W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 08:10 AM EDT

PDB ID	:	6MJJ
Title	:	Crystal structure of the mCD1d/xxm (JJ290) /iNKTCR ternary complex
Authors	:	Zajonc, D.M.; Bitra, A.; Janssens, J.
Deposited on	:	2018-09-21
Resolution	:	1.93 Å(reported)

The following versions of software and data (see references ⓘ) 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 ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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 ⓘ

There are 11 unique types of molecules in this entry. The entry contains 7333 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
1	C	201	Total	C	N	O	S	0	4	0
			1563	973	268	314	8			

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,Tcell receptor chain,T cell receptor beta constant 2, CHIMERIC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	239	Total	C	N	O	S	0	1	0
			1870	1174	331	359	6			

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
3	A	273	Total 2201	C 1404	N 376	O 408	S 13	0	4	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
4	B	97	Total 779	C 497	N 131	O 144	S 7	0	1	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
5	E	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 6 is an oligosaccharide called 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
6	F	3	Total 38	C 22	N 2	O 14	0	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total 6	C 3	O 3	0	0
7	C	1	Total 6	C 3	O 3	0	0
7	C	1	Total 6	C 3	O 3	0	0
7	C	1	Total 6	C 3	O 3	0	0
7	C	1	Total 6	C 3	O 3	0	0
7	D	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	5	Total 5	Na 5	0	0
8	D	3	Total 3	Na 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total Na 1 1		0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
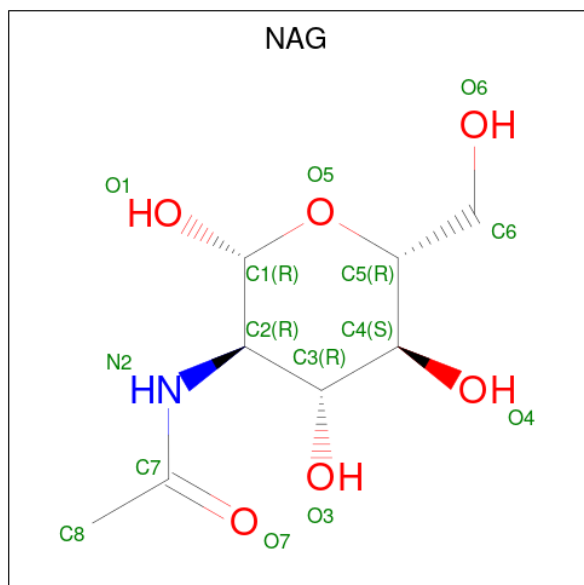
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total C N O 14 8 1 5				0	0

- Molecule 10 is N-[(2S,3S,4R)-1-({4-O-[(3,4-dichlorophenyl)methyl]-alpha-D-galactopyran osyl}oxy)-3,4-dihydroxyoctadecan-2-yl]hexacosanamide (three-letter code: JU4) (formula: $C_{57}H_{103}Cl_2NO_9$).
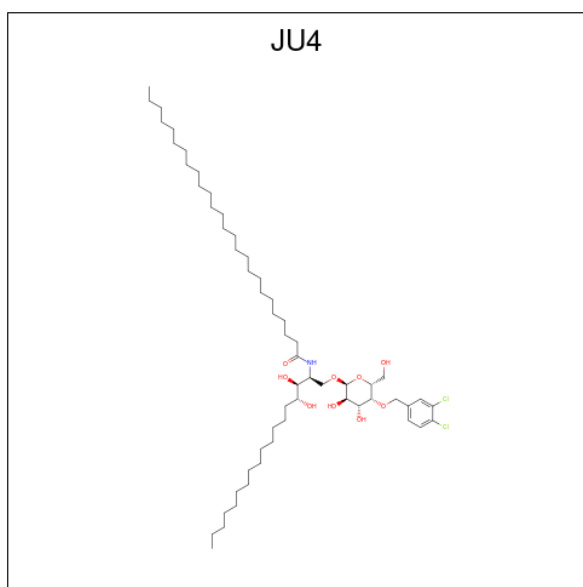
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	Cl	N	O	0	0
			69	57	2	1	9		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	156	Total	O	0	0
			156	156		
11	D	254	Total	O	0	0
			254	254		
11	A	215	Total	O	0	0
			215	215		
11	B	77	Total	O	0	0
			77	77		

