



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 04:44 PM EDT

PDB ID : 3OPM
Title : Crystal Structure of Human DPP4 Bound to TAK-294
Authors : Yano, J.K.; Aertgeerts, K.
Deposited on : 2010-09-01
Resolution : 2.72 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

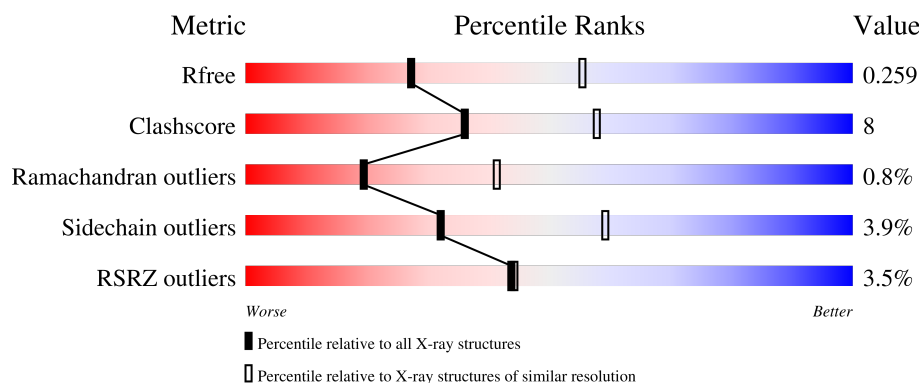
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	740	 3% 79% 18% ..
1	B	740	 2% 79% 19% ..
1	C	740	 5% 76% 20% ..
1	D	740	 4% 82% 16% .
2	E	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24713 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5950	3821	977	1126	26			
1	B	733	Total	C	N	O	S	0	0	0
			6013	3857	997	1133	26			
1	C	725	Total	C	N	O	S	0	0	0
			5937	3810	979	1122	26			
1	D	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	expression tag	UNP P27487
A	28	ASP	-	expression tag	UNP P27487
A	29	PRO	-	expression tag	UNP P27487
A	30	GLY	-	expression tag	UNP P27487
A	31	GLY	-	expression tag	UNP P27487
A	32	SER	-	expression tag	UNP P27487
A	33	HIS	-	expression tag	UNP P27487
A	34	HIS	-	expression tag	UNP P27487
A	35	HIS	-	expression tag	UNP P27487
A	36	HIS	-	expression tag	UNP P27487
A	37	HIS	-	expression tag	UNP P27487
A	38	HIS	-	expression tag	UNP P27487
B	27	ALA	-	expression tag	UNP P27487
B	28	ASP	-	expression tag	UNP P27487
B	29	PRO	-	expression tag	UNP P27487
B	30	GLY	-	expression tag	UNP P27487
B	31	GLY	-	expression tag	UNP P27487
B	32	SER	-	expression tag	UNP P27487
B	33	HIS	-	expression tag	UNP P27487
B	34	HIS	-	expression tag	UNP P27487
B	35	HIS	-	expression tag	UNP P27487

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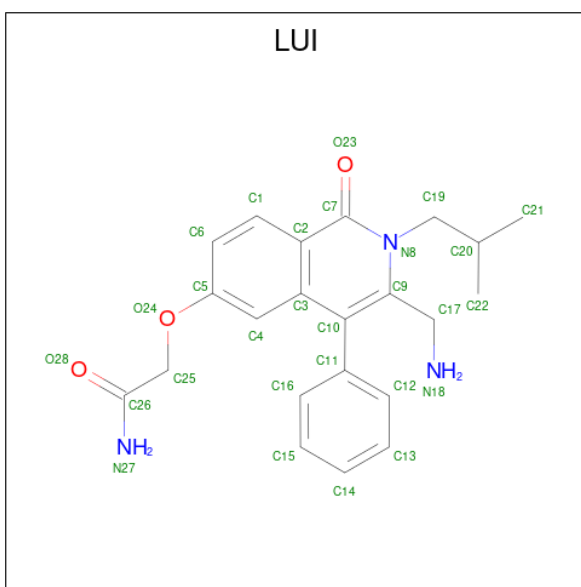
Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	expression tag	UNP P27487
B	37	HIS	-	expression tag	UNP P27487
B	38	HIS	-	expression tag	UNP P27487
C	27	ALA	-	expression tag	UNP P27487
C	28	ASP	-	expression tag	UNP P27487
C	29	PRO	-	expression tag	UNP P27487
C	30	GLY	-	expression tag	UNP P27487
C	31	GLY	-	expression tag	UNP P27487
C	32	SER	-	expression tag	UNP P27487
C	33	HIS	-	expression tag	UNP P27487
C	34	HIS	-	expression tag	UNP P27487
C	35	HIS	-	expression tag	UNP P27487
C	36	HIS	-	expression tag	UNP P27487
C	37	HIS	-	expression tag	UNP P27487
C	38	HIS	-	expression tag	UNP P27487
D	27	ALA	-	expression tag	UNP P27487
D	28	ASP	-	expression tag	UNP P27487
D	29	PRO	-	expression tag	UNP P27487
D	30	GLY	-	expression tag	UNP P27487
D	31	GLY	-	expression tag	UNP P27487
D	32	SER	-	expression tag	UNP P27487
D	33	HIS	-	expression tag	UNP P27487
D	34	HIS	-	expression tag	UNP P27487
D	35	HIS	-	expression tag	UNP P27487
D	36	HIS	-	expression tag	UNP P27487
D	37	HIS	-	expression tag	UNP P27487
D	38	HIS	-	expression tag	UNP P27487

