



## Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 12:09 AM JST

PDB ID : 8HNN  
EMDB ID : EMD-34913  
Title : Cryo-EM structure of human OATP1B1 in complex with simeprevir  
Authors : Shan, Z.; Yang, X.; Zhang, Y.  
Deposited on : 2022-12-07  
Resolution : 3.73 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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>.

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

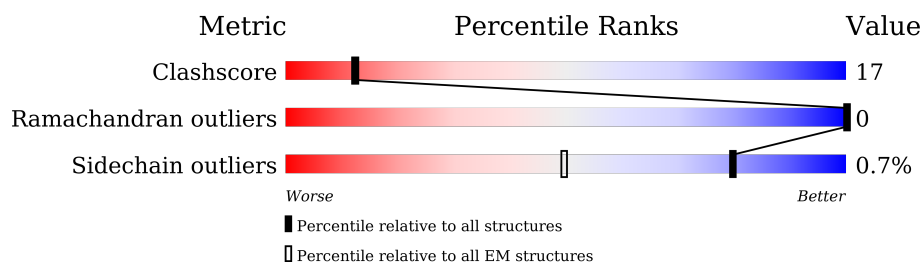
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.73 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	724	
2	B	2	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4236 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Solute carrier organic anion transporter family member 1B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	563	Total	C	N	O	S	0	0
			4142	2735	660	715	32		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	692	LEU	-	expression tag	UNP Q9Y6L6
A	693	GLU	-	expression tag	UNP Q9Y6L6
A	694	GLY	-	expression tag	UNP Q9Y6L6
A	695	SER	-	expression tag	UNP Q9Y6L6
A	696	ASP	-	expression tag	UNP Q9Y6L6
A	697	GLU	-	expression tag	UNP Q9Y6L6
A	698	VAL	-	expression tag	UNP Q9Y6L6
A	699	ASP	-	expression tag	UNP Q9Y6L6
A	700	ALA	-	expression tag	UNP Q9Y6L6
A	701	GLY	-	expression tag	UNP Q9Y6L6
A	702	SER	-	expression tag	UNP Q9Y6L6
A	703	HIS	-	expression tag	UNP Q9Y6L6
A	704	HIS	-	expression tag	UNP Q9Y6L6
A	705	HIS	-	expression tag	UNP Q9Y6L6
A	706	HIS	-	expression tag	UNP Q9Y6L6
A	707	HIS	-	expression tag	UNP Q9Y6L6
A	708	HIS	-	expression tag	UNP Q9Y6L6
A	709	HIS	-	expression tag	UNP Q9Y6L6
A	710	HIS	-	expression tag	UNP Q9Y6L6
A	711	HIS	-	expression tag	UNP Q9Y6L6
A	712	HIS	-	expression tag	UNP Q9Y6L6
A	713	GLY	-	expression tag	UNP Q9Y6L6
A	714	SER	-	expression tag	UNP Q9Y6L6
A	715	VAL	-	expression tag	UNP Q9Y6L6
A	716	GLU	-	expression tag	UNP Q9Y6L6
A	717	ASP	-	expression tag	UNP Q9Y6L6
A	718	TYR	-	expression tag	UNP Q9Y6L6
A	719	LYS	-	expression tag	UNP Q9Y6L6

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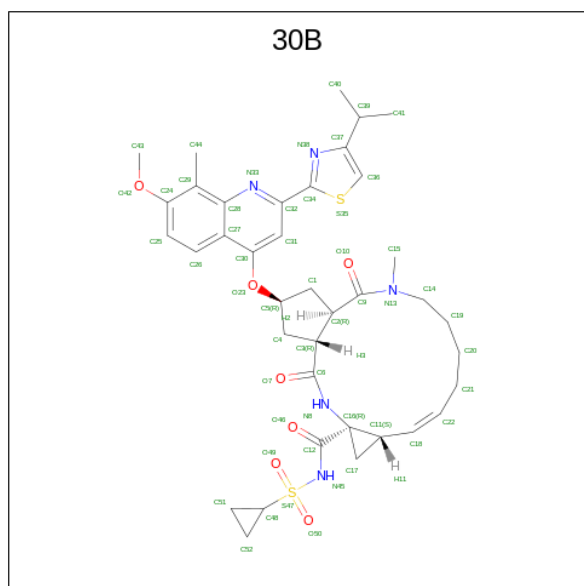
Chain	Residue	Modelled	Actual	Comment	Reference
A	720	ASP	-	expression tag	UNP Q9Y6L6
A	721	ASP	-	expression tag	UNP Q9Y6L6
A	722	ASP	-	expression tag	UNP Q9Y6L6
A	723	ASP	-	expression tag	UNP Q9Y6L6
A	724	LYS	-	expression tag	UNP Q9Y6L6

