	119.88
2	P	6	OMY	ODE-CB-CA	-4.10	98.64	107.28
2	O	2	3MY	CB-CA-C	4.10	119.15	111.47
2	N	2	3MY	CD2-CE2-CZ	-4.07	118.56	120.91
2	I	3	3FG	CD2-CG2-CB	4.05	123.59	120.11
2	P	5	GHP	C1-CA-N	4.04	122.06	112.40
2	N	2	3MY	CE1-CZ-CE2	4.02	122.45	118.55
2	J	6	OMY	ODE-CB-CG	3.99	119.89	111.19
2	K	2	3MY	CD2-CE2-CL	3.95	124.86	118.49
2	O	3	3FG	CD1-CG1-CB	3.94	123.50	120.11
2	P	5	GHP	C2-C3-C4	-3.93	115.56	119.88
2	M	2	3MY	CE1-CZ-CE2	3.86	122.30	118.55
2	J	3	3FG	CG2-CD2-CZ	-3.82	115.16	120.43
2	N	2	3MY	CB-CA-C	3.81	118.61	111.47
2	O	5	GHP	C1-CA-N	3.76	121.40	112.40
2	N	5	GHP	C2-C3-C4	-3.63	115.89	119.88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	6	OMY	CD1-CE1-CZ	-3.61	118.82	120.91
2	J	7	3FG	CD1-CG1-CB	-3.55	117.06	120.11
2	L	5	GHP	C2-C3-C4	-3.54	115.99	119.88
2	M	3	3FG	CD2-CG2-CB	3.52	123.13	120.11
2	P	3	3FG	CD2-CG2-CB	3.52	123.13	120.11
2	L	2	3MY	CE1-CZ-CE2	3.50	121.95	118.55
2	P	4	GHP	C5-C6-C1	3.48	124.70	121.20
2	J	5	GHP	C3-C2-C1	3.43	124.65	121.20
2	L	3	3FG	CD2-CG2-CB	3.28	122.93	120.11
2	J	2	3MY	CZ-CE2-CL	3.19	125.51	119.53
2	K	3	3FG	CB-CA-N	-3.14	104.89	112.40
2	J	6	OMY	CD2-CG-CB	3.14	125.40	120.73
2	I	6	OMY	CD1-CE1-CZ	-3.14	119.10	120.91
2	I	2	3MY	CB-CA-C	3.05	117.19	111.47
2	M	5	GHP	C6-C1-CA	3.04	125.56	120.65
2	L	6	OMY	O-C-CA	-3.04	116.81	124.78
2	N	6	OMY	O-C-CA	-3.03	116.83	124.78
2	L	7	3FG	CD1-CG1-CB	-3.02	117.52	120.11
2	P	4	GHP	C2-C1-CA	3.01	125.50	120.65
2	M	5	GHP	C2-C1-CA	-3.00	115.81	120.65
2	J	2	3MY	CB-CA-C	2.99	117.08	111.47
2	K	5	GHP	C1-CA-N	2.99	119.56	112.40
2	O	7	3FG	CB-CA-C	2.96	116.66	109.96
2	I	5	GHP	C2-C3-C4	-2.94	116.65	119.88
2	P	3	3FG	CG1-CB-CA	2.86	124.48	119.77
2	P	7	3FG	CD1-CG1-CB	-2.85	117.66	120.11
2	O	3	3FG	CB-CA-N	-2.84	105.60	112.40
2	K	5	GHP	C2-C1-CA	-2.83	116.09	120.65
2	L	5	GHP	C3-C2-C1	2.82	124.04	121.20
2	J	6	OMY	O-C-CA	-2.81	117.42	124.78
2	L	3	3FG	CB-CA-N	-2.81	105.68	112.40
2	O	7	3FG	CD1-CG1-CB	-2.80	117.71	120.11
2	J	5	GHP	C5-C6-C1	-2.80	118.38	121.20
2	P	5	GHP	C6-C1-C2	2.78	121.77	118.29
2	M	1	GHP	C2-C3-C4	-2.78	116.83	119.88
2	K	3	3FG	CG2-CD2-CZ	-2.77	116.61	120.43
2	K	7	3FG	CB-CA-C	2.76	116.20	109.96
2	L	6	OMY	CD1-CE1-CZ	-2.75	119.32	120.91
2	L	7	3FG	CB-CA-C	2.73	116.12	109.96
2	L	4	GHP	C2-C1-CA	2.71	125.02	120.65
2	I	2	3MY	CB-CG-CD2	-2.70	115.80	120.44
2	I	3	3FG	CG2-CD2-CZ	-2.70	116.71	120.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	3	3FG	CG2-CD2-CZ	-2.70	116.71	120.43
2	K	2	3MY	CE1-CZ-CE2	2.69	121.16	118.55
2	I	6	OMY	O-C-CA	-2.69	117.74	124.78
2	L	3	3FG	CG2-CD2-CZ	-2.67	116.74	120.43
2	L	6	OMY	CE2-CZ-CE1	2.67	121.14	118.55
2	J	1	GHP	C2-C3-C4	-2.63	116.99	119.88
2	O	2	3MY	CE2-CD2-CG	-2.63	118.66	120.46
2	I	6	OMY	CD2-CG-CB	2.62	124.63	120.73
2	M	5	GHP	C3-C2-C1	2.61	123.83	121.20
2	P	6	OMY	O-C-CA	-2.61	117.94	124.78
2	L	5	GHP	C6-C1-CA	2.61	124.86	120.65
2	P	4	GHP	C6-C5-C4	-2.61	117.01	119.88
2	N	7	3FG	CD2-CG2-CB	2.61	122.35	120.11
2	J	2	3MY	CD2-CE2-CL	-2.60	114.29	118.49
2	M	5	GHP	C2-C3-C4	-2.59	117.03	119.88
2	J	6	OMY	CZ-CE1-CL	2.59	124.39	119.53
2	K	5	GHP	C6-C1-CA	2.57	124.79	120.65
2	N	3	3FG	CB-CA-N	-2.54	106.31	112.40
2	M	6	OMY	CE2-CZ-CE1	2.54	121.02	118.55
2	N	2	3MY	CD1-CG-CD2	2.53	122.08	118.54
2	O	2	3MY	CD2-CE2-CL	2.51	122.55	118.49
2	J	2	3MY	CD1-CE1-CZ	-2.51	117.92	120.50
2	I	6	OMY	CZ-CE1-CL	2.49	124.20	119.53
2	P	6	OMY	CD1-CE1-CZ	2.48	122.35	120.91
2	I	7	3FG	CB-CA-C	2.47	115.55	109.96
2	J	1	GHP	C3-C2-C1	2.47	123.68	121.20
2	O	3	3FG	CD2-CG2-CB	2.46	122.22	120.11
2	P	2	3MY	CD1-CE1-CZ	-2.45	117.99	120.50
2	L	6	OMY	CZ-CE1-CL	2.44	124.10	119.53
2	O	4	GHP	C2-C3-C4	-2.43	117.21	119.88
2	K	6	OMY	O-C-CA	-2.43	118.41	124.78
2	L	7	3FG	OD1-CD1-CG1	-2.43	113.53	119.84
2	I	5	GHP	C2-C1-CA	-2.40	116.78	120.65
2	K	1	GHP	C2-C3-C4	-2.38	117.26	119.88
2	I	7	3FG	CG1-CB-CA	2.34	123.42	119.71
2	N	7	3FG	CD1-CG1-CB	-2.32	118.12	120.11
2	I	3	3FG	CB-CA-N	-2.32	106.85	112.40
2	K	7	3FG	OD1-CD1-CG1	-2.29	113.89	119.84
2	O	2	3MY	OBD-CZ-CE1	2.28	125.54	119.33
2	J	4	GHP	C1-CA-N	2.27	117.84	112.40
2	P	5	GHP	O4-C4-C3	-2.27	113.55	120.02
2	L	2	3MY	OBD-CZ-CE2	-2.26	113.56	119.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	3MY	CB-CG-CD2	-2.25	116.57	120.44
2	N	6	OMY	CD2-CE2-CZ	-2.25	118.19	120.50
2	M	6	OMY	CZ-CE1-CL	2.25	123.76	119.53
2	P	1	GHP	C1-CA-N	2.24	117.75	112.40
2	J	2	3MY	CE1-CZ-CE2	2.23	120.71	118.55
2	L	5	GHP	C2-C1-CA	-2.22	117.08	120.65
2	P	7	3FG	OD1-CD1-CG1	-2.21	114.10	119.84
2	I	2	3MY	CG-CB-CA	-2.19	109.67	114.10
2	O	2	3MY	CZ-CE2-CL	-2.18	115.43	119.53
2	P	4	GHP	C6-C1-C2	-2.16	115.59	118.29
2	O	5	GHP	C2-C1-CA	-2.16	117.17	120.65
2	M	6	OMY	O-C-CA	-2.15	119.14	124.78
2	P	2	3MY	CD2-CE2-CZ	2.15	122.16	120.91
2	N	5	GHP	O4-C4-C3	-2.14	113.92	120.02
2	N	6	OMY	ODE-CB-CG	2.14	115.86	111.19
2	M	7	3FG	CD2-CG2-CB	2.13	121.94	120.11
2	L	6	OMY	CD2-CE2-CZ	-2.11	118.33	120.50
2	N	2	3MY	OBD-CZ-CE2	-2.09	113.99	119.27
2	I	5	GHP	C6-C1-CA	2.09	124.02	120.65
2	J	3	3FG	CD2-CZ-CD1	2.09	121.70	119.20
2	O	6	OMY	O-C-CA	-2.08	119.31	124.78
2	K	6	OMY	CD2-CG-CB	2.07	123.81	120.73
2	M	3	3FG	CG2-CD2-CZ	-2.06	117.59	120.43
2	P	3	3FG	CB-CA-N	-2.05	107.48	112.40
2	K	6	OMY	CZ-CE1-CL	2.05	123.38	119.53
2	I	7	3FG	CD1-CG1-CB	-2.05	118.35	120.11
2	J	7	3FG	CB-CA-C	2.04	114.58	109.96
2	O	3	3FG	CG1-CB-CA	2.04	123.13	119.77
2	I	3	3FG	CG2-CB-CA	2.03	123.12	119.77
2	P	7	3FG	CB-CA-C	2.03	114.55	109.96
2	N	6	OMY	CZ-CE1-CL	2.02	123.32	119.53
2	I	4	GHP	C3-C2-C1	2.01	123.22	121.20
2	N	2	3MY	CE1-CD1-CG	-2.01	118.26	121.03

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	6	OMY	O-C-CA-CB
2	K	6	OMY	C-CA-CB-CG
2	K	6	OMY	C-CA-CB-ODE
2	L	6	OMY	O-C-CA-CB

