wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 09:21 AM EDT

PDB ID	:	6MJA
Title	:	Crystal structure of the mCD1d/xxo (JJ294) /iNKTCR ternary complex
Authors	:	Zajonc, D.M.; Bitra, A.; Janssens, J.
Deposited on	:	2018-09-20
Resolution	:	2.35 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.35 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 6950 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 T cell receptor alpha variable 11,T cell receptor alpha variable 11,T cell receptor alpha joining 18,Human nkt tcr alpha chain, CHIMERIC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	200	1546	959	265	314	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP A0A0B4J1J9
C	113	ILE	-	linker	UNP A0A0B4J1J9

- Molecule 2 is a protein called Beta-chain,T cell receptor chain,T cell receptor beta constant 2, CHIMERIC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	240	1888	1184	336	362	6	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	95	ASP	-	linker	UNP A2NTY6
D	96	GLU	-	linker	UNP A2NTY6
D	97	GLY	-	linker	UNP A2NTY6
D	98	TYR	-	linker	UNP A2NTY6
D	130	ALA	ALA	linker	UNP A0N8J3
D	168	CYS	SER	variant	UNP A0A5B9
D	186	SER	CYS	variant	UNP A0A5B9

- Molecule 3 is a protein called Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	269	2146	1372	365	396	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	HIS	-	expression tag	UNP A0A0R4J090
A	281	HIS	-	expression tag	UNP A0A0R4J090
A	282	HIS	-	expression tag	UNP A0A0R4J090
A	283	HIS	-	expression tag	UNP A0A0R4J090
A	284	HIS	-	expression tag	UNP A0A0R4J090
A	285	HIS	-	expression tag	UNP A0A0R4J090

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	98	802	513	137	146	6	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	2	28	16	2	10	0	0	0

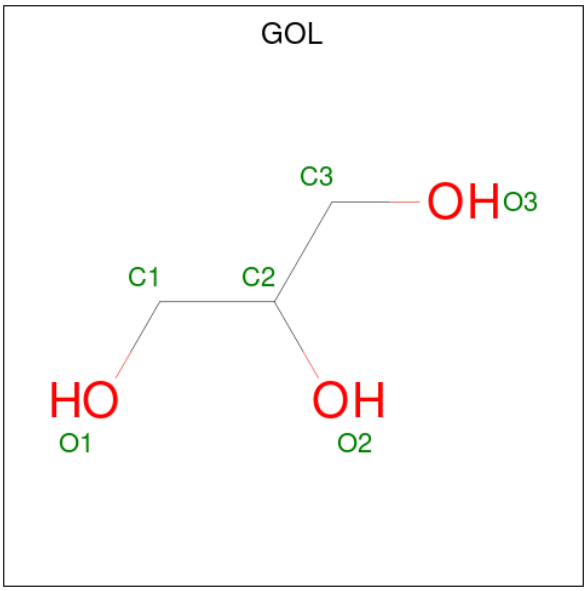
- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	F	4	49	28	2	19	0	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

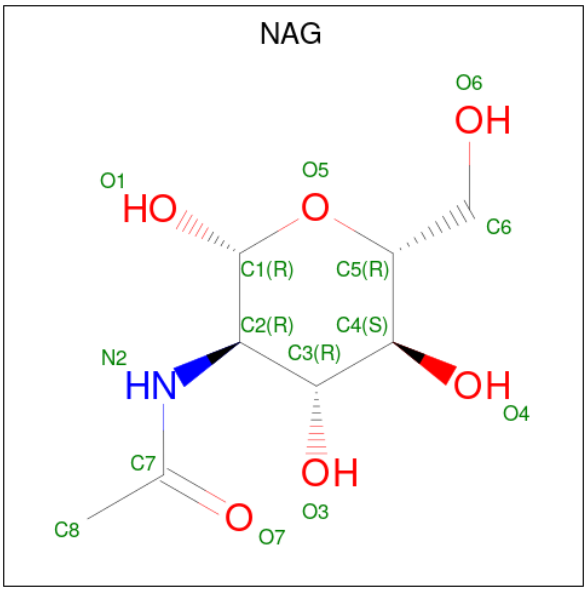
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
7	C	1	1	1	0	0
7	A	1	1	1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