- 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				AltConf	Trace
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is (2R,3aR,10Z,11aS,12aR,14aR)-N-(cyclopropylsulfonyl)-2-({7-methoxy-8-methyl-2-[4-(1-methylethyl)-1,3-thiazol-2-yl]quinolin-4-yl}oxy)-5-methyl-4,14-dioxo-2,3,3a,4,5,6,7,8,9,11a,12,13,14,14a-tetradecahydrocyclopenta[c]cyclopropa[g][1,6]diazacyclotetradecine-12a(1H)-carboxamide (three-letter code: 30B) (formula: C<sub>38</sub>H<sub>47</sub>N<sub>5</sub>O<sub>7</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	S	0
			52	38	5	7	2	

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).

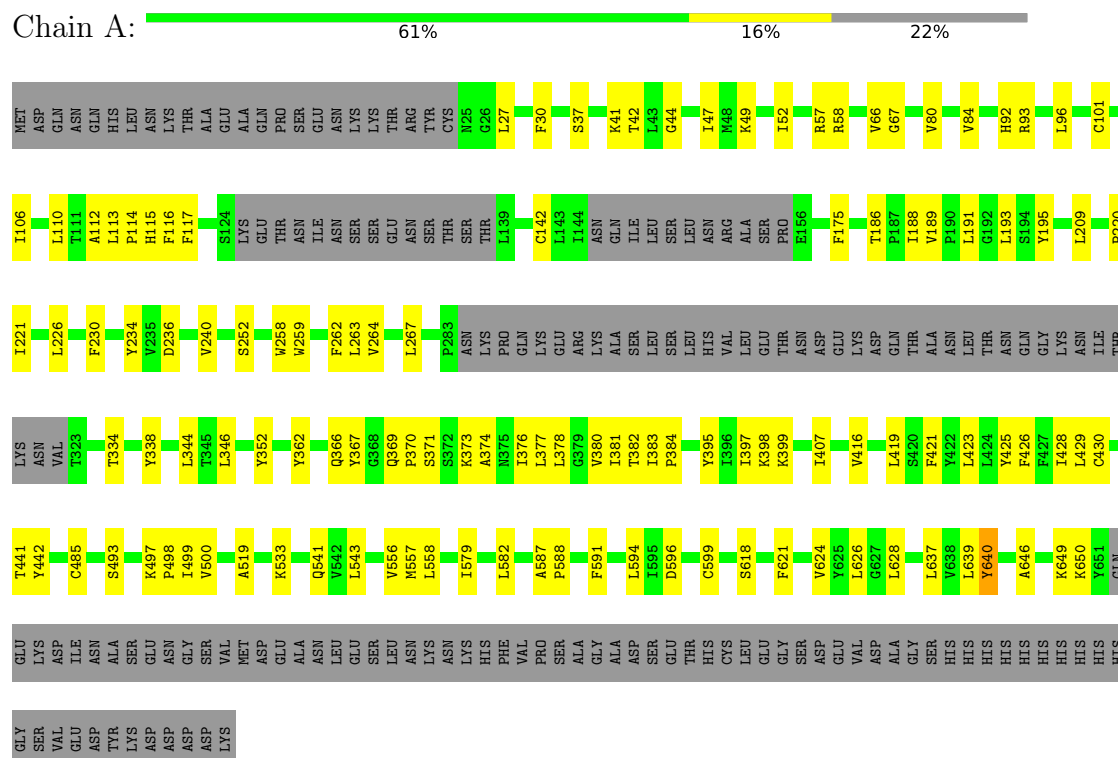


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	14	8	1	5	0

### 3 Residue-property plots

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. 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. 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: Solute carrier organic anion transporter family member 1B1



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	149222	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

## 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: 30B, NAG

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	0.36	0/4243	0.58	0/5761

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4142	0	3983	138	0
2	B	28	0	25	0	0
3	A	52	0	46	6	0
4	A	14	0	13	0	0
All	All	4236	0	4067	139	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 17.