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



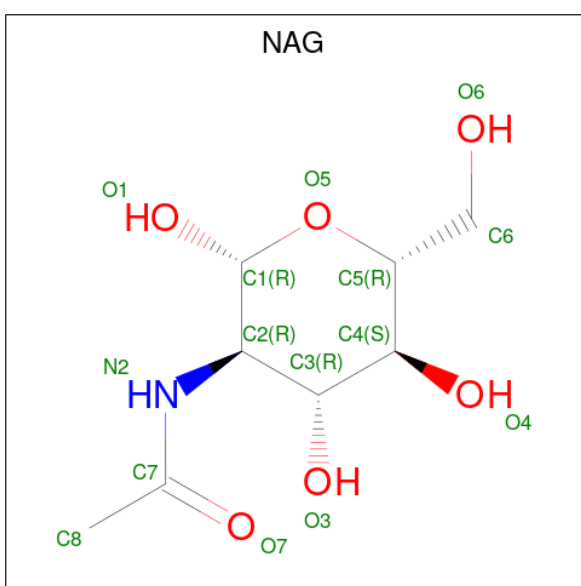
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-{[3-(aminomethyl)-2-(2-methylpropyl)-1-oxo-4-phenyl-1,2-dihydroisoquinolin-6-yl]oxy}acetamide (three-letter code: LUI) (formula: C₂₂H₂₅N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	22	3	3		
3	B	1	Total	C	N	O	0	0
			28	22	3	3		
3	C	1	Total	C	N	O	0	0
			28	22	3	3		
3	D	1	Total	C	N	O	0	0
			28	22	3	3		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

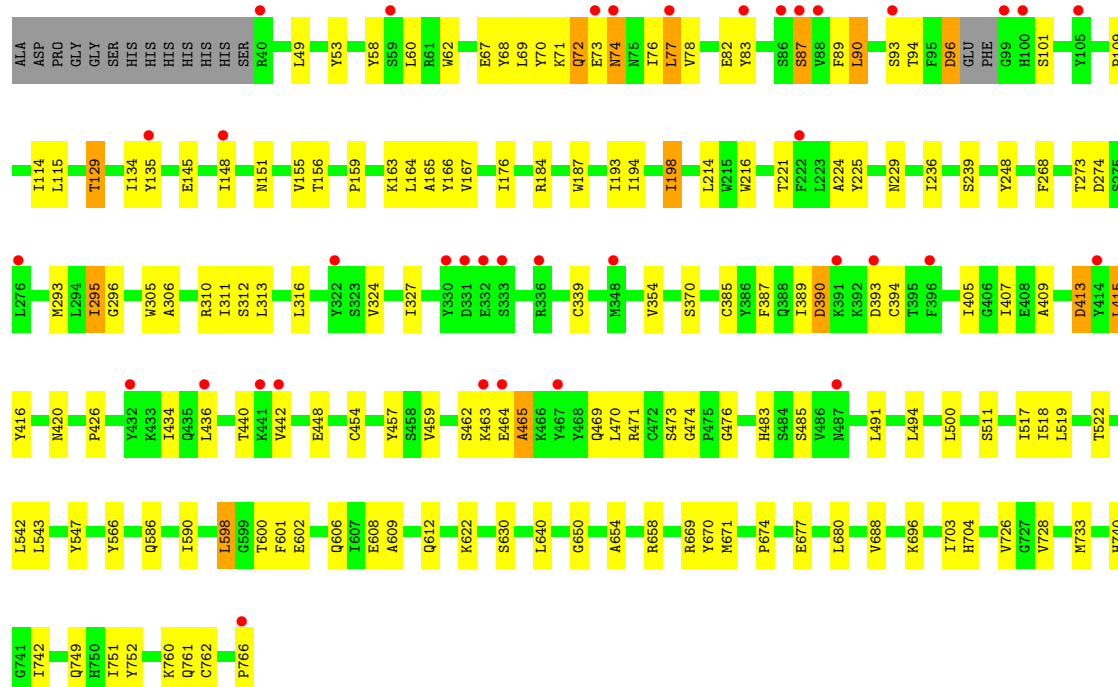
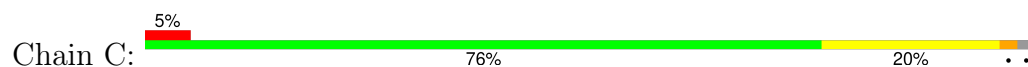
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	152	Total	O	0	0
			152	152		
5	B	142	Total	O	0	0
			142	142		
5	C	84	Total	O	0	0
			84	84		
5	D	128	Total	O	0	0
			128	128		

- Molecule 1: Dipeptidyl peptidase 4

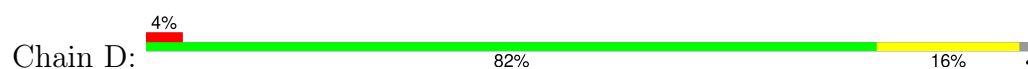




• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.77Å 122.56Å 144.74Å 90.00° 115.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.72 34.68 – 2.72	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.00-2.72) 97.5 (34.68-2.72)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.72Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.254 0.199 , 0.259	Depositor DCC
R_{free} test set	5038 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24713	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, LUI

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/6122	0.63	0/8327
1	B	0.50	0/6190	0.61	0/8419
1	C	0.46	0/6107	0.58	0/8305
1	D	0.49	0/6129	0.62	1/8336 (0.0%)
All	All	0.49	0/24548	0.61	1/33387 (0.0%)

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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	356	ARG	NE-CZ-NH1	5.34	122.97	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	96	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5950	0	5664	84	0
1	B	6013	0	5718	95	0
1	C	5937	0	5664	100	0
1	D	5957	0	5679	81	0
2	E	28	0	26	5	0
3	A	28	0	25	0	0
3	B	28	0	25	0	0
3	C	28	0	25	3	0
3	D	28	0	25	0	0
4	A	84	0	78	9	0
4	B	70	0	65	10	0
4	D	56	0	52	9	0
5	A	152	0	0	1	0
5	B	142	0	0	4	0
5	C	84	0	0	2	0
5	D	128	0	0	3	0
All	All	24713	0	23046	365	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 365 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASN:HD21	4:B:1501:NAG:C1	1.09	1.57
1:C:229:ASN:HD21	2:E:1:NAG:C1	1.07	1.55
1:B:229:ASN:HD21	4:B:2291:NAG:C1	0.94	1.54
1:B:281:ASN:HD21	4:B:2811:NAG:C1	1.16	1.51
1:D:229:ASN:HD21	4:D:2291:NAG:C1	1.15	1.51

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	725/740 (98%)	677 (93%)	42 (6%)	6 (1%)	19	41
1	B	731/740 (99%)	691 (94%)	39 (5%)	1 (0%)	51	77
1	C	721/740 (97%)	673 (93%)	39 (5%)	9 (1%)	13	30
1	D	725/740 (98%)	674 (93%)	45 (6%)	6 (1%)	19	41
All	All	2902/2960 (98%)	2715 (94%)	165 (6%)	22 (1%)	19	41