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	N	6	OMY	O-C-CA-CB
2	O	6	OMY	O-C-CA-CB
2	P	6	OMY	O-C-CA-CB
2	K	7	3FG	O-C-CA-CB
2	K	7	3FG	OXT-C-CA-CB
2	O	7	3FG	C-CA-CB-CG2
2	P	7	3FG	O-C-CA-CB
2	P	7	3FG	OXT-C-CA-CB
2	M	2	3MY	N-CA-CB-CG
2	O	2	3MY	N-CA-CB-CG
2	L	7	3FG	C-CA-CB-CG1
2	L	7	3FG	C-CA-CB-CG2
2	M	7	3FG	C-CA-CB-CG1
2	M	7	3FG	C-CA-CB-CG2
2	N	7	3FG	C-CA-CB-CG1
2	N	7	3FG	C-CA-CB-CG2
2	O	7	3FG	C-CA-CB-CG1
2	P	7	3FG	C-CA-CB-CG2
2	O	1	GHP	C2-C1-CA-C
2	O	4	GHP	C2-C1-CA-C
2	O	4	GHP	C6-C1-CA-C
2	P	4	GHP	C2-C1-CA-C
2	M	7	3FG	O-C-CA-N
2	K	7	3FG	OXT-C-CA-N
2	M	7	3FG	OXT-C-CA-N
2	M	1	GHP	C2-C1-CA-N
2	K	6	OMY	N-CA-CB-CG
2	L	6	OMY	C-CA-CB-CG
2	I	2	3MY	N-CA-CB-CG
2	K	2	3MY	N-CA-CB-CG
2	J	7	3FG	C-CA-CB-CG2
2	K	7	3FG	C-CA-CB-CG1
2	K	7	3FG	C-CA-CB-CG2
2	K	1	GHP	C6-C1-CA-N
2	L	1	GHP	C6-C1-CA-N
2	K	1	GHP	C2-C1-CA-C
2	L	1	GHP	C2-C1-CA-C
2	O	1	GHP	C6-C1-CA-C
2	K	1	GHP	C2-C1-CA-N
2	I	7	3FG	C-CA-CB-CG2
2	J	7	3FG	C-CA-CB-CG1
2	P	7	3FG	C-CA-CB-CG1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	P	7	3FG	OXT-C-CA-N
2	L	1	GHP	C2-C1-CA-N
2	M	1	GHP	C6-C1-CA-N
2	I	6	OMY	O-C-CA-CB
2	I	1	GHP	C2-C1-CA-C
2	I	1	GHP	C6-C1-CA-C
2	J	1	GHP	C6-C1-CA-C
2	K	1	GHP	C6-C1-CA-C
2	L	1	GHP	C6-C1-CA-C
2	M	1	GHP	C2-C1-CA-C
2	M	1	GHP	C6-C1-CA-C
2	N	1	GHP	C2-C1-CA-C
2	P	3	3FG	C-CA-CB-CG1
2	P	3	3FG	C-CA-CB-CG2
2	I	4	GHP	C2-C1-CA-C
2	I	4	GHP	C6-C1-CA-C
2	K	4	GHP	C2-C1-CA-C
2	L	4	GHP	C2-C1-CA-C
2	L	4	GHP	C6-C1-CA-C
2	N	4	GHP	C2-C1-CA-C
2	N	4	GHP	C6-C1-CA-C
2	I	4	GHP	C2-C1-CA-N
2	J	4	GHP	C2-C1-CA-N
2	J	4	GHP	C6-C1-CA-N

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	GHP	1	0
2	K	2	3MY	1	0
2	N	2	3MY	5	0
2	L	6	OMY	1	0
2	L	3	3FG	1	0
2	L	2	3MY	1	0
2	M	6	OMY	1	0
2	L	1	GHP	1	0
2	I	3	3FG	2	0



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

37 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CIT	D	602	-	12,12,12	1.19	1 (8%)	17,17,17	1.93	4 (23%)
6	MAN	K	102	2	11,11,12	1.27	1 (9%)	15,15,17	2.44	4 (26%)
4	CIT	C	602	-	12,12,12	1.18	1 (8%)	17,17,17	1.64	4 (23%)
8	N1L	L	103	5,2	12,12,13	3.30	6 (50%)	11,17,19	3.58	3 (27%)
3	FAD	A	601	1	53,58,58	1.76	10 (18%)	68,89,89	1.54	12 (17%)
5	T55	P	101	8	10,10,11	0.88	0	10,10,12	0.64	0
5	T55	M	101	8	10,10,11	0.41	0	10,10,12	1.11	1 (10%)
5	T55	N	101	8	10,10,11	0.55	0	10,10,12	1.57	3 (30%)
4	CIT	B	603	-	12,12,12	1.35	1 (8%)	17,17,17	1.61	4 (23%)
7	NAG	M	103	2	14,14,15	1.09	2 (14%)	17,19,21	1.55	5 (29%)
7	NAG	L	102	2	14,14,15	0.93	1 (7%)	17,19,21	1.75	4 (23%)
8	N1L	P	104	5,2	12,12,13	3.82	9 (75%)	11,17,19	2.38	3 (27%)
6	MAN	I	101	2	11,11,12	3.03	4 (36%)	15,15,17	3.19	4 (26%)
6	MAN	M	102	2	11,11,12	1.85	2 (18%)	15,15,17	1.93	4 (26%)
7	NAG	N	103	2	14,14,15	1.31	1 (7%)	17,19,21	1.52	4 (23%)
6	MAN	O	102	2	11,11,12	2.48	4 (36%)	15,15,17	1.69	4 (26%)
8	N1L	K	104	5,2	12,12,13	3.78	7 (58%)	11,17,19	3.14	3 (27%)
6	MAN	J	101	2	11,11,12	3.39	6 (54%)	15,15,17	2.23	1 (6%)
6	MAN	L	101	2	11,11,12	0.78	0	15,15,17	1.25	1 (6%)
8	N1L	O	104	5,2	12,12,13	3.97	7 (58%)	11,17,19	2.25	4 (36%)
3	FAD	C	601	1	53,58,58	1.84	8 (15%)	68,89,89	1.62	16 (23%)
7	NAG	J	102	2	14,14,15	2.78	6 (42%)	17,19,21	3.71	9 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAN	P	102	2	11,11,12	1.71	3 (27%)	15,15,17	1.67	4 (26%)
3	FAD	D	601	1	53,58,58	1.81	10 (18%)	68,89,89	1.54	15 (22%)
7	NAG	P	103	2	14,14,15	2.10	4 (28%)	17,19,21	1.40	2 (11%)
5	T55	B	602	8	10,10,11	0.52	0	10,10,12	1.07	0
5	T55	K	101	8	10,10,11	0.48	0	10,10,12	0.84	0
3	FAD	B	601	1	53,58,58	1.71	7 (13%)	68,89,89	1.59	15 (22%)
7	NAG	O	103	2	14,14,15	1.42	2 (14%)	17,19,21	1.63	3 (17%)
8	N1L	M	104	5,2	12,12,13	4.70	9 (75%)	11,17,19	3.14	7 (63%)
4	CIT	A	602	-	12,12,12	1.36	1 (8%)	17,17,17	1.43	2 (11%)
4	CIT	O	105	-	12,12,12	2.23	6 (50%)	17,17,17	4.39	8 (47%)
5	T55	O	101	8	10,10,11	0.57	0	10,10,12	0.63	0
7	NAG	K	103	2	14,14,15	1.03	2 (14%)	17,19,21	1.72	7 (41%)
6	MAN	N	102	2	11,11,12	2.34	3 (27%)	15,15,17	1.73	4 (26%)
8	N1L	N	104	5,2	12,12,13	4.01	7 (58%)	11,17,19	3.13	3 (27%)
7	NAG	I	102	2	14,14,15	1.93	5 (35%)	17,19,21	2.26	8 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	D	602	-	-	5/16/16/16	-
6	MAN	K	102	2	-	2/2/19/22	0/1/1/1
4	CIT	C	602	-	-	7/16/16/16	-
8	N1L	L	103	5,2	-	0/4/21/24	0/1/1/1
3	FAD	A	601	1	-	4/30/50/50	0/6/6/6
5	T55	P	101	8	-	5/7/8/9	-
5	T55	M	101	8	-	0/7/8/9	-
5	T55	N	101	8	-	0/7/8/9	-
4	CIT	B	603	-	-	5/16/16/16	-
7	NAG	M	103	2	-	3/6/23/26	0/1/1/1
7	NAG	L	102	2	-	4/6/23/26	0/1/1/1
8	N1L	P	104	5,2	-	2/4/21/24	0/1/1/1
6	MAN	I	101	2	-	0/2/19/22	0/1/1/1
6	MAN	M	102	2	-	0/2/19/22	1/1/1/1
7	NAG	N	103	2	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	O	102	2	-	2/2/19/22	0/1/1/1
8	N1L	K	104	5,2	-	1/4/21/24	0/1/1/1
6	MAN	J	101	2	-	2/2/19/22	0/1/1/1
6	MAN	L	101	2	-	2/2/19/22	0/1/1/1
8	N1L	O	104	5,2	-	1/4/21/24	0/1/1/1
3	FAD	C	601	1	-	4/30/50/50	0/6/6/6
7	NAG	J	102	2	-	2/6/23/26	0/1/1/1
6	MAN	P	102	2	-	0/2/19/22	0/1/1/1
3	FAD	D	601	1	-	5/30/50/50	0/6/6/6
7	NAG	P	103	2	-	2/6/23/26	0/1/1/1
5	T55	B	602	8	-	0/7/8/9	-
5	T55	K	101	8	-	0/7/8/9	-
3	FAD	B	601	1	-	4/30/50/50	0/6/6/6
7	NAG	O	103	2	-	4/6/23/26	0/1/1/1
8	N1L	M	104	5,2	-	1/4/21/24	0/1/1/1
4	CIT	A	602	-	-	1/16/16/16	-
4	CIT	O	105	-	-	12/16/16/16	-
5	T55	O	101	8	-	1/7/8/9	-
7	NAG	K	103	2	-	2/6/23/26	0/1/1/1
6	MAN	N	102	2	-	2/2/19/22	0/1/1/1
8	N1L	N	104	5,2	-	2/4/21/24	0/1/1/1
7	NAG	I	102	2	-	4/6/23/26	0/1/1/1

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	104	N1L	C1-C2	8.62	1.62	1.52
8	N	104	N1L	C1-C2	8.26	1.62	1.52
8	P	104	N1L	C1-C2	8.20	1.62	1.52
6	J	101	MAN	O5-C1	7.79	1.56	1.43
8	K	104	N1L	C1-C2	7.76	1.61	1.52
8	N	104	N1L	O6A-C6	7.67	1.45	1.22
8	M	104	N1L	O6A-C6	7.61	1.45	1.22
8	O	104	N1L	C1-C2	7.51	1.61	1.52
8	O	104	N1L	O6A-C6	7.28	1.44	1.22
8	L	103	N1L	O5-C1	7.02	1.54	1.43
6	I	101	MAN	O5-C1	6.70	1.54	1.43
7	J	102	NAG	O5-C1	6.66	1.54	1.43
8	P	104	N1L	O6A-C6	6.54	1.42	1.22