All (139) 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:116:PHE:HE1	1:A:259:TRP:CZ3	1.46	1.32
1:A:116:PHE:CE1	1:A:259:TRP:CZ3	2.21	1.28
1:A:116:PHE:CE1	1:A:259:TRP:CE3	2.22	1.26
1:A:116:PHE:CZ	1:A:259:TRP:HE3	1.60	1.19
1:A:421:PHE:CE1	1:A:543:LEU:HD23	1.83	1.13
1:A:92:HIS:O	1:A:96:LEU:HD23	1.47	1.13
1:A:594:LEU:HD11	1:A:624:VAL:HG13	1.35	1.07
1:A:116:PHE:CZ	1:A:259:TRP:CE3	2.42	1.05
1:A:114:PRO:HB2	1:A:258:TRP:HH2	1.24	1.03
1:A:594:LEU:HD11	1:A:624:VAL:CG1	1.93	0.98
1:A:114:PRO:HB2	1:A:258:TRP:CH2	2.02	0.93
1:A:428:ILE:HD11	1:A:533:LYS:HB3	1.50	0.89
1:A:421:PHE:HE1	1:A:543:LEU:HD23	1.39	0.87
1:A:421:PHE:CE1	1:A:543:LEU:CD2	2.61	0.83
1:A:628:LEU:HD23	1:A:628:LEU:O	1.79	0.81
1:A:116:PHE:HE1	1:A:259:TRP:HZ3	0.88	0.81
1:A:421:PHE:HE1	1:A:543:LEU:CD2	1.94	0.81
1:A:594:LEU:CD1	1:A:624:VAL:CG1	2.60	0.80
1:A:594:LEU:HD22	1:A:594:LEU:O	1.82	0.79
1:A:376:ILE:HG23	1:A:377:LEU:HG	1.66	0.78
1:A:344:LEU:HD11	1:A:640:TYR:HD2	1.52	0.74
1:A:209:LEU:HD12	1:A:209:LEU:O	1.88	0.74
1:A:57:ARG:NH2	1:A:252:SER:O	2.22	0.73
1:A:116:PHE:CE1	1:A:259:TRP:HZ3	1.80	0.73
1:A:41:LYS:HE3	3:A:801:30B:H18	1.70	0.72
1:A:115:HIS:CE1	1:A:259:TRP:CE2	2.79	0.71
1:A:27:LEU:HD23	1:A:27:LEU:O	1.91	0.70
1:A:112:ALA:HB1	1:A:259:TRP:HA	1.71	0.70
1:A:419:LEU:C	1:A:419:LEU:HD23	2.14	0.67
1:A:84:VAL:HB	1:A:186:THR:HG21	1.78	0.65
1:A:114:PRO:CB	1:A:258:TRP:HH2	2.04	0.64
1:A:113:LEU:HB3	1:A:117:PHE:CE2	2.33	0.64
1:A:113:LEU:HB3	1:A:117:PHE:HE2	1.63	0.64
1:A:41:LYS:HZ1	3:A:801:30B:H22	1.63	0.62
1:A:112:ALA:HA	1:A:258:TRP:CZ3	2.34	0.62
1:A:30:PHE:CE1	1:A:195:TYR:CD2	2.87	0.62
1:A:112:ALA:HA	1:A:258:TRP:HZ3	1.65	0.62
1:A:334:THR:HG22	1:A:334:THR:O	1.99	0.61
1:A:346:LEU:HD12	1:A:346:LEU:O	2.01	0.61
1:A:37:SER:HB3	1:A:188:ILE:HD12	1.83	0.60
1:A:84:VAL:HG11	1:A:186:THR:HG22	1.81	0.60
1:A:628:LEU:HD23	1:A:628:LEU:C	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:HD11	1:A:640:TYR:CD2	2.35	0.59
1:A:362:TYR:HA	1:A:621:PHE:CE2	2.38	0.58
1:A:428:ILE:O	1:A:428:ILE:HG23	2.03	0.58
1:A:352:TYR:CE2	3:A:801:30B:H5	2.37	0.58
1:A:115:HIS:ND1	1:A:259:TRP:CD2	2.73	0.56
1:A:416:VAL:HG22	1:A:637:LEU:HD11	1.88	0.55
1:A:594:LEU:C	1:A:594:LEU:HD13	2.27	0.55
1:A:115:HIS:CE1	1:A:259:TRP:CD2	2.95	0.55
1:A:423:LEU:O	1:A:423:LEU:HD23	2.07	0.55
1:A:558:LEU:HD12	1:A:558:LEU:O	2.07	0.53
1:A:493:SER:H	1:A:499:ILE:CB	2.21	0.53
1:A:371:SER:HA	1:A:374:ALA:HB3	1.89	0.53
1:A:209:LEU:HD21	1:A:556:VAL:HG11	1.91	0.52
1:A:209:LEU:HD21	1:A:556:VAL:CG1	2.39	0.51
1:A:582:LEU:HD12	1:A:582:LEU:N	2.24	0.51
1:A:234:TYR:HE1	1:A:240:VAL:HG11	1.75	0.51
1:A:367:TYR:C	1:A:369:GLN:H	2.14	0.51
1:A:30:PHE:CD1	1:A:195:TYR:CE2	2.99	0.51
1:A:370:PRO:HG2	1:A:373:LYS:HG2	1.93	0.51
1:A:366:GLN:OE1	1:A:618:SER:OG	2.29	0.50
1:A:112:ALA:HB2	1:A:262:PHE:HB2	1.94	0.50
1:A:344:LEU:CD1	1:A:639:LEU:HB3	2.42	0.49
1:A:646:ALA:O	1:A:650:LYS:HD3	2.11	0.49
1:A:30:PHE:CZ	1:A:195:TYR:CD2	3.00	0.49
1:A:399:LYS:O	1:A:399:LYS:HD2	2.12	0.49
1:A:541:GLN:HA	1:A:541:GLN:OE1	2.12	0.49
1:A:557:MET:HE1	1:A:557:MET:O	2.13	0.49
1:A:362:TYR:HA	1:A:621:PHE:HE2	1.76	0.48
1:A:395:TYR:C	1:A:395:TYR:CD1	2.86	0.48
1:A:101:CYS:SG	1:A:188:ILE:HD11	2.54	0.48
1:A:500:VAL:HA	1:A:519:ALA:O	2.14	0.48
1:A:84:VAL:HG11	1:A:186:THR:CG2	2.44	0.47
1:A:234:TYR:CE1	1:A:240:VAL:HG11	2.50	0.47
1:A:426:PHE:O	1:A:429:LEU:HG	2.14	0.47
1:A:497:LYS:O	1:A:498:PRO:C	2.53	0.47