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	73	GLU
1	C	90	LEU
1	C	93	SER
1	C	465	ALA

5.3.2 Protein sidechains ⓘ

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	651/662 (98%)	625 (96%)	26 (4%)	31	58
1	B	658/662 (99%)	631 (96%)	27 (4%)	30	57
1	C	650/662 (98%)	618 (95%)	32 (5%)	25	50
1	D	652/662 (98%)	634 (97%)	18 (3%)	43	71
All	All	2611/2648 (99%)	2508 (96%)	103 (4%)	32	59

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	83	TYR
1	C	413	ASP
1	D	501	ASP
1	C	96	ASP
1	C	316	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	344	GLN
1	C	612	GLN
1	D	761	GLN
1	C	592	HIS
1	D	92	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	2,1	14,14,15	0.45	0	17,19,21	1.35	2 (11%)
2	NAG	E	2	2	14,14,15	0.58	0	17,19,21	1.43	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
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	O5-C1-C2	-3.29	106.21	111.29
2	E	1	NAG	C1-C2-N2	3.07	115.27	110.43
2	E	2	NAG	O7-C7-N2	2.35	126.13	121.98
2	E	1	NAG	O4-C4-C3	-2.18	105.25	110.38

There are no chirality outliers.

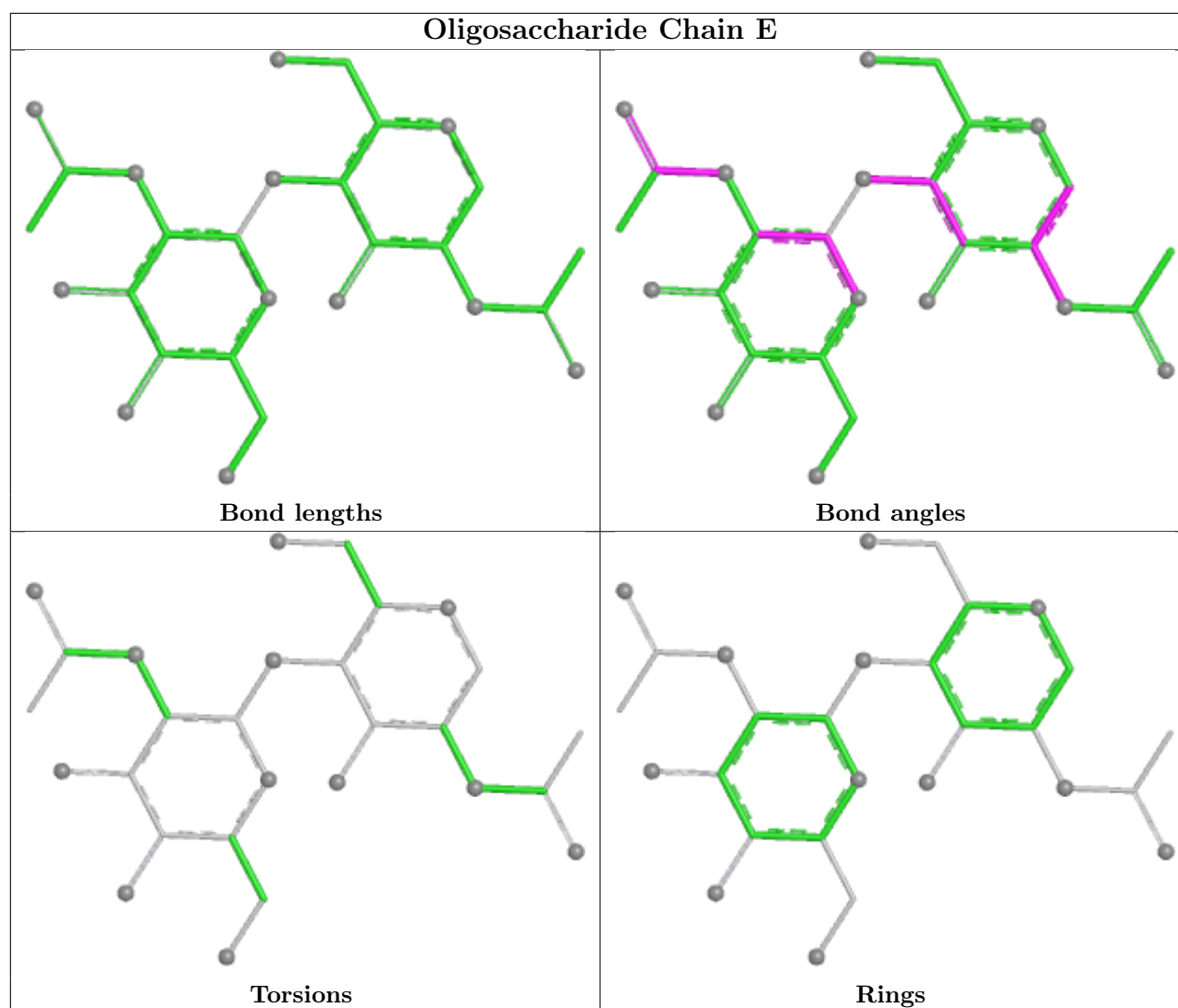
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	5	0
2	E	2	NAG	2	0