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	FAD	C9A-C5X	6.52	1.52	1.41
3	D	601	FAD	C9A-C5X	6.33	1.51	1.41
3	A	601	FAD	C9A-C5X	6.32	1.51	1.41
8	M	104	N1L	O3-C3	5.73	1.56	1.43
8	L	103	N1L	O6A-C6	5.69	1.39	1.22
6	O	102	MAN	O5-C1	5.67	1.52	1.43
8	K	104	N1L	O5-C1	5.64	1.52	1.43
3	C	601	FAD	C1'-C2'	-5.63	1.44	1.52
7	P	103	NAG	C1-C2	5.61	1.60	1.52
8	M	104	N1L	O5-C1	5.59	1.52	1.43
6	N	102	MAN	O5-C1	5.47	1.52	1.43
3	B	601	FAD	C1'-C2'	-5.36	1.45	1.52
8	K	104	N1L	O6A-C6	5.06	1.37	1.22
3	B	601	FAD	C9A-C5X	4.87	1.49	1.41
8	M	104	N1L	O6B-C6	4.87	1.46	1.30
3	D	601	FAD	O4B-C1B	4.74	1.47	1.41
6	I	101	MAN	O5-C5	4.73	1.53	1.43
6	J	101	MAN	O5-C5	4.70	1.53	1.43
3	D	601	FAD	C8-C7	4.67	1.52	1.40
8	L	103	N1L	C1-C2	4.67	1.58	1.52
8	O	104	N1L	O6B-C6	4.60	1.45	1.30
3	A	601	FAD	C8-C7	4.50	1.52	1.40
8	M	104	N1L	C2-N2	-4.44	1.32	1.47
7	J	102	NAG	O5-C5	4.38	1.52	1.43
7	J	102	NAG	C1-C2	4.37	1.58	1.52
3	B	601	FAD	C8-C7	4.31	1.51	1.40
3	C	601	FAD	C8-C7	4.29	1.51	1.40
6	M	102	MAN	O5-C5	4.28	1.52	1.43
8	N	104	N1L	O5-C5	4.12	1.51	1.43
8	N	104	N1L	C2-N2	-4.07	1.33	1.47
8	O	104	N1L	C2-N2	-4.02	1.33	1.47
8	P	104	N1L	C2-N2	-3.99	1.33	1.47
3	A	601	FAD	C4X-N5	3.95	1.38	1.30
8	K	104	N1L	O4-C4	3.88	1.52	1.43
3	B	601	FAD	C6-C7	3.87	1.45	1.39
8	O	104	N1L	O5-C5	3.87	1.50	1.43
4	O	105	CIT	C4-C3	3.81	1.58	1.53
6	M	102	MAN	O5-C1	3.80	1.49	1.43
8	K	104	N1L	O6B-C6	3.73	1.42	1.30
6	I	101	MAN	C1-C2	3.72	1.60	1.52
8	P	104	N1L	O3-C3	3.71	1.51	1.43
3	C	601	FAD	C4X-N5	3.65	1.37	1.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	FAD	C1'-C2'	-3.63	1.47	1.52
6	I	101	MAN	C2-C3	3.63	1.57	1.52
7	I	102	NAG	O5-C1	3.61	1.49	1.43
6	P	102	MAN	O5-C1	3.50	1.49	1.43
8	N	104	N1L	O5-C1	3.49	1.49	1.43
8	K	104	N1L	O3-C3	3.46	1.51	1.43
6	N	102	MAN	O5-C5	3.44	1.50	1.43
8	P	104	N1L	O5-C5	3.38	1.49	1.43
8	O	104	N1L	C3-C2	3.34	1.60	1.53
6	O	102	MAN	O3-C3	3.29	1.50	1.43
6	J	101	MAN	C4-C3	3.22	1.60	1.52
6	J	101	MAN	C1-C2	3.21	1.59	1.52
3	C	601	FAD	C6-C7	3.20	1.44	1.39
7	I	102	NAG	C8-C7	3.18	1.57	1.50
4	O	105	CIT	O1-C1	3.14	1.32	1.22
3	D	601	FAD	C8M-C8	3.07	1.57	1.51
8	N	104	N1L	O6B-C6	3.04	1.40	1.30
6	K	102	MAN	O5-C1	3.01	1.48	1.43
3	D	601	FAD	C5X-N5	-2.98	1.33	1.39
7	P	103	NAG	O3-C3	2.98	1.50	1.43
8	L	103	N1L	O6B-C6	2.94	1.40	1.30
7	N	103	NAG	C2-N2	2.94	1.51	1.46
8	K	104	N1L	O5-C5	2.92	1.48	1.43
7	L	102	NAG	C2-N2	2.89	1.51	1.46
4	B	603	CIT	C4-C3	2.87	1.57	1.53
7	O	103	NAG	C8-C7	2.86	1.56	1.50
3	A	601	FAD	C1'-C2'	-2.84	1.48	1.52
7	J	102	NAG	C3-C2	2.84	1.58	1.52
6	J	101	MAN	C4-C5	2.81	1.59	1.53
3	A	601	FAD	C2A-N3A	2.79	1.36	1.32
8	M	104	N1L	C4-C3	-2.74	1.45	1.52
7	I	102	NAG	C3-C2	2.74	1.58	1.52
6	P	102	MAN	C4-C3	2.74	1.59	1.52
7	J	102	NAG	C8-C7	2.72	1.56	1.50
7	P	103	NAG	C2-N2	2.72	1.50	1.46
6	O	102	MAN	O4-C4	-2.71	1.36	1.43
3	A	601	FAD	C2B-C1B	-2.68	1.49	1.53
3	C	601	FAD	O4B-C1B	2.66	1.44	1.41
8	O	104	N1L	C4-C5	2.65	1.57	1.53
4	O	105	CIT	O3-C5	2.62	1.30	1.22
3	D	601	FAD	C6-C7	2.60	1.43	1.39
4	O	105	CIT	C3-C6	2.59	1.56	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	103	N1L	O5-C5	2.59	1.48	1.43
4	O	105	CIT	O2-C1	-2.58	1.22	1.30
6	P	102	MAN	O3-C3	2.56	1.49	1.43
3	C	601	FAD	O4-C4	2.56	1.28	1.23
7	J	102	NAG	C2-N2	2.56	1.50	1.46
7	I	102	NAG	O5-C5	2.54	1.48	1.43
8	M	104	N1L	C4-C5	2.54	1.57	1.53
4	O	105	CIT	C2-C1	2.53	1.58	1.50
3	C	601	FAD	C8M-C8	2.53	1.56	1.51
3	A	601	FAD	C2'-C3'	-2.51	1.48	1.53
3	D	601	FAD	C2B-C1B	-2.49	1.50	1.53
3	B	601	FAD	C4X-N5	2.49	1.35	1.30
6	O	102	MAN	O2-C2	-2.48	1.38	1.43
4	A	602	CIT	C4-C3	2.47	1.56	1.53
7	K	103	NAG	C8-C7	2.45	1.55	1.50
6	N	102	MAN	C4-C3	2.44	1.58	1.52
7	O	103	NAG	O5-C1	2.42	1.47	1.43
3	D	601	FAD	C4X-N5	2.41	1.35	1.30
8	L	103	N1L	O3-C3	2.40	1.48	1.43
8	M	104	N1L	C3-C2	2.40	1.58	1.53
8	P	104	N1L	C3-C2	2.36	1.58	1.53
6	J	101	MAN	O2-C2	2.33	1.48	1.43
7	P	103	NAG	C4-C5	2.31	1.57	1.53
3	A	601	FAD	C7M-C7	2.23	1.55	1.51
3	A	601	FAD	C5A-C4A	2.21	1.46	1.40
3	B	601	FAD	C5X-N5	-2.18	1.35	1.39
4	C	602	CIT	C4-C3	2.14	1.56	1.53
8	P	104	N1L	C4-C5	2.14	1.56	1.53
3	B	601	FAD	C8M-C8	2.14	1.55	1.51
7	K	103	NAG	O5-C5	2.13	1.47	1.43
7	M	103	NAG	C8-C7	2.11	1.54	1.50
4	D	602	CIT	C4-C3	2.08	1.56	1.53
7	I	102	NAG	C4-C3	2.07	1.57	1.52
8	N	104	N1L	C3-C2	2.06	1.58	1.53
3	D	601	FAD	C4-N3	-2.04	1.35	1.38
8	P	104	N1L	C5-C6	2.03	1.57	1.53
7	M	103	NAG	O5-C5	2.03	1.47	1.43
8	P	104	N1L	O4-C4	2.02	1.47	1.43
3	A	601	FAD	C6-C7	2.01	1.42	1.39