1:A:209:LEU:CD2	1:A:556:VAL:CG1	2.93	0.46
1:A:27:LEU:HD23	1:A:27:LEU:C	2.35	0.46
1:A:84:VAL:CB	1:A:186:THR:HG21	2.45	0.46
1:A:381:ILE:O	1:A:384:PRO:HD2	2.15	0.46
1:A:397:ILE:HG23	1:A:407:ILE:HD11	1.98	0.46
1:A:425:TYR:HB3	1:A:626:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:ALA:HB3	1:A:588:PRO:CD	2.45	0.46
1:A:58:ARG:O	1:A:58:ARG:HD2	2.16	0.45
1:A:175:PHE:CD2	1:A:175:PHE:C	2.89	0.45
1:A:430:CYS:SG	1:A:533:LYS:HD3	2.56	0.45
1:A:338:TYR:CD1	1:A:338:TYR:C	2.89	0.45
1:A:236:ASP:O	1:A:240:VAL:HG12	2.16	0.45
1:A:41:LYS:CE	3:A:801:30B:H18	2.43	0.45
1:A:93:ARG:HG2	1:A:191:LEU:HD22	1.99	0.44
1:A:557:MET:CE	1:A:557:MET:C	2.85	0.44
1:A:30:PHE:CZ	1:A:195:TYR:HD2	2.36	0.44
1:A:80:VAL:O	1:A:80:VAL:HG12	2.16	0.44
1:A:226:LEU:HD21	1:A:264:VAL:HG21	1.99	0.44
1:A:649:LYS:HE3	1:A:650:LYS:HE2	1.99	0.44
1:A:49:LYS:O	1:A:52:ILE:HG22	2.18	0.44
1:A:441:THR:HG22	1:A:442:TYR:N	2.32	0.44
1:A:344:LEU:HG	1:A:639:LEU:CB	2.48	0.44
1:A:352:TYR:CD1	1:A:352:TYR:O	2.70	0.44
1:A:344:LEU:HG	1:A:639:LEU:HB3	2.00	0.44
1:A:628:LEU:C	1:A:628:LEU:CD2	2.86	0.44
1:A:42:THR:HG21	1:A:220:PRO:HD3	2.00	0.43
1:A:594:LEU:CD1	1:A:624:VAL:HG11	2.46	0.43
1:A:142:CYS:HA	1:A:485:CYS:SG	2.57	0.43
1:A:41:LYS:NZ	3:A:801:30B:H22	2.29	0.43
1:A:44:GLY:O	1:A:47:ILE:HG22	2.18	0.43
1:A:579:ILE:HD13	1:A:579:ILE:HA	1.88	0.43
1:A:380:VAL:C	1:A:382:THR:N	2.71	0.43
1:A:221:ILE:CD1	1:A:383:ILE:HG21	2.49	0.43
1:A:374:ALA:HA	1:A:378:LEU:HD23	2.01	0.43
1:A:380:VAL:O	1:A:381:ILE:C	2.56	0.43
1:A:110:LEU:HD12	1:A:110:LEU:O	2.19	0.42
1:A:428:ILE:O	1:A:428:ILE:HG13	2.19	0.42
1:A:221:ILE:HD11	1:A:383:ILE:HG21	2.01	0.42
1:A:113:LEU:N	1:A:114:PRO:CD	2.83	0.42
1:A:115:HIS:CB	1:A:259:TRP:HB3	2.50	0.41
1:A:189:VAL:HG13	1:A:193:LEU:HD12	2.03	0.41
1:A:380:VAL:O	1:A:382:THR:N	2.53	0.41
1:A:398:LYS:C	1:A:398:LYS:HD3	2.41	0.41
3:A:801:30B:H20A	3:A:801:30B:HN45	1.86	0.41
1:A:419:LEU:HD23	1:A:419:LEU:O	2.20	0.41
1:A:344:LEU:HD12	1:A:639:LEU:HB3	2.02	0.41
1:A:191:LEU:HD23	1:A:191:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LEU:CD1	1:A:267:LEU:HD23	2.51	0.41
1:A:226:LEU:CD2	1:A:264:VAL:HG11	2.51	0.41
1:A:209:LEU:CD2	1:A:556:VAL:HG11	2.49	0.41
1:A:557:MET:O	1:A:557:MET:SD	2.79	0.40
1:A:557:MET:HB3	1:A:557:MET:HE3	1.85	0.40
1:A:596:ASP:O	1:A:599:CYS:HB3	2.21	0.40
1:A:626:LEU:HD23	1:A:626:LEU:HA	1.87	0.40
1:A:84:VAL:HB	1:A:186:THR:CG2	2.48	0.40
1:A:84:VAL:CG1	1:A:186:THR:CG2	3.00	0.40
1:A:96:LEU:HD13	1:A:96:LEU:HA	1.89	0.40
1:A:112:ALA:CB	1:A:259:TRP:HA	2.46	0.40
1:A:80:VAL:O	1:A:80:VAL:CG1	2.70	0.40
1:A:106:ILE:HA	1:A:106:ILE:HD13	1.83	0.40
1:A:66:VAL:O	1:A:67:GLY:C	2.58	0.40
1:A:639:LEU:HD13	1:A:639:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	555/724 (77%)	538 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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	409/631 (65%)	406 (99%)	3 (1%)	81 88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	PHE
1	A	591	PHE
1	A	640	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	B	1	1,2	14,14,15	1.45	1 (7%)	17,19,21	1.48	3 (17%)
2	NAG	B	2	2	14,14,15	0.36	0	17,19,21	0.69	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
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	O4-C4	5.15	1.55	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O4-C4-C5	3.71	118.51	109.30
2	B	1	NAG	O4-C4-C3	2.65	116.48	110.35
2	B	1	NAG	C4-C3-C2	-2.52	107.33	111.02

