



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2021 – 12:51 PM EDT

PDB ID : 6XKD
Title : Structure of ligand-bound mouse cGAMP hydrolase ENPP1
Authors : Fernandez, D.; Li, L.
Deposited on : 2020-06-26
Resolution : 3.20 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.18
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) : 2.18

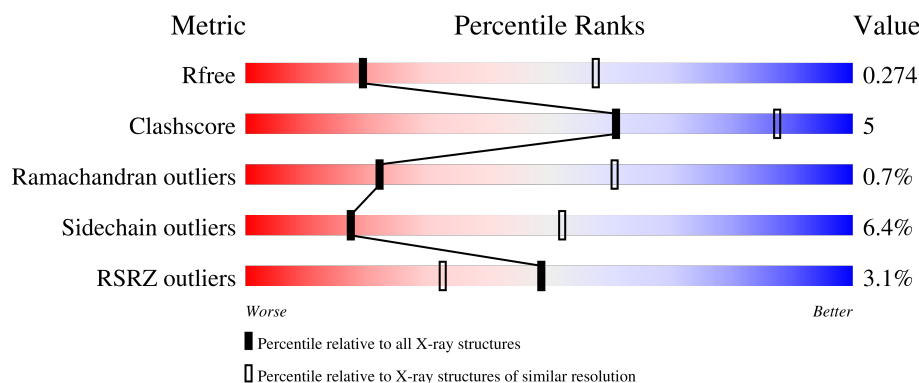
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	823	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>13%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	823	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>12%</div> <div>•</div> <div>17%</div> </div> </div>
2	C	4	<div> <div></div> <div>100%</div> </div>
2	D	4	<div> <div></div> <div>100%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10875 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.

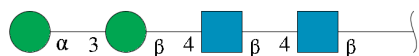
- Molecule 1 is a protein called Ectonucleotide pyrophosphatase/phosphodiesterase family member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	679	Total	C	N	O	S	0	0	0
			5374	3466	882	997	29			
1	B	681	Total	C	N	O	S	0	0	0
			5308	3436	870	976	26			

There are 18 discrepancies between the modelled and reference sequences:

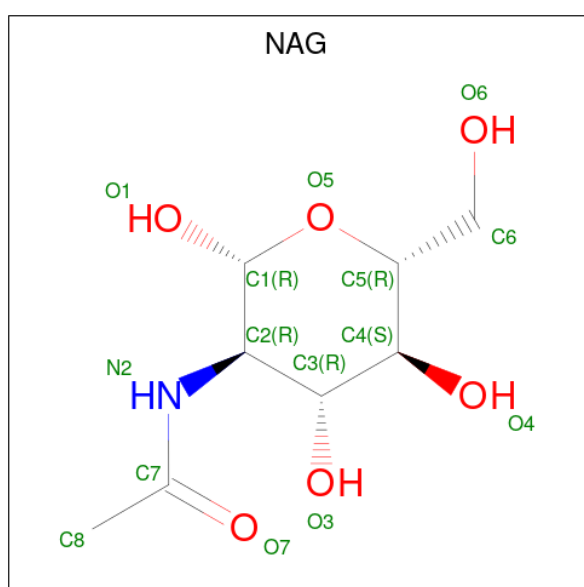
Chain	Residue	Modelled	Actual	Comment	Reference
A	83	TRP	-	expression tag	UNP G3X9S2
A	84	THR	-	expression tag	UNP G3X9S2
A	85	ASN	-	expression tag	UNP G3X9S2
A	86	THR	-	expression tag	UNP G3X9S2
A	87	SER	-	expression tag	UNP G3X9S2
A	88	GLY	-	expression tag	UNP G3X9S2
A	89	SER	-	expression tag	UNP G3X9S2
A	90	CYS	-	expression tag	UNP G3X9S2
A	91	ARG	-	expression tag	UNP G3X9S2
B	83	TRP	-	expression tag	UNP G3X9S2
B	84	THR	-	expression tag	UNP G3X9S2
B	85	ASN	-	expression tag	UNP G3X9S2
B	86	THR	-	expression tag	UNP G3X9S2
B	87	SER	-	expression tag	UNP G3X9S2
B	88	GLY	-	expression tag	UNP G3X9S2
B	89	SER	-	expression tag	UNP G3X9S2
B	90	CYS	-	expression tag	UNP G3X9S2
B	91	ARG	-	expression tag	UNP G3X9S2