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



5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
3	LUI	B	800	-	29,30,30	0.84	1 (3%)	38,42,42	1.41	3 (7%)
4	NAG	A	2811	1	14,14,15	0.89	0	17,19,21	1.39	5 (29%)
4	NAG	D	2291	1	14,14,15	0.51	0	17,19,21	2.53	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	901	1	14,14,15	0.79	0	17,19,21	2.14	4 (23%)
4	NAG	B	3211	1	14,14,15	0.72	0	17,19,21	1.32	1 (5%)
4	NAG	D	1501	1	14,14,15	0.88	0	17,19,21	1.65	3 (17%)
4	NAG	A	2292	-	14,14,15	0.66	0	17,19,21	1.22	2 (11%)
4	NAG	A	1501	1	14,14,15	0.68	0	17,19,21	2.04	5 (29%)
4	NAG	A	3211	1	14,14,15	0.59	0	17,19,21	0.85	0
3	LUI	A	800	-	29,30,30	0.86	2 (6%)	38,42,42	1.36	4 (10%)
3	LUI	D	800	-	29,30,30	0.84	1 (3%)	38,42,42	1.47	4 (10%)
4	NAG	B	2291	1	14,14,15	0.51	0	17,19,21	1.09	1 (5%)
4	NAG	B	1501	1	14,14,15	0.59	0	17,19,21	1.25	1 (5%)
4	NAG	A	2191	1	14,14,15	0.67	0	17,19,21	0.94	1 (5%)
4	NAG	A	2291	1	14,14,15	0.66	0	17,19,21	1.32	2 (11%)
4	NAG	D	2811	1	14,14,15	0.87	0	17,19,21	1.98	4 (23%)
4	NAG	D	2191	1	14,14,15	0.61	0	17,19,21	1.06	1 (5%)
4	NAG	B	2811	1	14,14,15	0.51	0	17,19,21	0.88	0
3	LUI	C	800	-	29,30,30	0.85	1 (3%)	38,42,42	1.33	3 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LUI	B	800	-	-	1/13/15/15	0/3/3/3
4	NAG	A	2811	1	-	2/6/23/26	0/1/1/1
4	NAG	D	2291	1	-	2/6/23/26	0/1/1/1
4	NAG	B	901	1	-	1/6/23/26	0/1/1/1
4	NAG	B	3211	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1501	1	-	3/6/23/26	0/1/1/1
4	NAG	A	2292	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1501	1	-	3/6/23/26	0/1/1/1
4	NAG	A	3211	1	-	0/6/23/26	0/1/1/1
3	LUI	A	800	-	-	4/13/15/15	0/3/3/3
3	LUI	D	800	-	-	3/13/15/15	0/3/3/3
4	NAG	B	2291	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1501	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2191	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	2291	1	-	1/6/23/26	0/1/1/1
4	NAG	D	2811	1	-	0/6/23/26	0/1/1/1
4	NAG	D	2191	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2811	1	-	2/6/23/26	0/1/1/1
3	LUI	C	800	-	-	2/13/15/15	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	LUI	C7-N8	-2.54	1.34	1.40
3	B	800	LUI	C7-N8	-2.28	1.35	1.40
3	A	800	LUI	C9-N8	-2.23	1.35	1.39
3	C	800	LUI	C7-N8	-2.21	1.35	1.40
3	D	800	LUI	C7-N8	-2.15	1.35	1.40

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2291	NAG	C1-O5-C5	7.19	121.82	112.19
3	B	800	LUI	C2-C7-N8	5.02	122.62	115.26
3	D	800	LUI	C2-C7-N8	5.01	122.60	115.26
3	A	800	LUI	C2-C7-N8	4.86	122.38	115.26
3	C	800	LUI	C2-C7-N8	4.74	122.20	115.26

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	800	LUI	O24-C25-C26-N27
4	A	1501	NAG	C3-C2-N2-C7
4	D	1501	NAG	C1-C2-N2-C7
4	B	2811	NAG	O5-C5-C6-O6
4	B	1501	NAG	O5-C5-C6-O6

There are no ring outliers.

13 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2811	NAG	3	0
4	D	2291	NAG	3	0