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

3 Data and refinement statistics ⓘ

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	79.00Å 191.28Å 151.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.87 – 1.93	Depositor
% Data completeness (in resolution range)	99.7 (47.87-1.93)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.01 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.184 , 0.216	Depositor
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.010	Xtriage
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7333	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

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

4.2 Too-close contacts ⓘ

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

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

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

4.3.2 Protein sidechains ⓘ

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

4.3.3 RNA ⓘ

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

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

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

4.5 Carbohydrates ⓘ

5 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	0.36	0	17,19,21	0.63	0
5	NAG	E	2	5	14,14,15	0.29	0	17,19,21	0.65	0
6	NAG	F	1	3,6	14,14,15	0.24	0	17,19,21	0.97	1 (5%)
6	NAG	F	2	6	14,14,15	0.26	0	17,19,21	0.82	1 (5%)
6	FUC	F	3	6	10,10,11	0.47	0	14,14,16	0.62	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	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	1/6/23/26	0/1/1/1
6	FUC	F	3	6	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	1	NAG	O5-C5-C6	3.04	111.96	107.20
6	F	2	NAG	C1-O5-C5	2.36	115.38	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
6	F	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

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths | Bond angles

Torsions | Rings
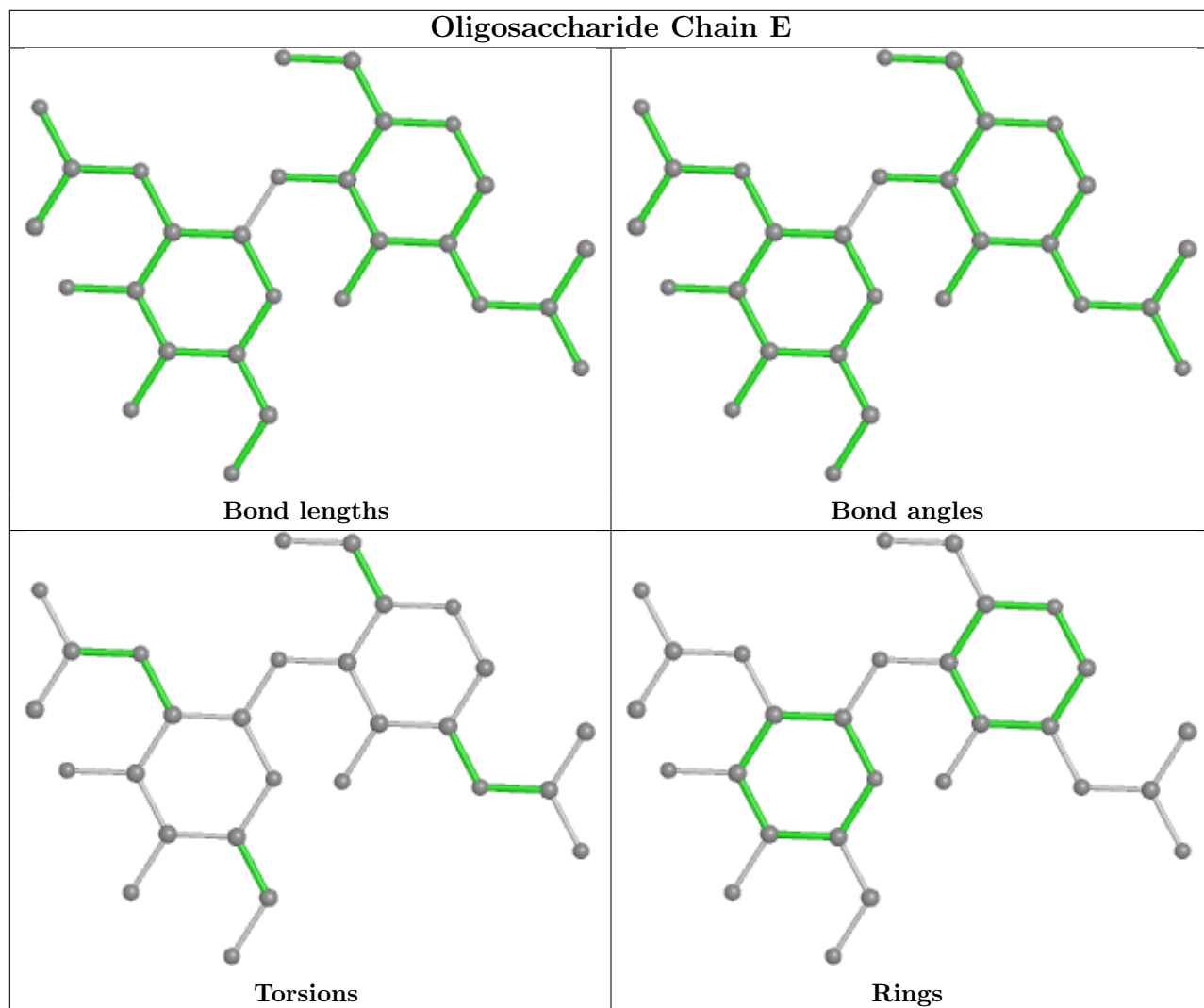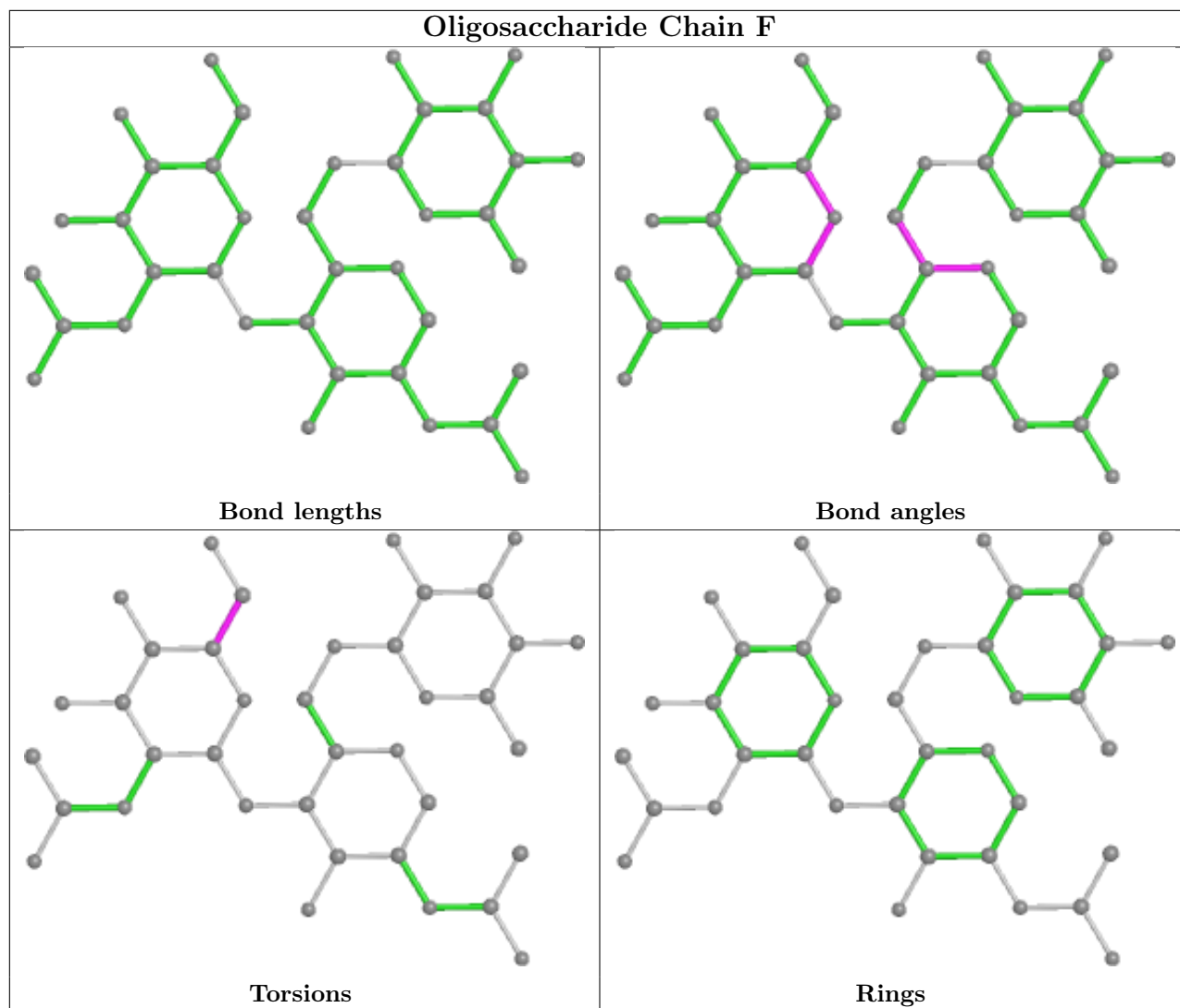
4.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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	#$|Z| > 2$
7	GOL	C	604	-	5,5,5	0.33	0	5,5,5	0.15	0
7	GOL	B	101	-	5,5,5	0.41	0	5,5,5	0.42	0
7	GOL	B	102	-	5,5,5	0.29	0	5,5,5	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
7	GOL	C	602	-	5,5,5	0.38	0	5,5,5	0.65	0
7	GOL	C	601	-	5,5,5	0.31	0	5,5,5	0.19	0
7	GOL	C	609	8	5,5,5	0.31	0	5,5,5	0.18	0
7	GOL	D	301	-	5,5,5	0.38	0	5,5,5	0.27	0
7	GOL	B	103	-	5,5,5	0.33	0	5,5,5	0.36	0
9	NAG	A	304	3	14,14,15	0.41	0	17,19,21	0.92	0
7	GOL	C	603	-	5,5,5	0.43	0	5,5,5	0.41	0
10	JU4	A	308	-	70,70,70	0.77	1 (1%)	79,83,83	0.84	0
7	GOL	A	301	-	5,5,5	0.34	0	5,5,5	0.18	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