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	102	NAG	O5-C5-C6	13.11	127.75	107.20
4	O	105	CIT	O7-C3-C6	-13.05	90.54	108.86
8	L	103	N1L	O6B-C6-O6A	-10.74	99.71	124.09
8	K	104	N1L	O6B-C6-O6A	-9.46	102.61	124.09
8	N	104	N1L	O6B-C6-O6A	-8.91	103.85	124.09
6	J	101	MAN	O5-C5-C6	8.08	119.87	107.20
6	I	101	MAN	C1-O5-C5	8.05	123.09	112.19
4	O	105	CIT	C2-C3-C6	7.51	126.25	110.11
6	K	102	MAN	C1-O5-C5	7.29	122.08	112.19
8	P	104	N1L	O6B-C6-O6A	-6.92	108.37	124.09
6	I	101	MAN	O5-C5-C6	6.44	117.30	107.20
8	M	104	N1L	O6B-C6-O6A	-5.75	111.04	124.09
6	M	102	MAN	C1-O5-C5	5.61	119.79	112.19
6	I	101	MAN	C1-C2-C3	5.58	116.52	109.67
8	M	104	N1L	O4-C4-C3	-5.06	98.65	110.35
7	I	102	NAG	O5-C5-C6	5.02	115.08	107.20
4	O	105	CIT	O6-C6-C3	4.95	121.65	113.05
4	O	105	CIT	O7-C3-C4	4.93	120.93	109.40
3	B	601	FAD	N3A-C2A-N1A	-4.52	121.62	128.68
4	D	602	CIT	O5-C6-C3	-4.34	116.11	122.25
4	D	602	CIT	O6-C6-C3	4.33	120.57	113.05
6	O	102	MAN	O5-C5-C6	4.31	113.95	107.20
8	M	104	N1L	C3-C2-N2	-4.17	102.72	110.97
7	O	103	NAG	C4-C3-C2	-4.11	105.00	111.02
3	C	601	FAD	C9A-C5X-N5	-4.10	117.97	122.43
6	P	102	MAN	C1-O5-C5	4.07	117.71	112.19
7	I	102	NAG	C1-O5-C5	-4.05	106.70	112.19
4	O	105	CIT	C3-C2-C1	-3.98	104.17	113.81
3	D	601	FAD	C4-C4X-N5	3.87	123.75	118.23
3	B	601	FAD	C9A-C5X-N5	-3.86	118.23	122.43
6	N	102	MAN	O5-C5-C6	3.86	113.26	107.20
6	K	102	MAN	O5-C5-C6	3.84	113.22	107.20
8	O	104	N1L	O3-C3-C2	-3.83	102.78	109.81
4	C	602	CIT	O6-C6-C3	3.83	119.70	113.05
3	C	601	FAD	N3A-C2A-N1A	-3.82	122.71	128.68
8	O	104	N1L	O6B-C6-O6A	-3.81	115.43	124.09
7	L	102	NAG	O5-C5-C6	3.54	112.75	107.20
4	A	602	CIT	O6-C6-C3	3.53	119.17	113.05
8	N	104	N1L	O6A-C6-C5	-3.52	107.91	120.81
3	B	601	FAD	C5X-N5-C4X	3.50	123.89	118.07
4	O	105	CIT	O5-C6-C3	-3.48	117.33	122.25
3	A	601	FAD	C9A-C5X-N5	-3.47	118.66	122.43
8	N	104	N1L	O3-C3-C2	-3.46	103.46	109.81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	FAD	C4-C4X-N5	3.33	122.98	118.23
3	C	601	FAD	N6A-C6A-N1A	3.32	125.47	118.57
7	J	102	NAG	C6-C5-C4	-3.32	105.22	113.00
4	B	603	CIT	O6-C6-C3	3.25	118.69	113.05
3	A	601	FAD	C5X-C6-C7	-3.22	114.81	120.71
7	L	102	NAG	C2-N2-C7	3.21	127.48	122.90
4	O	105	CIT	O7-C3-C2	-3.19	101.93	109.40
8	M	104	N1L	O3-C3-C4	-3.19	102.98	110.35
6	P	102	MAN	O5-C1-C2	3.17	115.66	110.77
8	M	104	N1L	O6A-C6-C5	-3.16	109.22	120.81
7	N	103	NAG	O6-C6-C5	-3.16	100.46	111.29
3	C	601	FAD	C5X-N5-C4X	3.15	123.31	118.07
4	B	603	CIT	O7-C3-C4	3.10	116.66	109.40
3	D	601	FAD	N3A-C2A-N1A	-3.06	123.89	128.68
3	B	601	FAD	O4-C4-C4X	-3.06	118.49	126.60
8	O	104	N1L	O6A-C6-C5	-3.04	109.64	120.81
3	A	601	FAD	C4-C4X-N5	3.03	122.55	118.23
7	J	102	NAG	C4-C3-C2	-3.03	106.58	111.02
3	D	601	FAD	O4-C4-C4X	-3.02	118.59	126.60
6	L	101	MAN	O5-C5-C6	3.02	111.93	107.20
3	A	601	FAD	N6A-C6A-N1A	3.00	124.80	118.57
8	L	103	N1L	O4-C4-C3	-2.99	103.44	110.35
7	P	103	NAG	O6-C6-C5	-2.98	101.06	111.29
7	I	102	NAG	C4-C3-C2	2.97	115.38	111.02
7	K	103	NAG	O5-C1-C2	-2.95	106.64	111.29
3	D	601	FAD	C10-N1-C2	2.95	122.79	116.90
7	I	102	NAG	C8-C7-N2	2.92	121.05	116.10
6	O	102	MAN	O4-C4-C3	-2.92	103.61	110.35
7	K	103	NAG	O5-C5-C6	2.89	111.74	107.20
3	B	601	FAD	C2A-N1A-C6A	2.88	123.69	118.75
3	D	601	FAD	C4X-C4-N3	2.88	120.50	113.19
7	O	103	NAG	O6-C6-C5	-2.87	101.44	111.29
7	M	103	NAG	C1-C2-N2	-2.87	105.59	110.49
6	N	102	MAN	C1-O5-C5	2.84	116.04	112.19
6	M	102	MAN	O5-C5-C6	2.81	111.62	107.20
7	O	103	NAG	C1-O5-C5	-2.78	108.42	112.19
3	C	601	FAD	O4-C4-C4X	-2.78	119.23	126.60
3	A	601	FAD	N3A-C2A-N1A	-2.77	124.34	128.68
7	J	102	NAG	O5-C5-C4	-2.76	104.11	110.83
3	A	601	FAD	C5X-N5-C4X	2.74	122.64	118.07
4	B	603	CIT	O7-C3-C2	-2.72	103.03	109.40
7	K	103	NAG	O6-C6-C5	-2.71	101.99	111.29

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	FAD	C6-C7-C8	2.70	123.54	119.67
8	L	103	N1L	O6A-C6-C5	-2.70	110.91	120.81
6	M	102	MAN	O6-C6-C5	-2.66	102.17	111.29
8	K	104	N1L	O6A-C6-C5	-2.65	111.08	120.81
3	A	601	FAD	C1B-N9A-C4A	-2.65	121.98	126.64
3	C	601	FAD	C6-C7-C8	2.60	123.39	119.67
3	B	601	FAD	C5'-C4'-C3'	-2.59	107.19	112.20
8	O	104	N1L	O4-C4-C3	-2.59	104.37	110.35
5	N	101	T55	CAF-CAE-CAG	2.58	127.48	111.54
7	J	102	NAG	C8-C7-N2	2.57	120.45	116.10
3	B	601	FAD	O2'-C2'-C1'	-2.57	103.59	109.80
3	B	601	FAD	C5X-C6-C7	-2.55	116.02	120.71
3	D	601	FAD	C4'-C3'-C2'	-2.55	108.06	113.36
7	L	102	NAG	C1-C2-N2	-2.55	106.14	110.49
3	C	601	FAD	C5A-C6A-N6A	-2.55	116.48	120.35
4	D	602	CIT	O7-C3-C2	-2.54	103.45	109.40
3	A	601	FAD	C6-C5X-C9A	2.54	122.53	118.94
6	N	102	MAN	O5-C1-C2	2.54	114.69	110.77
3	A	601	FAD	O4-C4-C4X	-2.53	119.90	126.60
7	M	103	NAG	O6-C6-C5	-2.52	102.63	111.29
3	C	601	FAD	C5X-C6-C7	-2.52	116.09	120.71
6	K	102	MAN	C1-C2-C3	2.52	112.76	109.67
6	P	102	MAN	O3-C3-C4	2.51	116.16	110.35
7	N	103	NAG	C2-N2-C7	2.51	126.48	122.90
3	C	601	FAD	C5'-C4'-C3'	-2.50	107.37	112.20
3	C	601	FAD	C9A-C9-C8	2.50	124.33	119.30
3	D	601	FAD	C1'-N10-C9A	2.49	124.66	120.51
3	C	601	FAD	C4'-C3'-C2'	-2.48	108.20	113.36
7	J	102	NAG	C2-N2-C7	2.48	126.43	122.90
3	B	601	FAD	C9-C8-C7	-2.47	116.13	119.67
3	D	601	FAD	C1'-C2'-C3'	-2.47	102.89	109.79
4	A	602	CIT	O5-C6-C3	-2.46	118.77	122.25
6	O	102	MAN	O5-C1-C2	2.44	114.53	110.77
8	K	104	N1L	C4-C3-C2	-2.43	107.27	111.37
7	K	103	NAG	C8-C7-N2	2.42	120.20	116.10
3	C	601	FAD	C9-C8-C7	-2.41	116.22	119.67
7	M	103	NAG	O5-C5-C6	2.41	110.98	107.20
3	D	601	FAD	C9A-C5X-N5	-2.40	119.83	122.43
6	P	102	MAN	O6-C6-C5	-2.40	103.07	111.29
7	J	102	NAG	C3-C4-C5	-2.38	105.99	110.24
8	M	104	N1L	C3-C4-C5	2.37	113.30	109.25
4	C	602	CIT	O7-C3-C2	-2.37	103.86	109.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	102	MAN	O5-C1-C2	2.35	114.40	110.77
4	C	602	CIT	O7-C3-C4	2.35	114.89	109.40
7	L	102	NAG	C6-C5-C4	-2.34	107.51	113.00
6	N	102	MAN	O2-C2-C1	2.34	113.95	109.15
8	P	104	N1L	O5-C5-C6	2.31	113.92	106.31
3	B	601	FAD	C6-C7-C8	2.30	122.97	119.67
3	C	601	FAD	C6-C5X-C9A	2.30	122.19	118.94
8	M	104	N1L	O4-C4-C5	2.28	114.86	109.74
6	I	101	MAN	C3-C4-C5	-2.28	106.18	110.24
3	C	601	FAD	C4-C4X-N5	2.28	121.47	118.23
3	A	601	FAD	C4X-C10-N1	-2.26	119.47	124.73
3	D	601	FAD	O5B-PA-O1A	2.26	117.90	109.07
3	B	601	FAD	O4-C4-N3	2.26	124.44	120.12
4	D	602	CIT	O4-C5-C4	2.25	121.58	114.35
7	J	102	NAG	O3-C3-C2	2.25	114.12	109.47
6	O	102	MAN	C1-O5-C5	2.25	115.24	112.19
5	N	101	T55	CAF-CAE-CAD	-2.24	100.18	110.51
3	D	601	FAD	O4'-C4'-C5'	2.21	114.89	109.92
5	M	101	T55	CAK-CAJ-CAI	-2.21	103.19	114.42
3	D	601	FAD	C5X-N5-C4X	2.21	121.75	118.07
3	B	601	FAD	N6A-C6A-N1A	2.21	123.16	118.57
3	D	601	FAD	C4X-C10-N1	-2.21	119.61	124.73
7	I	102	NAG	C2-N2-C7	2.20	126.04	122.90
3	B	601	FAD	C4'-C3'-C2'	-2.17	108.84	113.36
7	N	103	NAG	O7-C7-C8	-2.17	118.02	122.06
5	N	101	T55	CAJ-CAK-CAL	2.17	123.25	113.79
7	M	103	NAG	C2-N2-C7	2.17	125.99	122.90
7	I	102	NAG	O7-C7-C8	-2.16	118.05	122.06
7	K	103	NAG	C6-C5-C4	-2.15	107.96	113.00
3	D	601	FAD	C5X-C6-C7	-2.13	116.79	120.71
6	M	102	MAN	C6-C5-C4	-2.13	108.01	113.00
3	B	601	FAD	C9A-C9-C8	2.12	123.57	119.30
3	A	601	FAD	C4X-C4-N3	2.11	118.56	113.19
7	J	102	NAG	O7-C7-C8	-2.09	118.18	122.06
7	I	102	NAG	O5-C1-C2	-2.09	107.99	111.29
3	C	601	FAD	O4-C4-N3	2.08	124.10	120.12
8	P	104	N1L	O6B-C6-C5	-2.07	106.06	113.65
7	P	103	NAG	O7-C7-C8	-2.07	118.21	122.06
4	B	603	CIT	C3-C4-C5	2.07	118.83	113.81
7	M	103	NAG	C6-C5-C4	-2.05	108.20	113.00
7	N	103	NAG	C8-C7-N2	2.04	119.56	116.10
7	I	102	NAG	O6-C6-C5	-2.04	104.29	111.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	602	CIT	O3-C5-C4	-2.04	116.98	122.94
7	K	103	NAG	C1-C2-N2	-2.04	107.01	110.49
3	C	601	FAD	C7M-C7-C8	-2.03	116.57	120.74
3	D	601	FAD	O2A-PA-O1A	2.03	122.27	112.24
7	K	103	NAG	C2-N2-C7	2.01	125.77	122.90
4	O	105	CIT	O2-C1-O1	-2.00	118.30	123.30