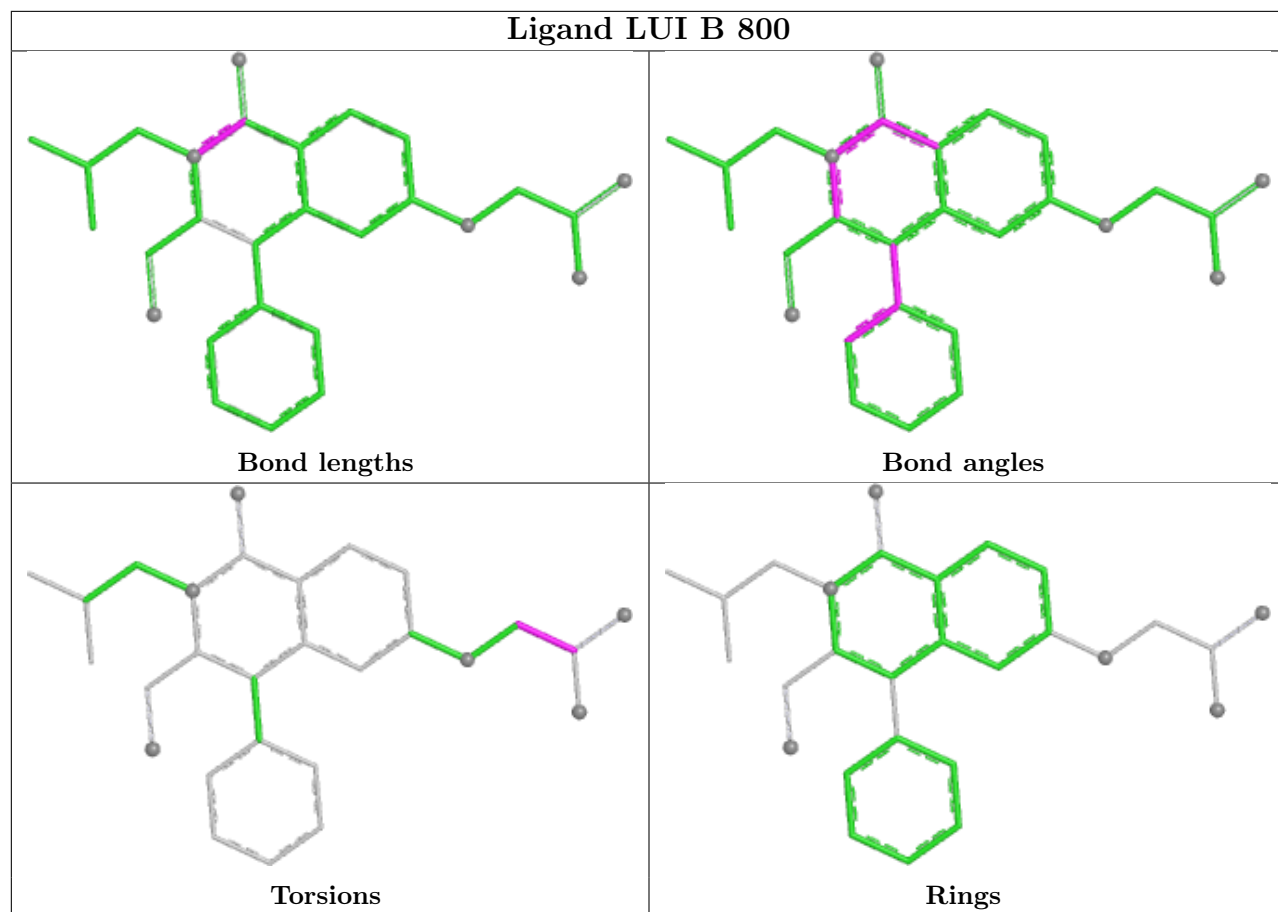
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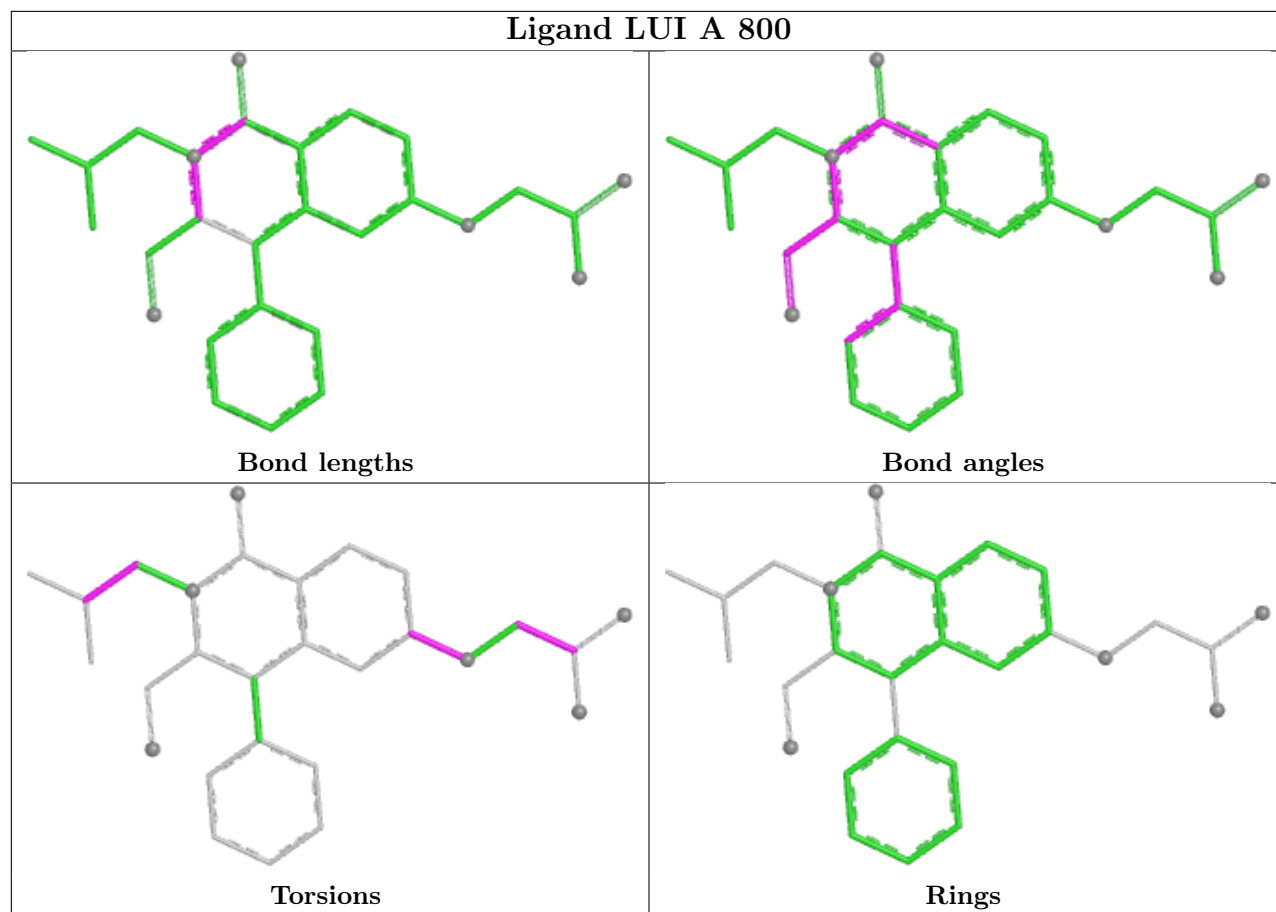
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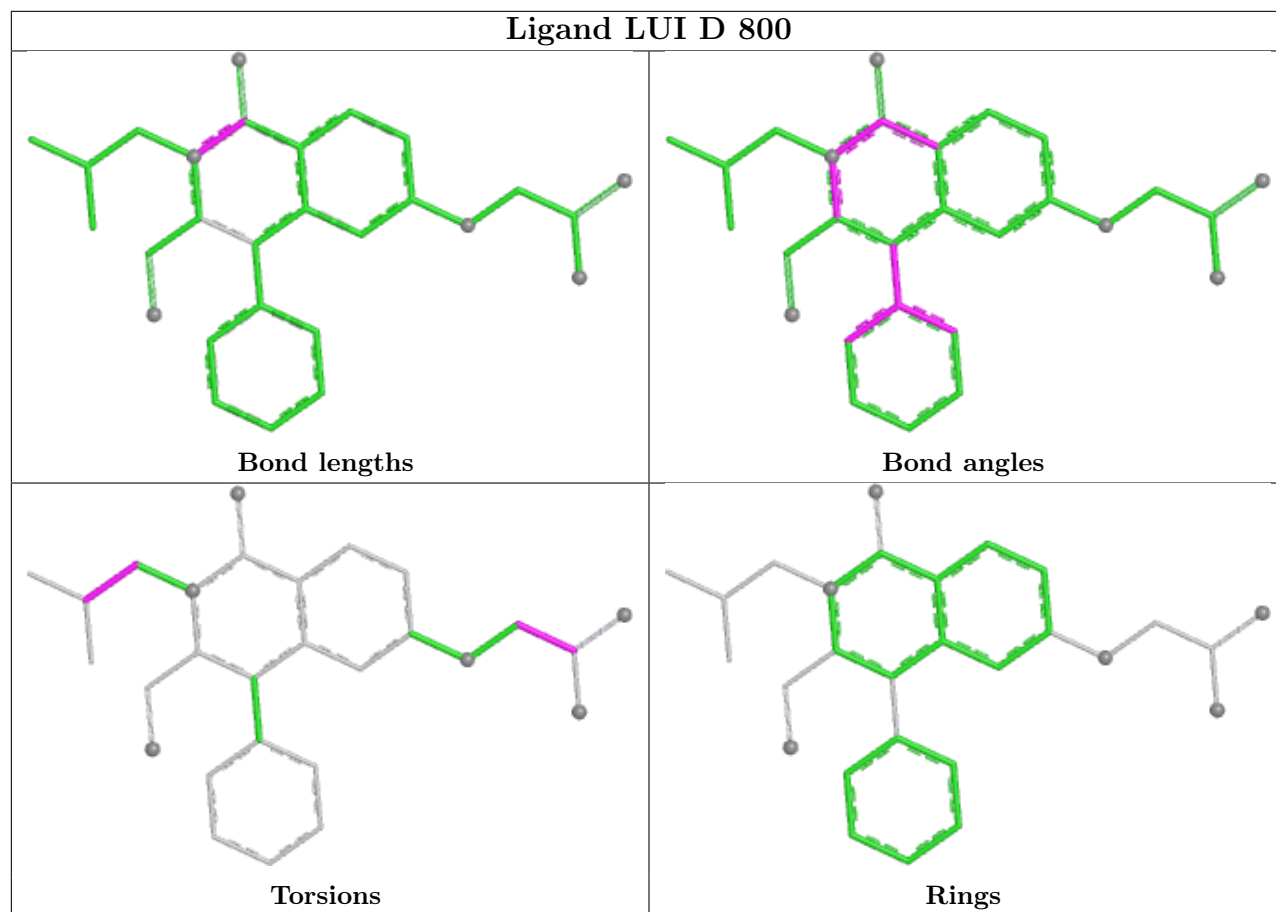
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	901	NAG	2	0
4	D	1501	NAG	1	0
4	A	2292	NAG	3	0
4	A	3211	NAG	2	0
4	B	2291	NAG	2	0
4	B	1501	NAG	4	0
4	A	2291	NAG	4	0
4	D	2811	NAG	3	0
4	D	2191	NAG	2	0
4	B	2811	NAG	2	0
3	C	800	LUI	3	0