7	GOL	C	604	-	-	2/4/4/4	-
7	GOL	B	101	-	-	2/4/4/4	-
7	GOL	B	102	-	-	3/4/4/4	-
7	GOL	C	602	-	-	1/4/4/4	-
7	GOL	C	601	-	-	2/4/4/4	-
7	GOL	C	609	8	-	0/4/4/4	-
7	GOL	D	301	-	-	3/4/4/4	-
7	GOL	B	103	-	-	4/4/4/4	-
9	NAG	A	304	3	-	0/6/23/26	0/1/1/1
7	GOL	C	603	-	-	3/4/4/4	-
10	JU4	A	308	-	-	11/63/83/83	0/2/2/2
7	GOL	A	301	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	308	JU4	CAT-CAU	-4.36	1.40	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	601	GOL	C1-C2-C3-O3
7	C	603	GOL	C1-C2-C3-O3
7	C	604	GOL	O1-C1-C2-C3
7	B	101	GOL	O1-C1-C2-C3
7	B	102	GOL	C1-C2-C3-O3
7	B	103	GOL	O1-C1-C2-C3
7	B	103	GOL	C1-C2-C3-O3
7	C	603	GOL	O2-C2-C3-O3
10	A	308	JU4	CCG-CCH-CCI-CCJ
10	A	308	JU4	CCK-CCL-CCM-CCN
7	D	301	GOL	O1-C1-C2-C3
10	A	308	JU4	CBZ-CCA-CCB-CCC
10	A	308	JU4	CCD-CCE-CCF-CCG
10	A	308	JU4	CBP-CBQ-CBR-CBS
7	B	103	GOL	O2-C2-C3-O3
10	A	308	JU4	O6-C2-C3-O2
10	A	308	JU4	CCN-CCO-CCP-CCQ
7	C	601	GOL	O2-C2-C3-O3
7	C	604	GOL	O1-C1-C2-O2
7	B	101	GOL	O1-C1-C2-O2
7	B	102	GOL	O2-C2-C3-O3
10	A	308	JU4	CCL-CCM-CCN-CCO
7	C	603	GOL	O1-C1-C2-C3
7	C	602	GOL	O2-C2-C3-O3
7	D	301	GOL	C1-C2-C3-O3
7	B	103	GOL	O1-C1-C2-O2
10	A	308	JU4	CBK-CBL-CBM-CBN
7	B	102	GOL	O1-C1-C2-C3
10	A	308	JU4	CBX-CBY-CBZ-CCA
7	D	301	GOL	O2-C2-C3-O3
10	A	308	JU4	CCC-CCD-CCE-CCF
7	A	301	GOL	C1-C2-C3-O3