There are no chirality outliers.

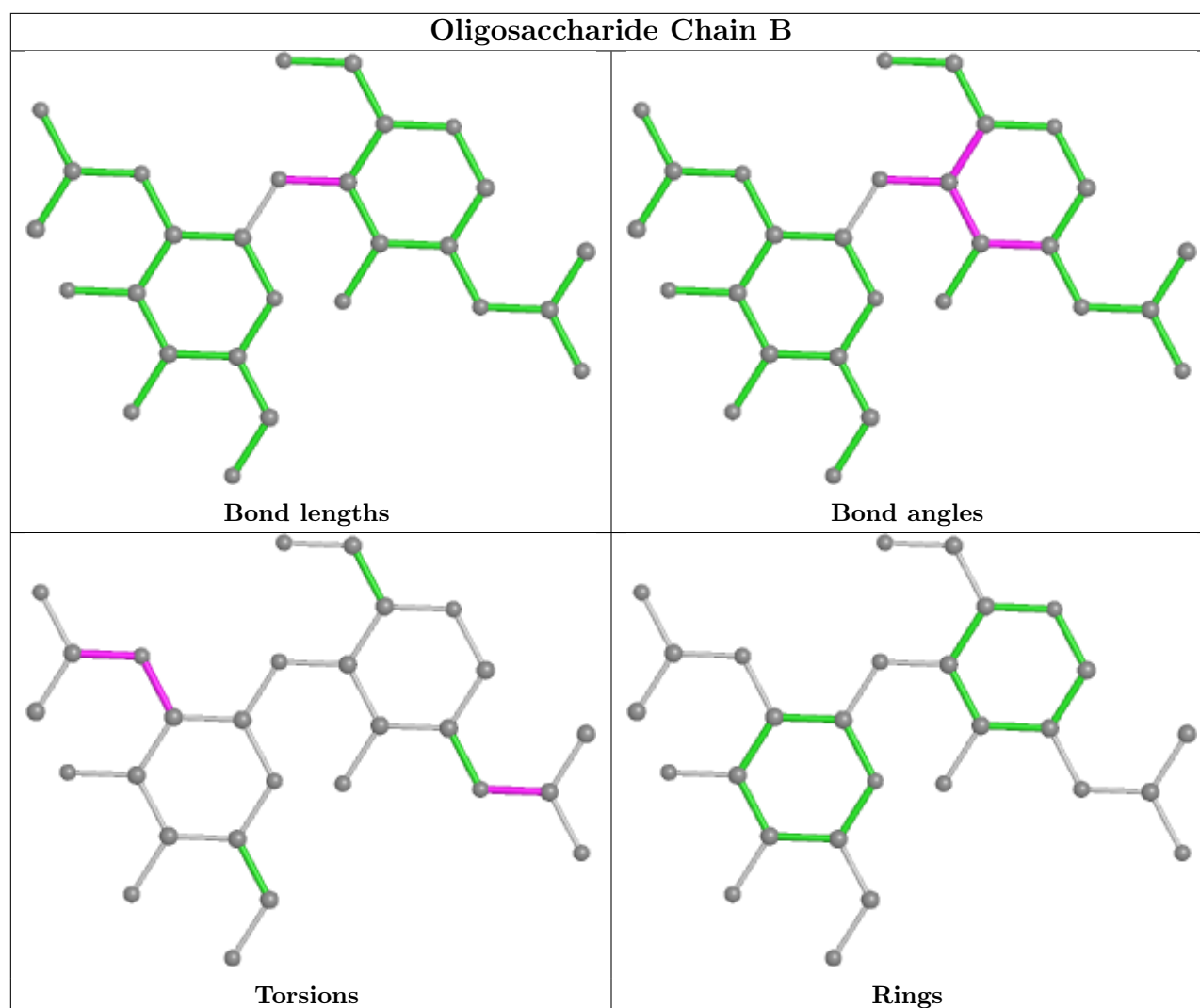
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	2	NAG	C1-C2-N2-C7