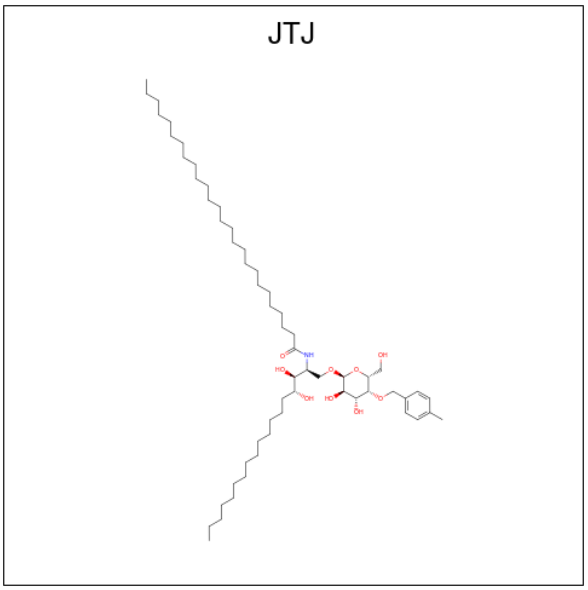
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	C	1	6	3	3	0	0
			Total	C	O		
8	D	1	6	3	3	0	0
			Total	C	O		
8	D	1	6	3	3	0	0

- Molecule 9 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		
9	A	1	14	8	1	5	0	0

- Molecule 10 is N-[(2S,3S,4R)-3,4-dihydroxy-1-({4-O-[(4-methylphenyl)methyl]-alpha-D-galactopyranosyl}oxy)octadecan-2-yl]hexacosanamide (three-letter code: JTJ) (formula: $C_{58}H_{107}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	A	1	68	58	1	9	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	C	91	91	91	0	0
11	D	140	Total 140	O 140	0	0
11	A	111	Total 111	O 111	0	0
11	B	47	Total 47	O 47	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	79.04Å 191.49Å 151.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.68 – 2.35	Depositor
% Data completeness (in resolution range)	99.6 (45.68-2.35)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.196 , 0.237	Depositor
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.066	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6950	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates (i)

6 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	$\#\|Z\| > 2$
5	NAG	E	1	3,5	14,14,15	0.44	0	17,19,21	0.87	1 (5%)
5	NAG	E	2	5	14,14,15	0.41	0	17,19,21	1.03	1 (5%)
6	NAG	F	1	6,3	14,14,15	0.40	0	17,19,21	0.70	0
6	NAG	F	2	6	14,14,15	0.38	0	17,19,21	0.86	1 (5%)
6	BMA	F	3	6	11,11,12	0.47	0	15,15,17	0.85	0
6	FUC	F	4	6	10,10,11	0.56	0	14,14,16	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1	3,5	-	1/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
6	NAG	F	1	6,3	-	1/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	BMA	F	3	6	-	2/2/19/22	0/1/1/1
6	FUC	F	4	6	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	2	NAG	C4-C3-C2	3.36	115.95	111.02
6	F	2	NAG	C1-O5-C5	2.89	116.10	112.19
5	E	1	NAG	C1-O5-C5	2.30	115.30	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

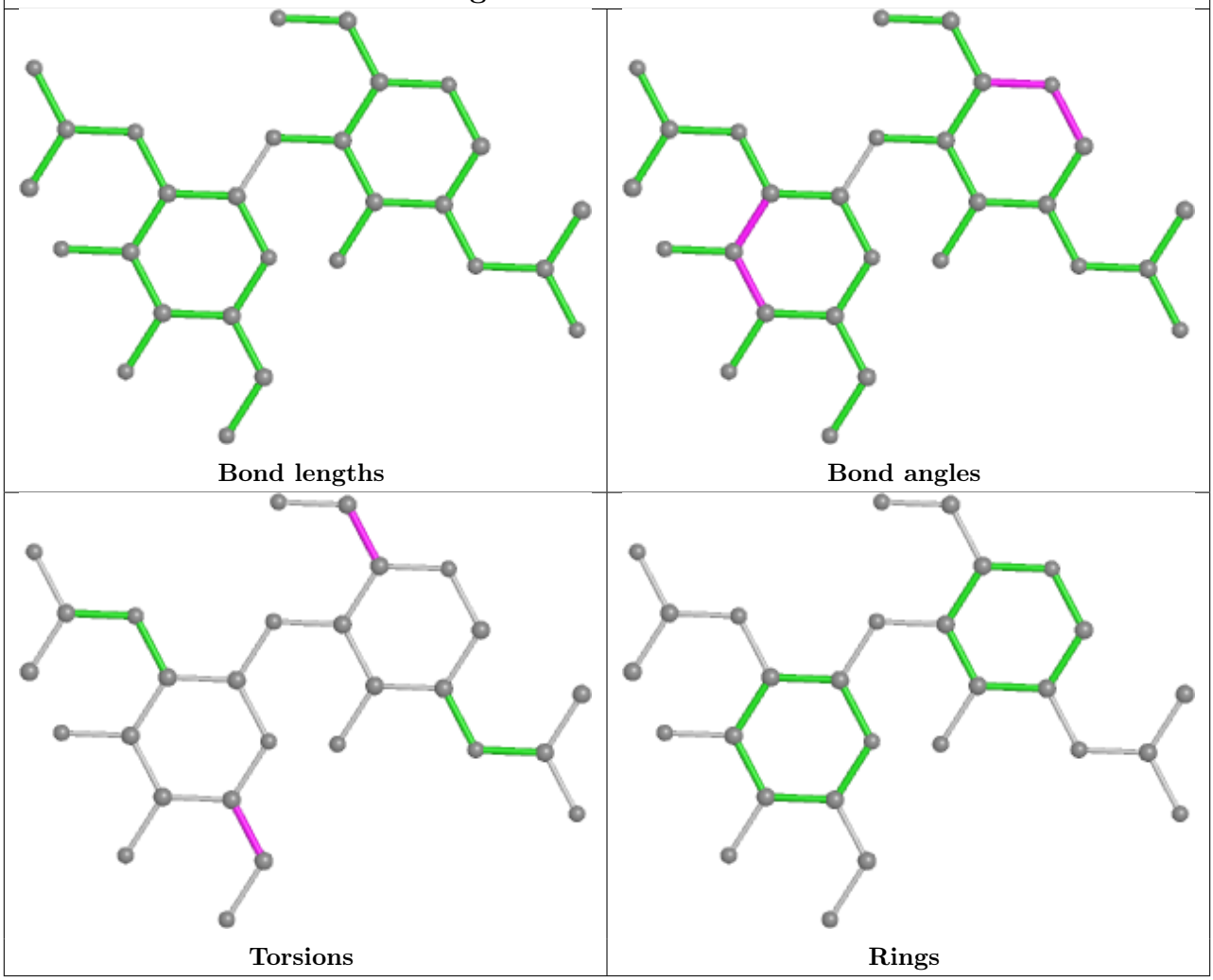
Mol	Chain	Res	Type	Atoms
6	F	3	BMA	C4-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
6	F	3	BMA	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