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 JU4 A 308

Bond lengths | Bond angles

Torsions | Rings
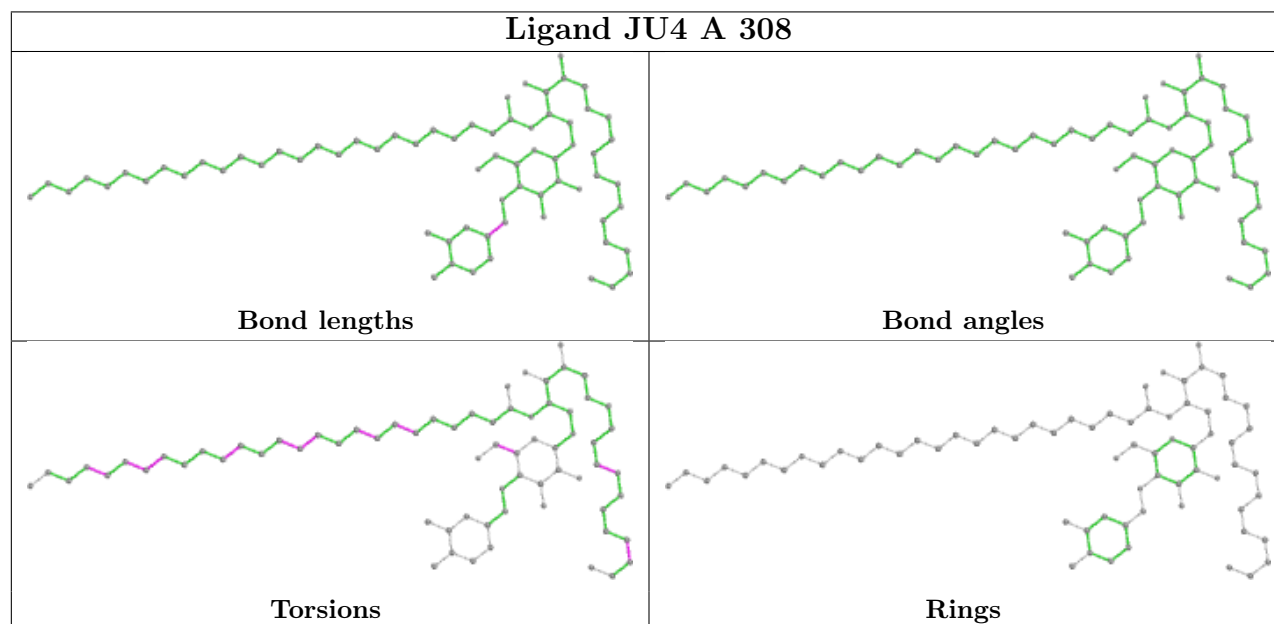
4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

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

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

5.3 Carbohydrates ⓘ

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

5.4 Ligands ⓘ

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

5.5 Other polymers ⓘ

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