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	O	105	CIT	C2-C3-C4-C5
4	O	105	CIT	O7-C3-C4-C5
4	O	105	CIT	C2-C3-C6-O5
4	O	105	CIT	O7-C3-C6-O5
4	O	105	CIT	O7-C3-C6-O6
4	O	105	CIT	C4-C3-C6-O5
4	O	105	CIT	C4-C3-C6-O6
8	M	104	N1L	C4-C5-C6-O6A
8	N	104	N1L	C4-C5-C6-O6B
8	O	104	N1L	C4-C5-C6-O6B
6	J	101	MAN	O5-C5-C6-O6
6	N	102	MAN	O5-C5-C6-O6
3	D	601	FAD	O3'-C3'-C4'-O4'
7	I	102	NAG	O5-C5-C6-O6
7	L	102	NAG	O5-C5-C6-O6
6	N	102	MAN	C4-C5-C6-O6
6	J	101	MAN	C4-C5-C6-O6
6	K	102	MAN	C4-C5-C6-O6
6	K	102	MAN	O5-C5-C6-O6
7	I	102	NAG	C8-C7-N2-C2
7	I	102	NAG	O7-C7-N2-C2
7	J	102	NAG	C8-C7-N2-C2
7	J	102	NAG	O7-C7-N2-C2
7	K	103	NAG	C8-C7-N2-C2
7	K	103	NAG	O7-C7-N2-C2
7	L	102	NAG	C8-C7-N2-C2
7	L	102	NAG	O7-C7-N2-C2
7	M	103	NAG	C8-C7-N2-C2
7	M	103	NAG	O7-C7-N2-C2
7	N	103	NAG	C8-C7-N2-C2
7	N	103	NAG	O7-C7-N2-C2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
7	O	103	NAG	C8-C7-N2-C2
7	O	103	NAG	O7-C7-N2-C2
7	P	103	NAG	C8-C7-N2-C2
7	P	103	NAG	O7-C7-N2-C2
7	L	102	NAG	C4-C5-C6-O6
7	I	102	NAG	C4-C5-C6-O6
7	O	103	NAG	C4-C5-C6-O6
3	D	601	FAD	C2'-C3'-C4'-O4'
6	L	101	MAN	O5-C5-C6-O6
3	D	601	FAD	O3'-C3'-C4'-C5'
3	C	601	FAD	C2'-C3'-C4'-O4'
4	O	105	CIT	C1-C2-C3-C6
5	P	101	T55	CAH-CAI-CAJ-CAK
5	P	101	T55	CAI-CAJ-CAK-CAL
3	B	601	FAD	O3'-C3'-C4'-C5'
4	O	105	CIT	C2-C3-C6-O6
3	B	601	FAD	C2'-C3'-C4'-C5'
3	B	601	FAD	O3'-C3'-C4'-O4'
3	C	601	FAD	O3'-C3'-C4'-O4'
7	O	103	NAG	O5-C5-C6-O6
3	B	601	FAD	C2'-C3'-C4'-O4'
5	P	101	T55	CAE-CAG-CAH-CAI
4	A	602	CIT	C1-C2-C3-O7
4	B	603	CIT	C1-C2-C3-O7
4	C	602	CIT	C1-C2-C3-O7
5	P	101	T55	CAF-CAE-CAG-CAH
3	C	601	FAD	C2'-C3'-C4'-C5'
3	D	601	FAD	C2'-C3'-C4'-C5'
3	A	601	FAD	O3'-C3'-C4'-C5'
4	B	603	CIT	C4-C3-C6-O5
4	B	603	CIT	C4-C3-C6-O6
4	C	602	CIT	C2-C3-C6-O5
4	C	602	CIT	C2-C3-C6-O6
4	C	602	CIT	C4-C3-C6-O5
4	C	602	CIT	C4-C3-C6-O6
4	C	602	CIT	C3-C4-C5-O3
3	A	601	FAD	C2'-C3'-C4'-C5'
3	A	601	FAD	O3'-C3'-C4'-O4'
4	O	105	CIT	C6-C3-C4-C5
6	O	102	MAN	C4-C5-C6-O6
4	C	602	CIT	C3-C4-C5-O4
5	P	101	T55	CAD-CAE-CAG-CAH

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	601	FAD	C2'-C3'-C4'-O4'
6	L	101	MAN	C4-C5-C6-O6
8	P	104	N1L	C4-C5-C6-O6B
4	B	603	CIT	C2-C3-C6-O5
4	B	603	CIT	C2-C3-C6-O6
4	D	602	CIT	C2-C3-C6-O5
4	D	602	CIT	C2-C3-C6-O6
4	D	602	CIT	C1-C2-C3-O7
7	M	103	NAG	C4-C5-C6-O6
6	O	102	MAN	O5-C5-C6-O6
5	O	101	T55	CAF-CAE-CAG-CAH
4	O	105	CIT	C3-C4-C5-O3
4	O	105	CIT	C3-C4-C5-O4
3	D	601	FAD	PA-O3P-P-O2P
4	D	602	CIT	C3-C4-C5-O3
8	K	104	N1L	O5-C5-C6-O6B
8	N	104	N1L	O5-C5-C6-O6A
8	P	104	N1L	O5-C5-C6-O6B
3	C	601	FAD	O3'-C3'-C4'-C5'
4	D	602	CIT	C3-C4-C5-O4

All (1) ring outliers are listed below:

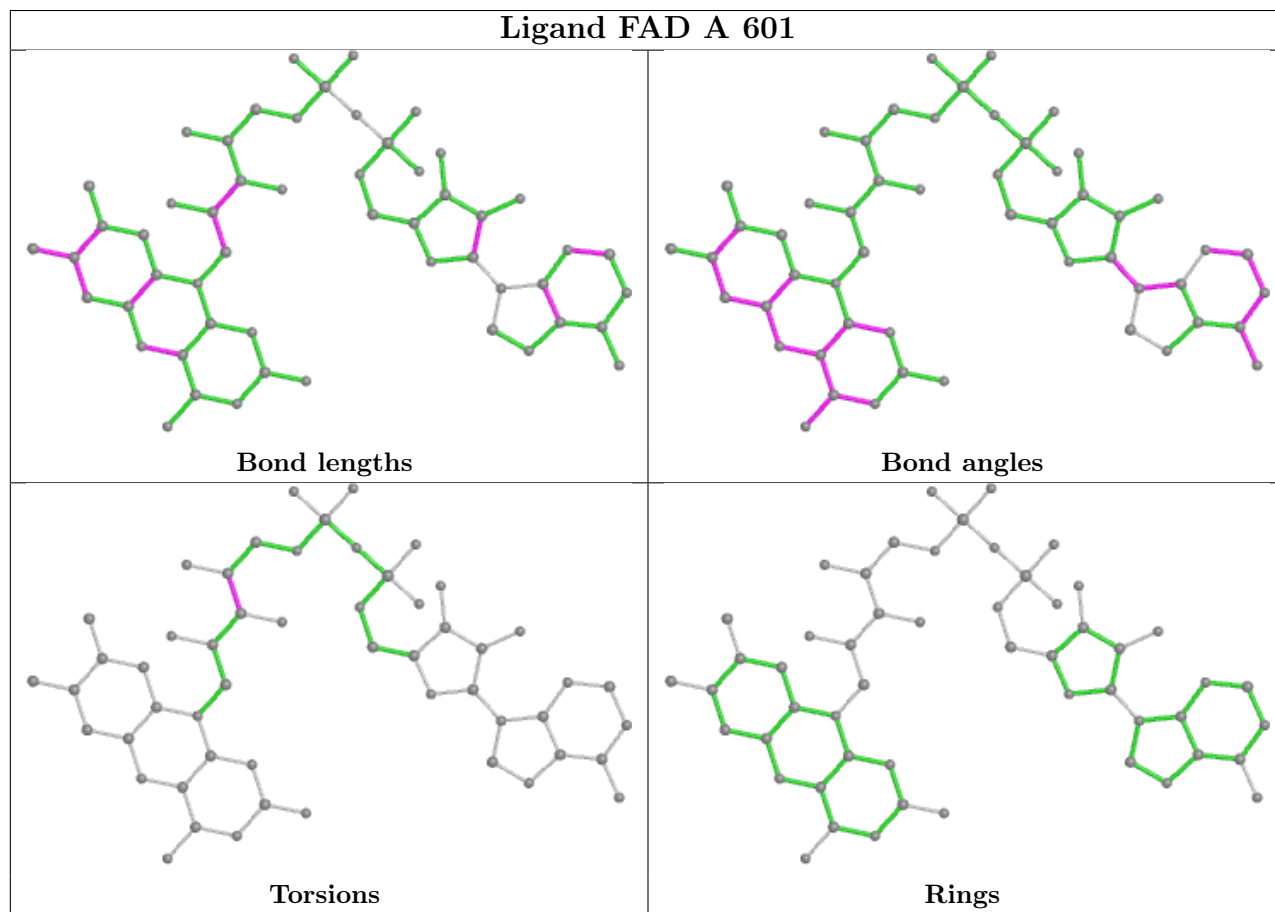
Mol	Chain	Res	Type	Atoms
6	M	102	MAN	C1-C2-C3-C4-C5-O5