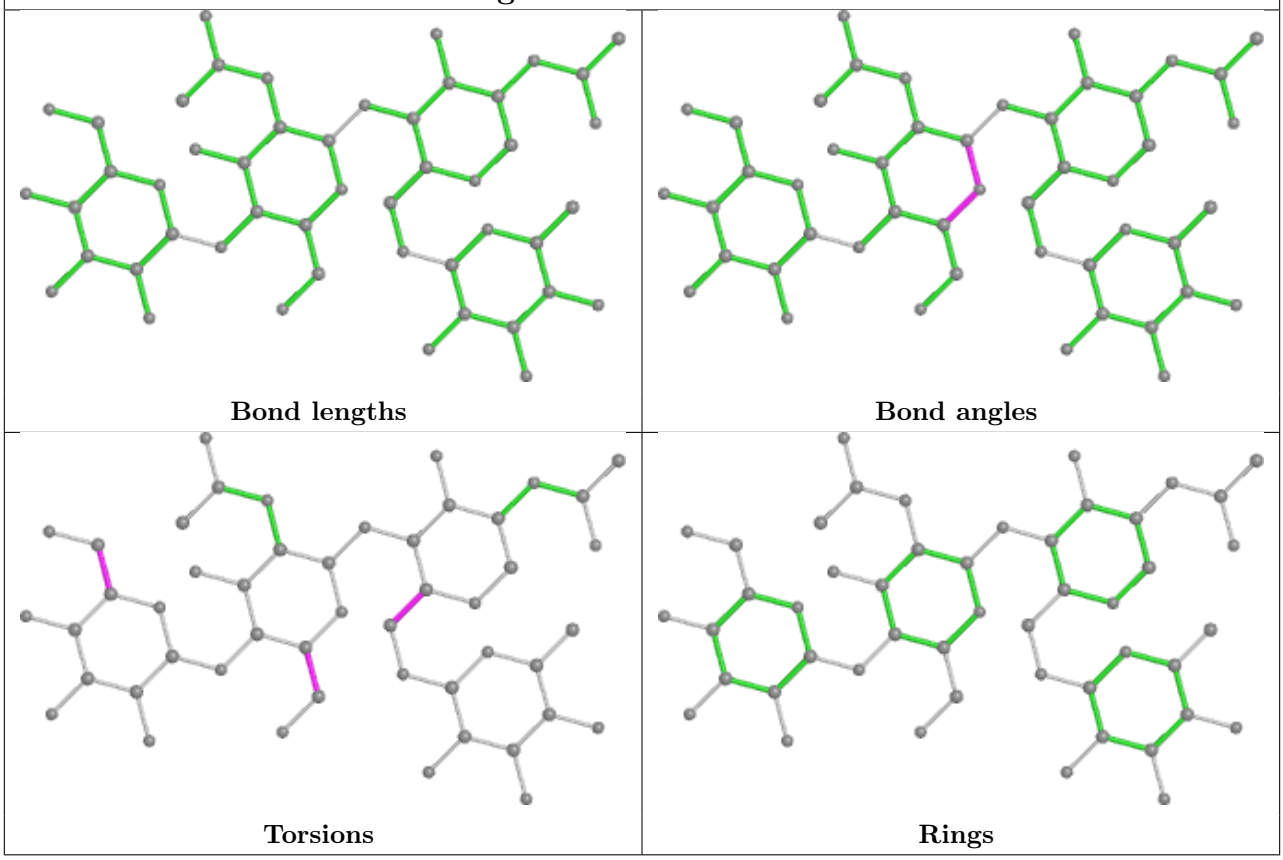
No monomer is involved in short contacts.