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.



## 5.6 Ligand geometry [i](#)

2 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	NAG	A	802	1	14,14,15	0.28	0	17,19,21	0.61	0
3	30B	A	801	-	49,58,58	1.95	10 (20%)	60,88,88	1.97	13 (21%)

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	NAG	A	802	1	-	2/6/23/26	0/1/1/1
3	30B	A	801	-	-	20/51/79/79	0/6/7/7

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	30B	C9-N13	8.04	1.49	1.35
3	A	801	30B	C17-C16	4.20	1.55	1.51
3	A	801	30B	C24-C29	4.11	1.46	1.40
3	A	801	30B	C11-C18	-3.98	1.45	1.49
3	A	801	30B	C16-N8	2.61	1.50	1.45
3	A	801	30B	O7-C6	-2.35	1.18	1.23
3	A	801	30B	C16-C12	-2.13	1.49	1.53
3	A	801	30B	C36-S35	2.06	1.73	1.70
3	A	801	30B	C29-C28	2.03	1.46	1.43
3	A	801	30B	C27-C28	2.03	1.47	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	30B	C4-C3-C2	5.25	108.62	103.02
3	A	801	30B	O42-C24-C29	5.12	118.98	115.03
3	A	801	30B	O46-C12-C16	-4.67	115.18	120.74
3	A	801	30B	O23-C30-C27	4.55	120.20	114.22
3	A	801	30B	C17-C16-N8	4.36	123.66	117.80
3	A	801	30B	C31-C30-C27	-4.35	116.52	121.88
3	A	801	30B	C16-N8-C6	3.85	131.67	121.89
3	A	801	30B	C28-N33-C32	3.28	120.76	117.02
3	A	801	30B	C39-C37-N38	-3.13	115.20	120.30
3	A	801	30B	C19-C20-C21	-2.54	102.70	113.79
3	A	801	30B	O42-C24-C25	-2.46	120.15	124.37
3	A	801	30B	C20-C21-C22	-2.41	98.64	112.43
3	A	801	30B	O7-C6-C3	2.03	124.18	121.73

There are no chirality outliers.