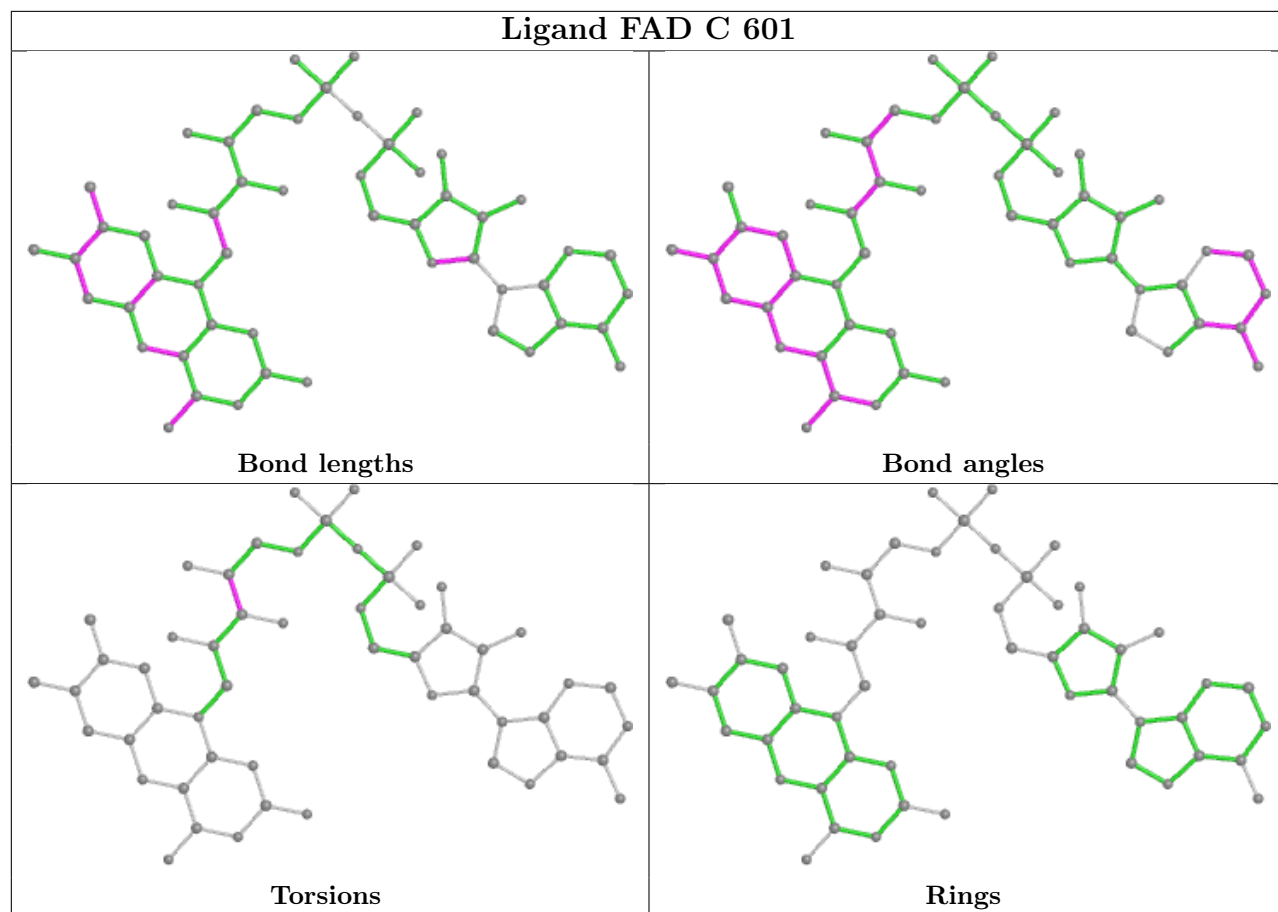
9 monomers are involved in 28 short contacts:

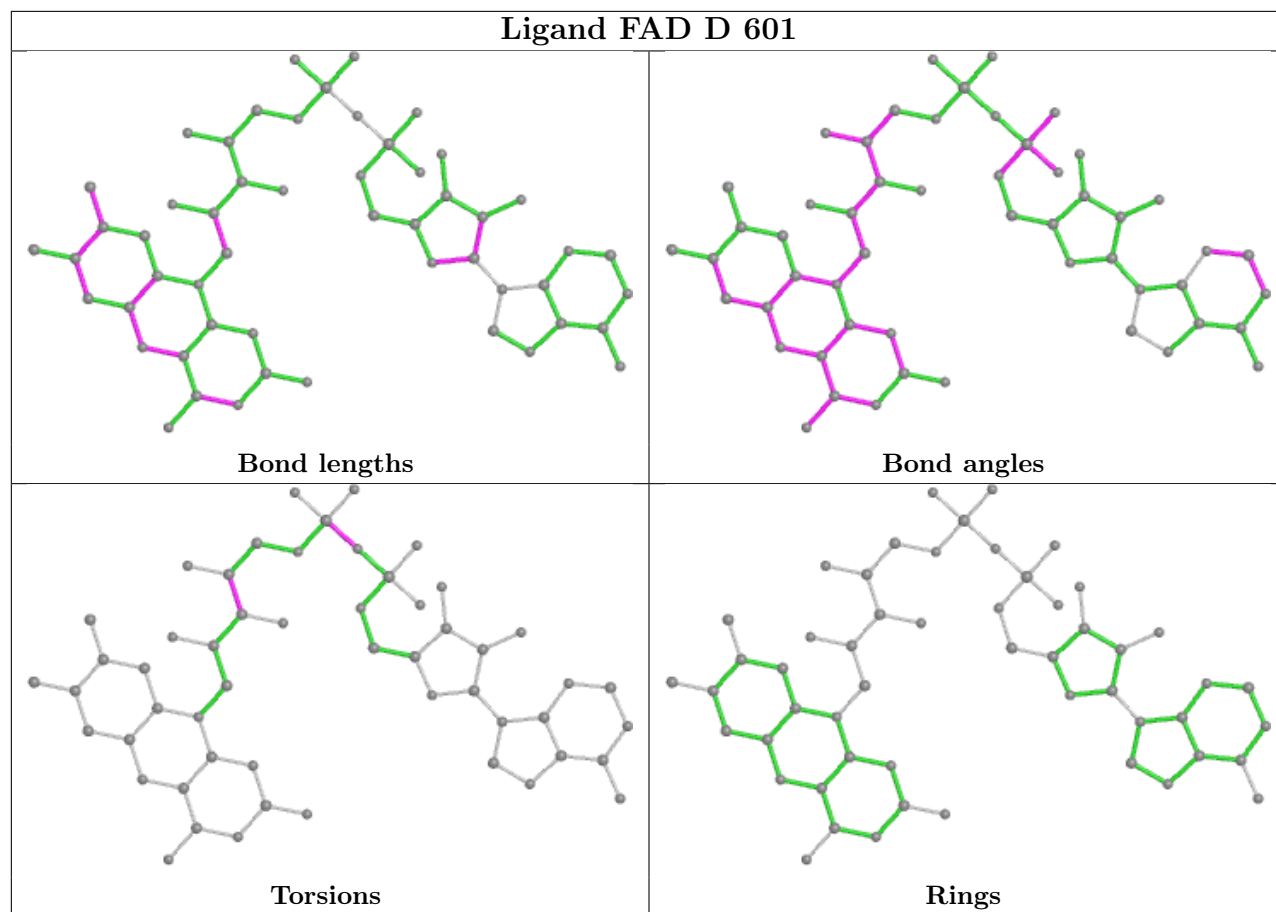
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	103	N1L	2	0
5	P	101	T55	0	1
5	M	101	T55	4	0
5	N	101	T55	14	0
7	L	102	NAG	3	0
8	K	104	N1L	1	0
5	B	602	T55	1	0
5	K	101	T55	1	0
8	M	104	N1L	1	0

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

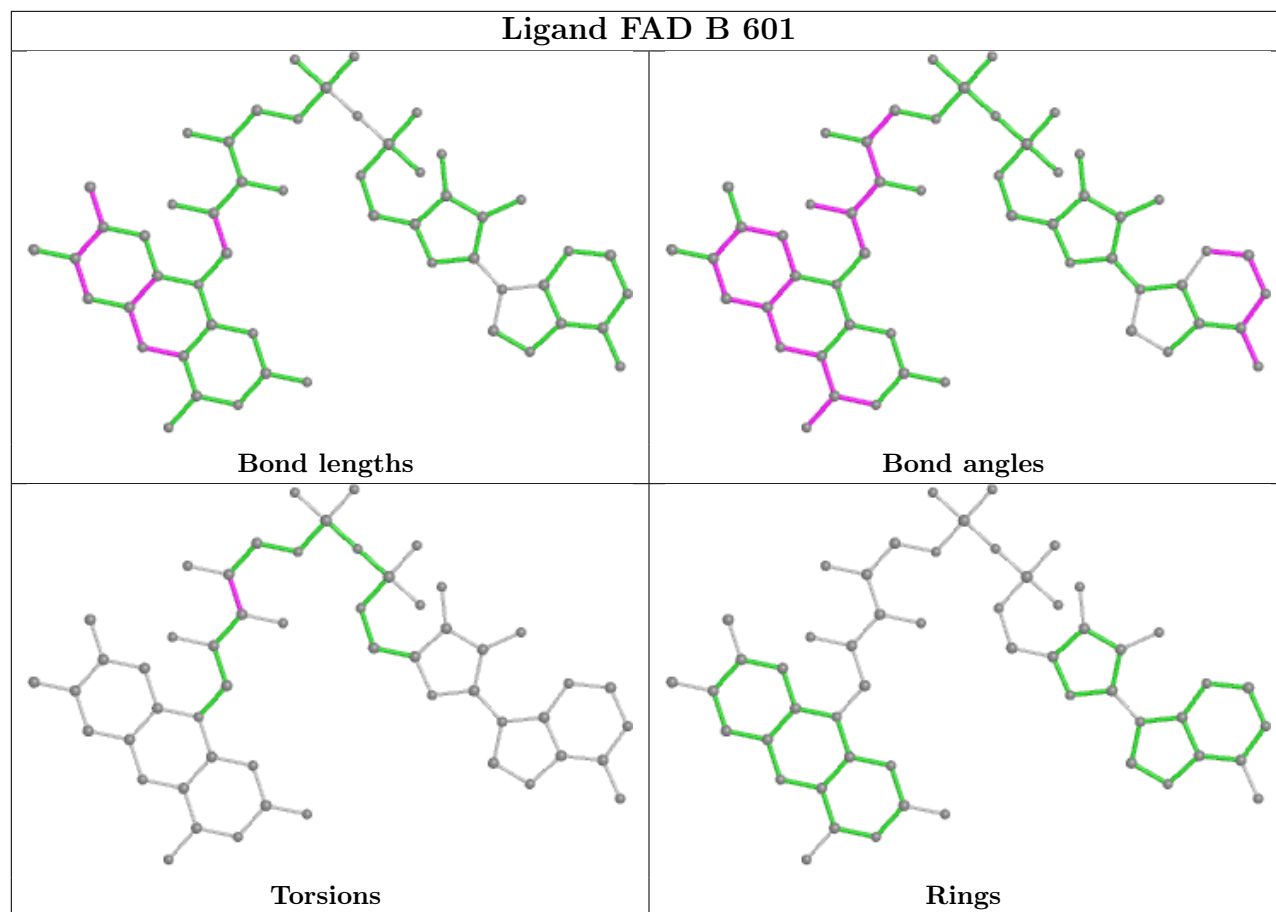
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.











## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	498/523 (95%)	-0.24	10 (2%) 65 71	12, 21, 42, 137	0
1	B	498/523 (95%)	-0.16	10 (2%) 65 71	14, 24, 48, 120	0
1	C	498/523 (95%)	-0.12	19 (3%) 40 48	17, 28, 52, 110	0
1	D	498/523 (95%)	0.28	35 (7%) 16 22	20, 39, 61, 109	0
2	I	0/7	-	-	-	-
2	J	0/7	-	-	-	-
2	K	0/7	-	-	-	-
2	L	0/7	-	-	-	-
2	M	0/7	-	-	-	-
2	N	0/7	-	-	-	-
2	O	0/7	-	-	-	-
2	P	0/7	-	-	-	-
All	All	1992/2148 (92%)	-0.06	74 (3%) 41 49	12, 27, 55, 137	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	GLY	9.2
1	D	357	ARG	8.3
1	D	302	PRO	8.3
1	B	356	GLY	7.3
1	D	356	GLY	6.8
1	A	357	ARG	6.3
1	C	355	PRO	6.3
1	B	357	ARG	6.3
1	D	355	PRO	6.0
1	D	303	GLY	5.9
1	D	304	MET	5.3
1	C	357	ARG	5.2
1	D	358	GLY	5.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	354	THR	5.0
1	D	26	CYS	4.9
1	C	302	PRO	4.6
1	D	301	VAL	4.5
1	A	356	GLY	4.5
1	D	359	GLY	4.2
1	B	354	THR	4.1
1	C	354	THR	4.1
1	C	359	GLY	4.1
1	A	302	PRO	4.1
1	C	356	GLY	4.0
1	D	305	GLY	4.0
1	D	433	ALA	4.0
1	A	355	PRO	3.8
1	D	378	ARG	3.8
1	D	202	ARG	3.7
1	B	302	PRO	3.7
1	D	434	ASN	3.6
1	D	436	GLY	3.6
1	C	303	GLY	3.5
1	B	26	CYS	3.4
1	B	303	GLY	3.4
1	C	26	CYS	3.2
1	D	482	GLY	3.2
1	A	26	CYS	3.1
1	D	457	GLY	3.1
1	D	487	GLY	3.1
1	D	435	PRO	3.1
1	B	305	GLY	3.0
1	C	358	GLY	2.9
1	B	355	PRO	2.9
1	C	119	SER	2.8
1	D	285	ASP	2.8
1	D	481	PRO	2.8
1	D	392	GLY	2.8
1	D	205	PRO	2.7
1	C	523	PRO	2.7
1	D	265	ALA	2.6
1	C	304	MET	2.6
1	A	354	THR	2.6
1	B	320	PRO	2.6
1	C	305	GLY	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	203	ASP	2.6
1	B	304	MET	2.5
1	D	523	PRO	2.5
1	A	436	GLY	2.5
1	C	481	PRO	2.4
1	A	303	GLY	2.4
1	D	471	ILE	2.4
1	D	400	LEU	2.4
1	C	297	ILE	2.4
1	D	353	SER	2.3
1	A	304	MET	2.3
1	D	194	ARG	2.3
1	C	38	ASP	2.3
1	D	488	VAL	2.2
1	C	202	ARG	2.2
1	C	434	ASN	2.2
1	D	437	ASN	2.1
1	C	86	VAL	2.0
1	D	189	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	3FG	L	7	13/13	0.10	0.70	101,144,162,174	0
2	3FG	M	7	13/13	0.15	0.79	116,143,162,171	0
2	GHP	M	5	11/12	0.34	0.62	112,143,167,185	0
2	GHP	K	5	11/12	0.41	0.54	108,137,152,169	0
2	3FG	K	7	13/13	0.42	0.70	107,144,168,176	0
2	3FG	I	7	13/13	0.51	0.43	69,100,119,129	0
2	OMY	K	6	14/15	0.54	0.36	91,123,147,148	0
2	GHP	L	5	11/12	0.55	0.49	102,132,149,172	0
2	GHP	M	1	11/12	0.57	0.46	80,89,97,99	0
2	OMY	M	6	14/15	0.62	0.42	88,128,160,170	0
2	GHP	I	1	11/12	0.63	0.48	102,108,111,117	0
2	GHP	I	5	11/12	0.70	0.32	58,76,103,104	0
2	GHP	K	4	11/12	0.70	0.15	60,66,78,85	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	OMY	L	6	14/15	0.72	0.31	84,114,150,151	0
2	GHP	M	4	11/12	0.74	0.21	59,80,94,105	0
2	3FG	I	3	12/13	0.75	0.36	53,89,99,104	0
2	GHP	J	4	11/12	0.75	0.28	40,55,61,63	0
2	GHP	K	1	11/12	0.75	0.18	50,59,70,71	0
2	GHP	L	4	11/12	0.75	0.12	54,66,75,78	0
2	GHP	L	1	11/12	0.76	0.25	54,62,72,72	0
2	3FG	L	3	12/13	0.79	0.25	66,75,83,87	0
2	OMY	I	6	14/15	0.80	0.36	57,70,75,79	0
2	OMY	J	6	14/15	0.80	0.33	52,66,72,85	0
2	3FG	M	3	12/13	0.80	0.25	69,77,84,85	0
2	3FG	J	7	13/13	0.81	0.31	40,50,56,59	0
2	3MY	M	2	13/14	0.81	0.23	74,77,97,132	0
2	3FG	O	7	13/13	0.81	0.26	40,45,52,54	0
2	3MY	K	2	13/14	0.83	0.16	50,56,66,112	0
2	3MY	I	2	13/14	0.84	0.35	49,83,94,99	0
2	3MY	J	2	13/14	0.84	0.34	44,55,65,77	0
2	3FG	K	3	12/13	0.85	0.19	58,72,78,80	0
2	GHP	J	1	11/12	0.85	0.24	44,49,51,52	0
2	GHP	I	4	11/12	0.86	0.21	41,50,55,55	0
2	3MY	L	2	13/14	0.87	0.16	52,62,72,104	0
2	GHP	J	5	11/12	0.88	0.25	45,50,56,60	0
2	3MY	O	2	13/14	0.90	0.22	29,33,35,43	0
2	GHP	P	1	11/12	0.90	0.18	32,34,38,38	0
2	3FG	J	3	12/13	0.90	0.29	43,50,53,66	0
2	GHP	P	5	11/12	0.91	0.12	26,31,40,41	0
2	3MY	N	2	13/14	0.91	0.20	25,33,40,58	0
2	OMY	O	6	14/15	0.91	0.23	34,40,48,56	0
2	GHP	O	5	11/12	0.92	0.17	27,34,40,40	0
2	OMY	P	6	14/15	0.92	0.13	30,39,40,68	0
2	3FG	N	7	13/13	0.93	0.27	34,41,47,51	0
2	3FG	P	7	13/13	0.93	0.17	35,42,47,50	0
2	GHP	O	4	11/12	0.94	0.14	25,30,32,33	0
2	3FG	O	3	12/13	0.94	0.16	27,31,32,36	0
2	GHP	N	5	11/12	0.94	0.21	29,32,36,38	0
2	3MY	P	2	13/14	0.94	0.21	28,31,35,46	0
2	GHP	O	1	11/12	0.94	0.15	28,31,36,37	0
2	GHP	N	1	11/12	0.95	0.21	25,30,33,34	0
2	OMY	N	6	14/15	0.95	0.22	32,36,39,60	0
2	GHP	N	4	11/12	0.95	0.16	25,29,36,40	0
2	3FG	P	3	12/13	0.95	0.20	31,38,40,42	0
2	3FG	N	3	12/13	0.96	0.20	28,31,34,34	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GHP	P	4	11/12	0.97	0.10	27,30,31,34	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

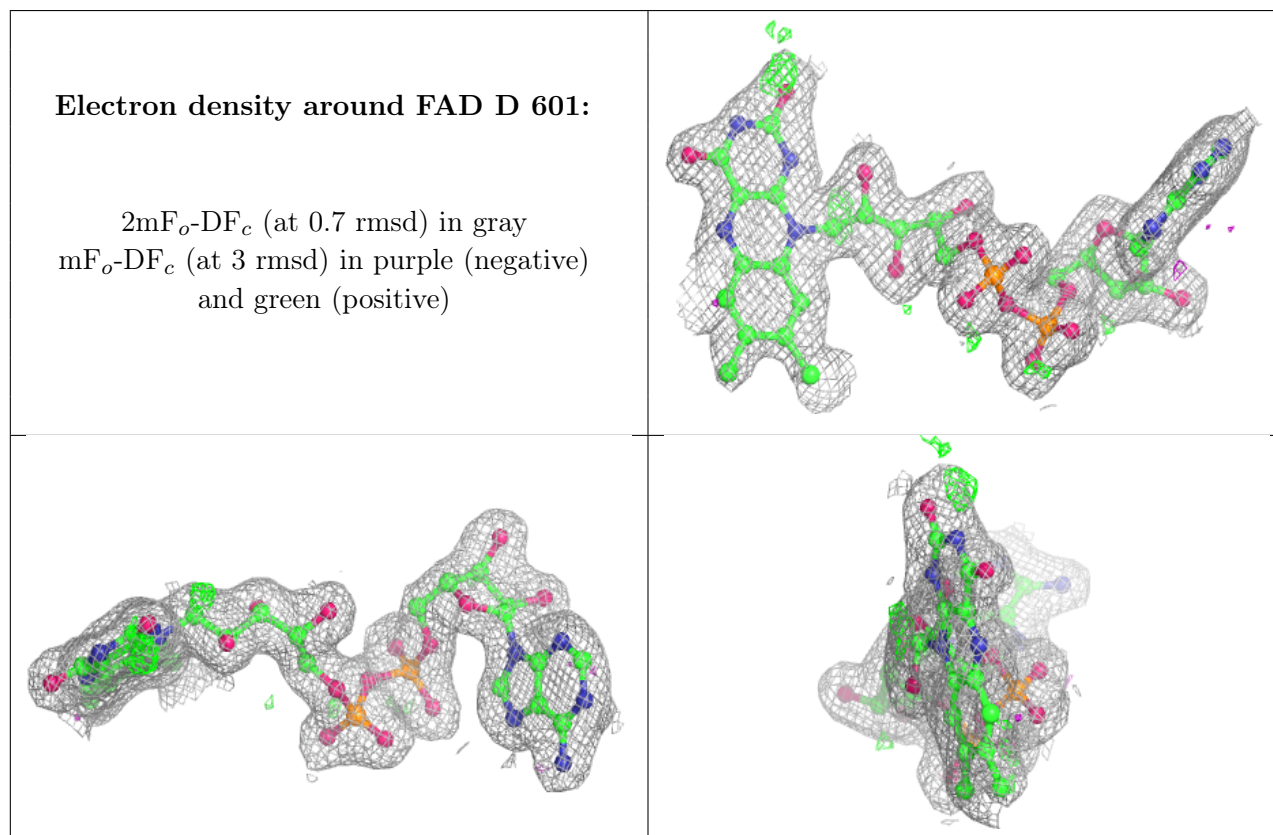
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MAN	I	101	11/12	0.09	1.04	103,132,139,141	0
6	MAN	K	102	11/12	0.43	0.76	136,145,157,161	0
7	NAG	K	103	14/15	0.44	0.77	107,133,142,154	0
7	NAG	M	103	14/15	0.47	0.92	108,139,149,151	0
6	MAN	M	102	11/12	0.50	0.72	112,144,153,160	0
6	MAN	L	101	11/12	0.56	0.73	128,153,162,166	0
7	NAG	I	102	14/15	0.56	0.49	71,83,106,107	0
7	NAG	J	102	14/15	0.63	0.42	81,93,113,114	0
5	T55	N	101	11/12	0.67	0.27	40,45,56,73	0
7	NAG	L	102	14/15	0.69	0.62	107,135,149,153	0
7	NAG	O	103	14/15	0.71	0.42	66,77,92,94	0
8	N1L	M	104	12/13	0.72	0.30	52,59,75,78	0
5	T55	M	101	11/12	0.73	0.39	53,56,87,94	0
5	T55	P	101	11/12	0.75	0.36	33,41,78,79	0
5	T55	B	602	11/12	0.75	0.43	48,50,65,72	0
5	T55	O	101	11/12	0.76	0.52	43,51,75,78	0
8	N1L	L	103	12/13	0.78	0.24	40,54,66,66	0
5	T55	K	101	11/12	0.78	0.30	51,56,62,71	0
6	MAN	J	101	11/12	0.79	0.27	52,62,67,77	0
8	N1L	K	104	12/13	0.83	0.20	36,56,70,73	0
4	CIT	A	602	13/13	0.85	0.19	37,46,55,59	0
7	NAG	P	103	14/15	0.86	0.16	40,45,48,54	0
4	CIT	O	105	13/13	0.88	0.21	31,40,50,51	0
4	CIT	B	603	13/13	0.88	0.20	38,56,71,78	0
8	N1L	N	104	12/13	0.88	0.30	40,42,50,50	0
8	N1L	O	104	12/13	0.88	0.24	33,40,48,55	0