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

Oligosaccharide Chain E



Oligosaccharide Chain F



4.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
8	GOL	C	302	-	5,5,5	0.29	0	5,5,5	0.24	0
8	GOL	D	602	-	5,5,5	0.29	0	5,5,5	0.23	0
10	JTJ	A	308	-	69,69,69	0.88	2 (2%)	77,81,81	0.87	2 (2%)
8	GOL	D	601	-	5,5,5	0.34	0	5,5,5	0.41	0
9	NAG	A	301	3	14,14,15	0.56	0	17,19,21	1.35	2 (11%)

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
8	GOL	C	302	-	-	0/4/4/4	-
8	GOL	D	602	-	-	2/4/4/4	-
10	JTJ	A	308	-	-	18/63/83/83	0/2/2/2
8	GOL	D	601	-	-	3/4/4/4	-
9	NAG	A	301	3	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	308	JTJ	CAT-CAU	-4.42	1.40	1.50
10	A	308	JTJ	CBA-CAX	-3.18	1.39	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	301	NAG	C4-C3-C2	3.92	116.77	111.02
9	A	301	NAG	C1-O5-C5	2.29	115.30	112.19
10	A	308	JTJ	CAM-CAN-CAP	-2.08	108.61	112.71
10	A	308	JTJ	O4-CAT-CAU	2.05	114.64	109.91

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	601	GOL	O1-C1-C2-C3
9	A	301	NAG	C8-C7-N2-C2
9	A	301	NAG	O7-C7-N2-C2
10	A	308	JTJ	OAR-CAQ-CBG-CBH
10	A	308	JTJ	O6-C2-C3-O2

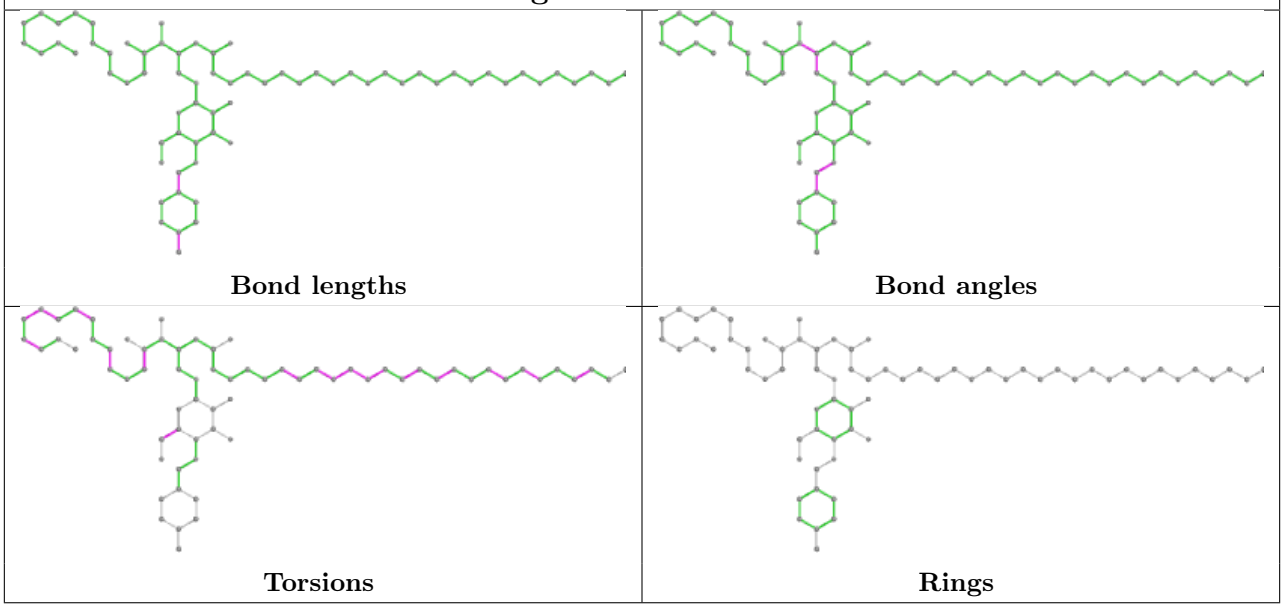
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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 JTJ A 308



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.