All (22) torsion outliers are listed below:



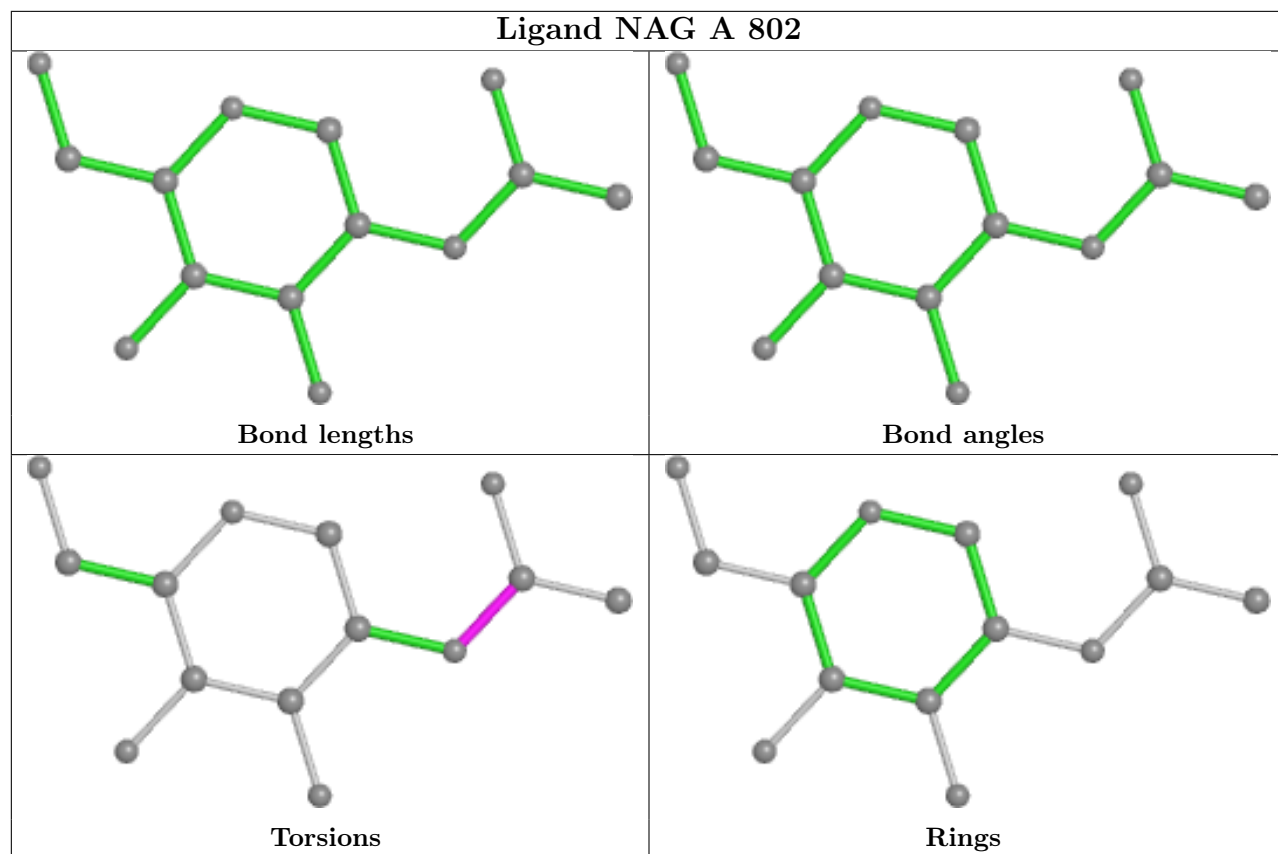
Mol	Chain	Res	Type	Atoms
3	A	801	30B	C1-C5-O23-C30
3	A	801	30B	C4-C5-O23-C30
3	A	801	30B	C12-C16-N8-C6
3	A	801	30B	N45-C12-C16-C11
3	A	801	30B	O46-C12-C16-N8
3	A	801	30B	O46-C12-C16-C11
3	A	801	30B	C51-C48-S47-O50
4	A	802	NAG	C8-C7-N2-C2
3	A	801	30B	O7-C6-N8-C16
3	A	801	30B	C14-C19-C20-C21
3	A	801	30B	C25-C24-O42-C43
3	A	801	30B	C29-C24-O42-C43
4	A	802	NAG	O7-C7-N2-C2
3	A	801	30B	C27-C30-O23-C5
3	A	801	30B	C31-C30-O23-C5
3	A	801	30B	C3-C6-N8-C16
3	A	801	30B	C52-C48-S47-O49
3	A	801	30B	C52-C48-S47-O50
3	A	801	30B	C4-C3-C6-N8
3	A	801	30B	C19-C14-N13-C15
3	A	801	30B	C4-C3-C6-O7
3	A	801	30B	C16-C11-C18-C22