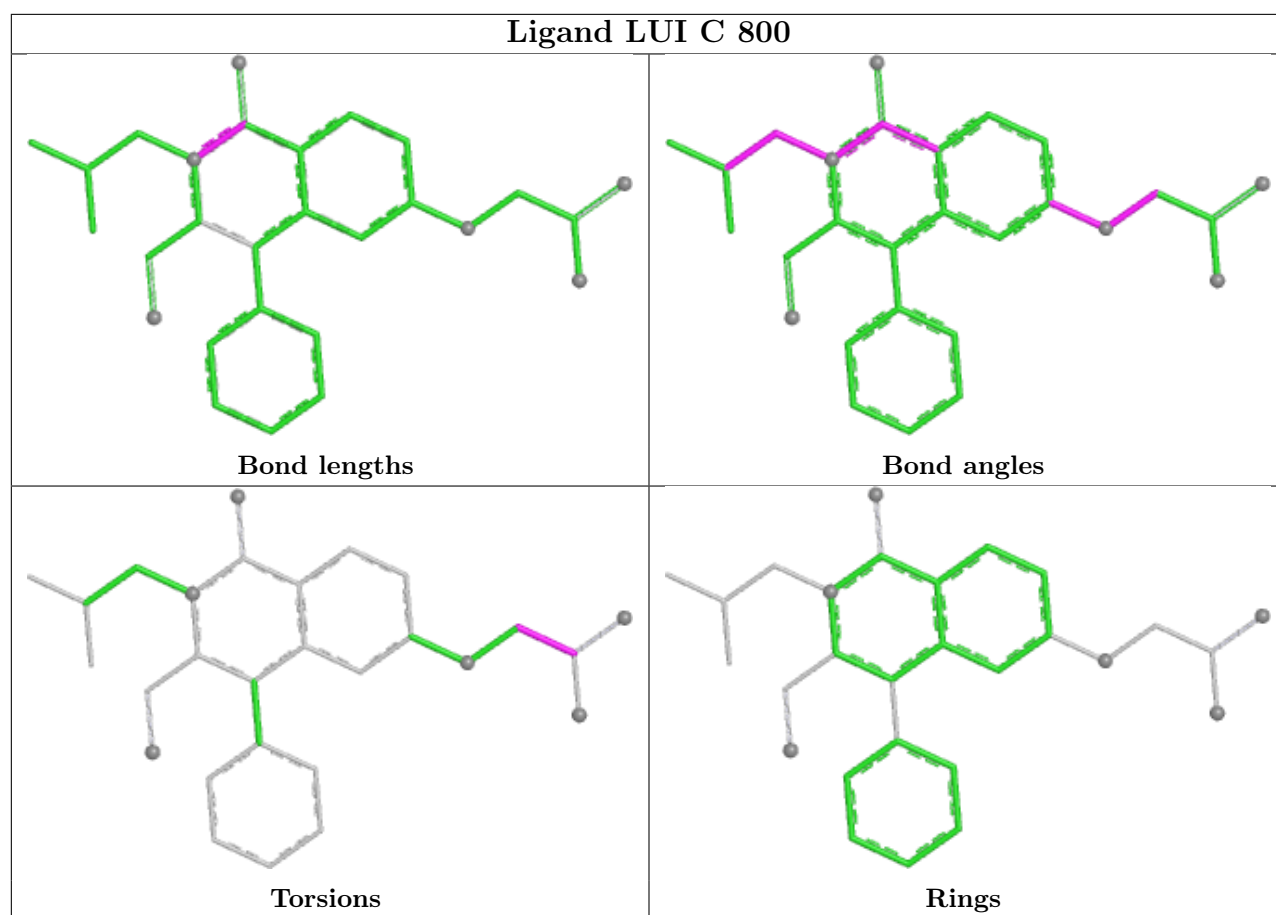
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand LUI B 800









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	727/740 (98%)	-0.07	23 (3%) 47 48	21, 42, 79, 100	0
1	B	733/740 (99%)	-0.19	13 (1%) 68 70	24, 46, 69, 85	0
1	C	725/740 (97%)	0.16	37 (5%) 28 27	25, 61, 101, 122	0
1	D	727/740 (98%)	-0.01	30 (4%) 37 36	24, 47, 91, 117	0
All	All	2912/2960 (98%)	-0.03	103 (3%) 44 44	21, 48, 91, 122	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	SER	4.6
1	D	92	ASN	4.6
1	C	73	GLU	4.5
1	D	81	ALA	4.4
1	D	97	GLU	4.4