Continued on next page...

Continued from previous page...

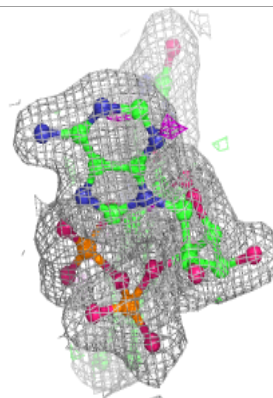
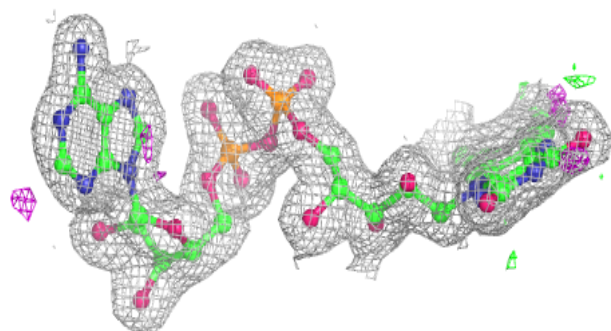
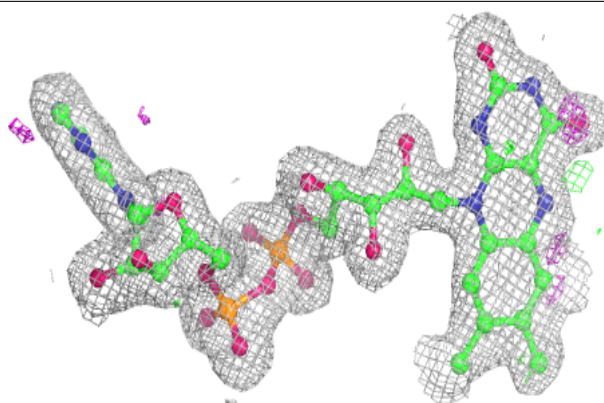
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CIT	C	602	13/13	0.91	0.27	45,55,62,67	0
6	MAN	N	102	11/12	0.92	0.21	38,45,53,54	0
6	MAN	O	102	11/12	0.92	0.10	34,40,45,49	0
6	MAN	P	102	11/12	0.92	0.20	28,39,50,57	0
4	CIT	D	602	13/13	0.93	0.23	39,43,51,54	0
8	N1L	P	104	12/13	0.93	0.22	29,32,37,51	0
7	NAG	N	103	14/15	0.94	0.15	30,40,45,48	0
3	FAD	D	601	53/53	0.97	0.11	20,26,38,43	0
3	FAD	C	601	53/53	0.97	0.13	19,22,28,32	0
3	FAD	B	601	53/53	0.98	0.10	10,14,24,29	0
3	FAD	A	601	53/53	0.99	0.10	11,15,22,26	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.

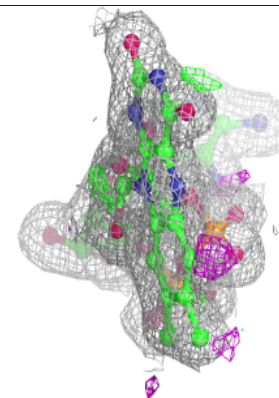
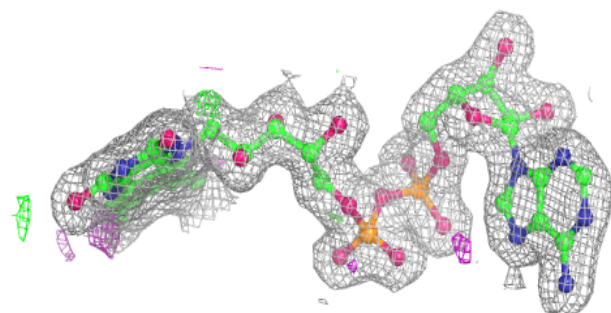
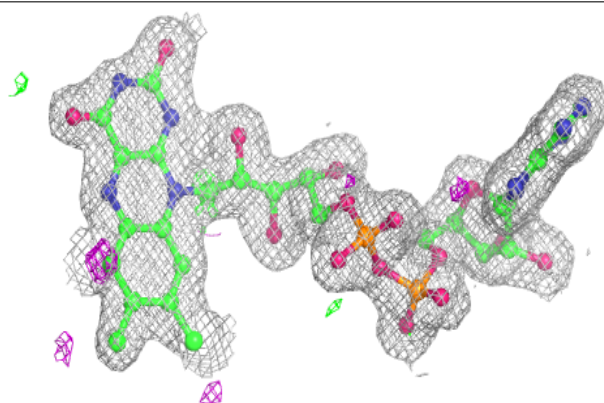


**Electron density around FAD C 601:**

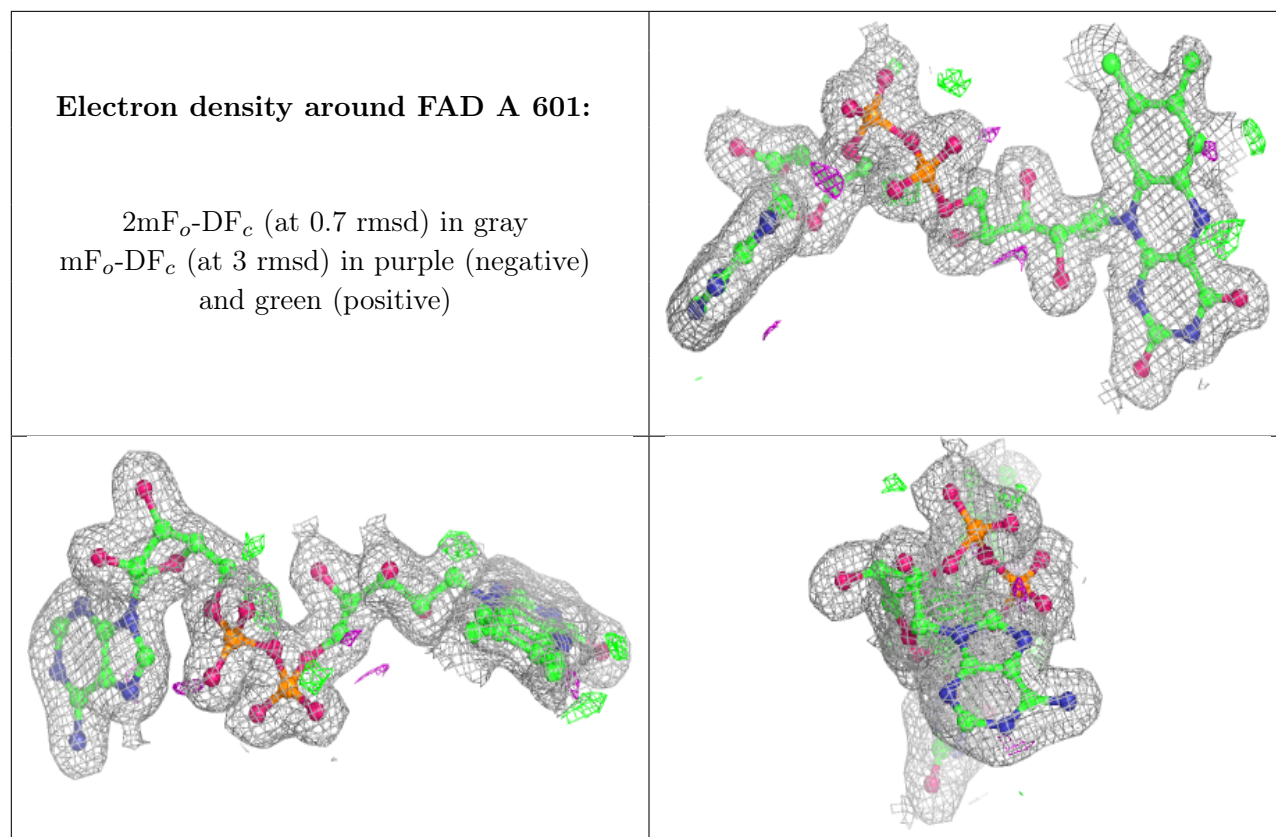
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around FAD B 601:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.