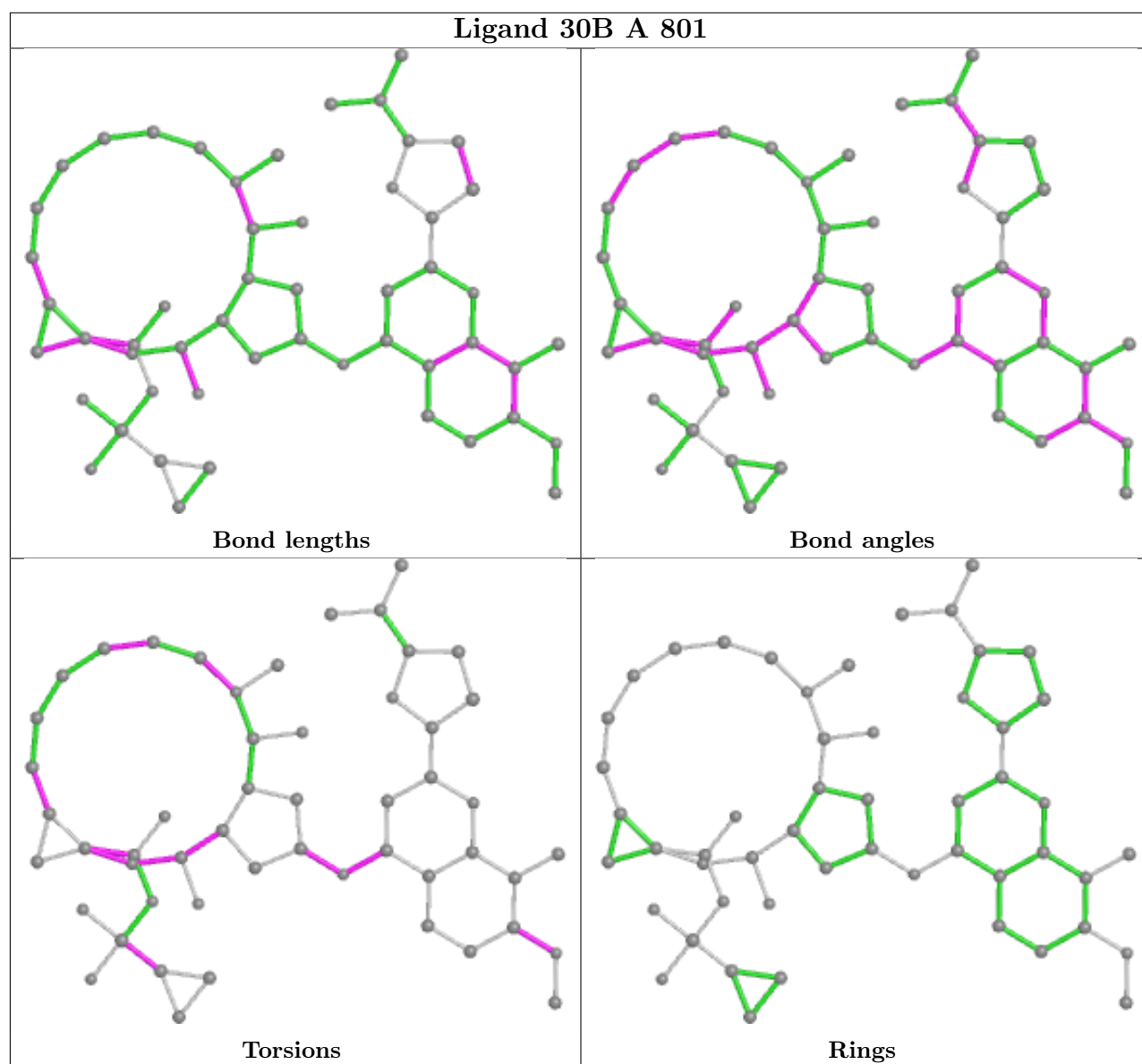
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	30B	6	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.