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

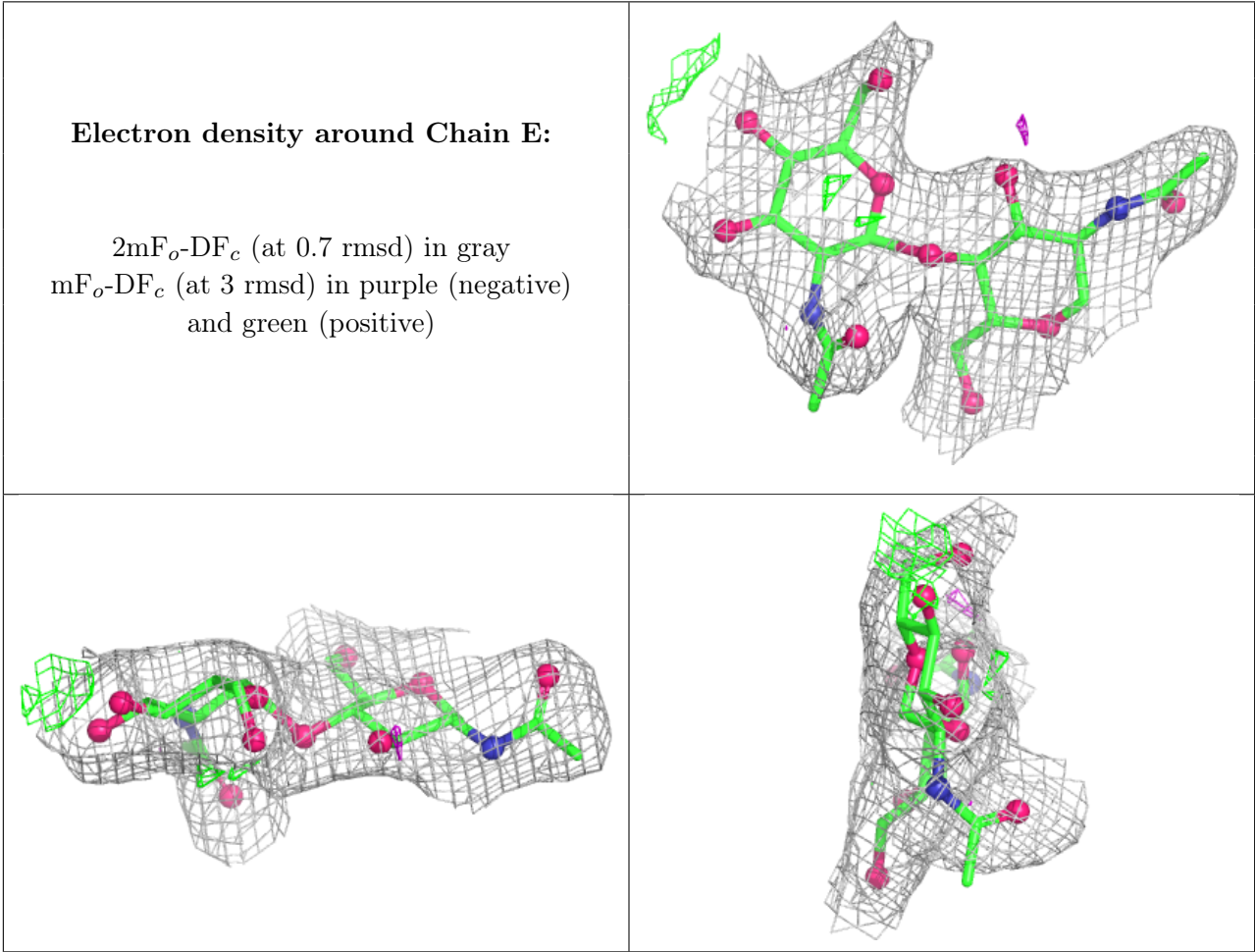
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.82	0.24	55,55,56,56	0
2	NAG	E	1	14/15	0.94	0.13	42,44,46,46	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
4	NAG	B	901	14/15	0.75	0.15	53,54,55,55	0
4	NAG	A	2811	14/15	0.76	0.17	48,51,54,54	0
4	NAG	A	1501	14/15	0.80	0.32	53,55,57,59	0
4	NAG	A	2191	14/15	0.81	0.34	53,56,59,60	0
4	NAG	D	1501	14/15	0.82	0.28	51,53,54,54	0
4	NAG	D	2811	14/15	0.83	0.23	52,53,54,54	0
4	NAG	B	3211	14/15	0.84	0.37	55,57,57,58	0
4	NAG	A	2292	14/15	0.86	0.24	50,51,52,52	0

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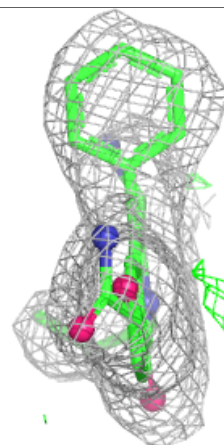
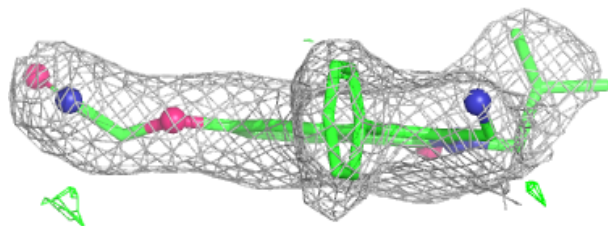
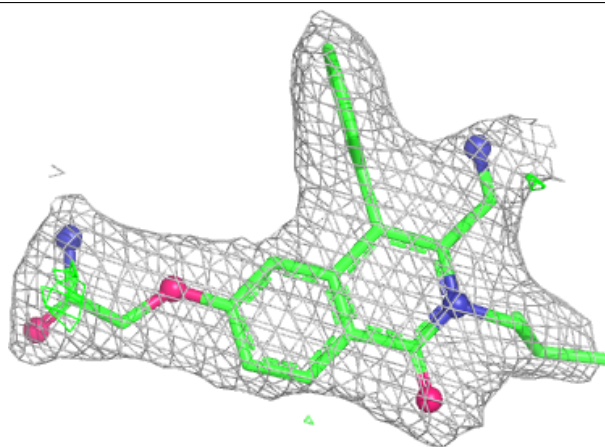
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	D	2191	14/15	0.87	0.27	51,53,57,58	0
4	NAG	B	2811	14/15	0.87	0.13	51,52,55,55	0
4	NAG	D	2291	14/15	0.89	0.21	50,51,53,54	0
4	NAG	B	1501	14/15	0.89	0.27	50,51,52,52	0
4	NAG	B	2291	14/15	0.90	0.15	45,48,49,49	0
4	NAG	A	3211	14/15	0.93	0.26	49,52,54,55	0
4	NAG	A	2291	14/15	0.93	0.19	45,48,50,51	0
3	LUI	C	800	28/28	0.95	0.16	39,41,46,47	0
3	LUI	A	800	28/28	0.95	0.21	36,40,47,50	0
3	LUI	D	800	28/28	0.96	0.15	35,38,42,43	0
3	LUI	B	800	28/28	0.97	0.17	37,39,40,40	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.

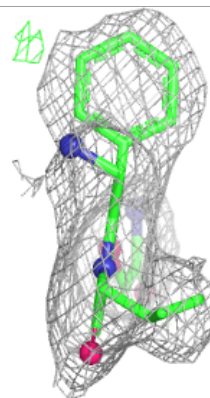
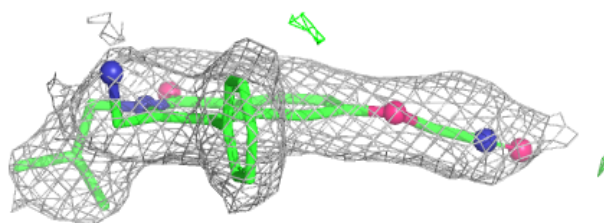
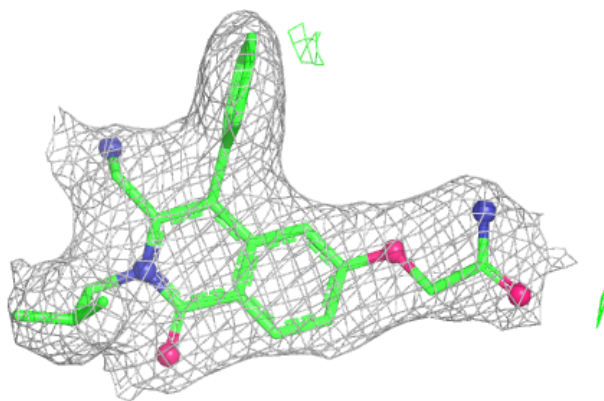
Electron density around LUI C 800:

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

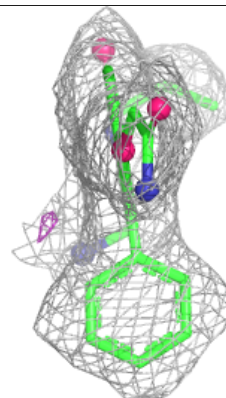
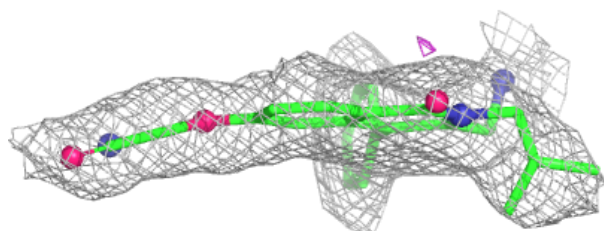
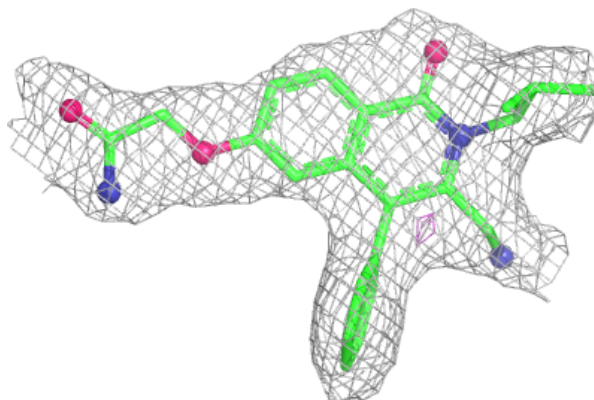


Electron density around LUI A 800:

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

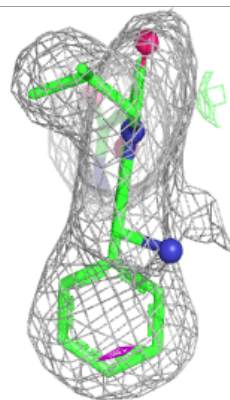
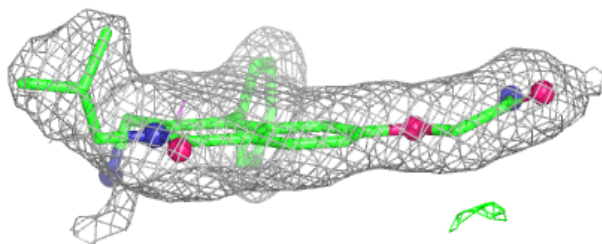
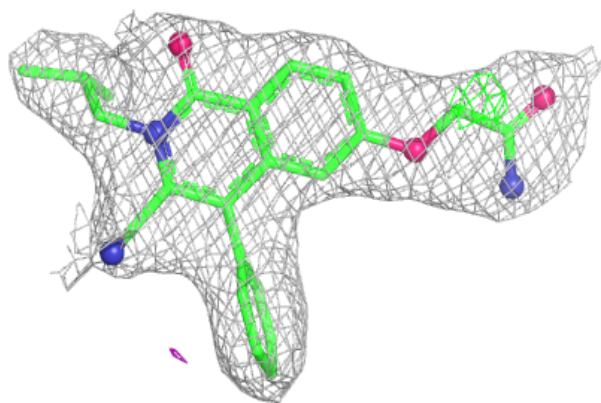
**Electron density around LUI D 800:**

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



Electron density around LUI B 800:

$2mF_o-DF_c$ (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.