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		

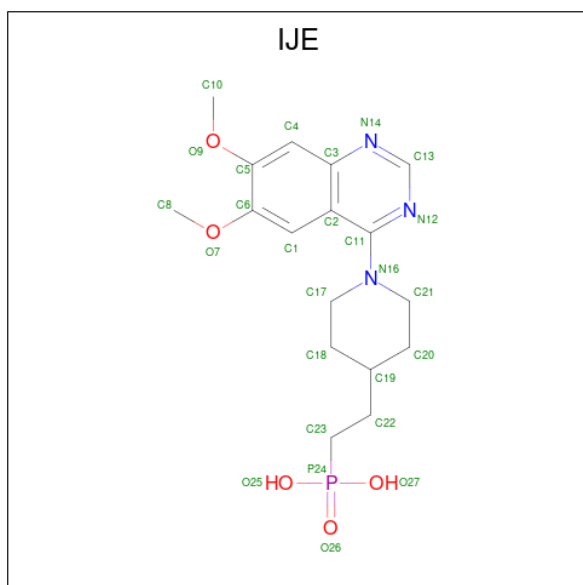
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

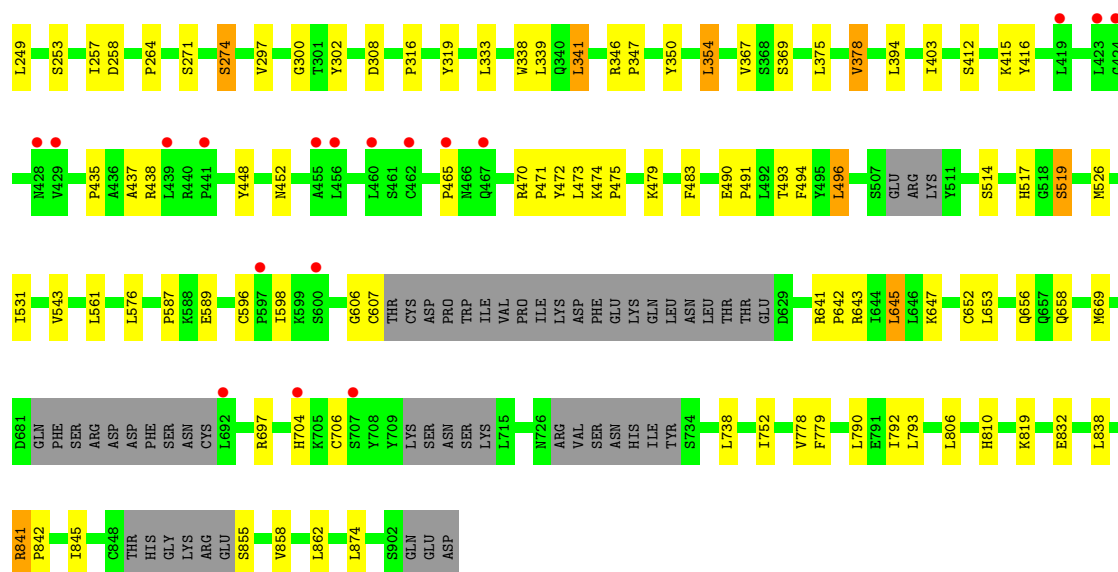
- Molecule 7 is {2-[1-(6,7-dimethoxyquinazolin-4-yl)piperidin-4-yl]ethyl}phosphonic acid (three-letter code: IJE) (formula: C₁₇H₂₄N₃O₅P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O P 26 17 3 5 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	18	Total O 18 18	0	0
8	B	14	Total O 14 14	0	0



- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%

MAG1
MAG2
BMA3
MAN4

- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	102.35Å 102.35Å 172.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.64 – 3.20 51.18 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.7 (30.64-3.20) 91.8 (51.18-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.201 , 0.273 0.202 , 0.274	Depositor DCC
R_{free} test set	1522 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	64.3	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.043 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10875	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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, MAN, BMA, CA, ZN, CL, IJE

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	0.47	0/5530	0.67	0/7539
1	B	0.46	0/5465	0.67	1/7465 (0.0%)
All	All	0.46	0/10995	0.67	1/15004 (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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	855	SER	N-CA-CB	6.13	119.70	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	411	GLY	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	5374	0	5119	52	0
1	B	5308	0	5006	43	0
2	C	50	0	43	0	0
2	D	50	0	43	0	0
3	A	28	0	26	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	A	26	0	0	3	0
8	A	18	0	0	0	0
8	B	14	0	0	0	0
All	All	10875	0	10237	95	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 5.

All (95) 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:778:VAL:HB	1:A:810:HIS:HB2	1.73	0.71
1:A:238:THR:OG1	7:A:1011:IJE:O26	2.12	0.67
1:A:438:ARG:HG2	1:A:493:THR:HG22	1.77	0.66
1:A:238:THR:OG1	7:A:1011:IJE:P24	2.55	0.65
1:A:193:PRO:HG2	1:A:398:LEU:HD12	1.79	0.63
1:B:474:LYS:HG3	1:B:475:PRO:HD3	1.82	0.61
1:B:437:ALA:HB3	1:B:494:PHE:HB2	1.81	0.61
1:A:485:LYS:HD3	1:A:784:ASP:HB3	1.83	0.60
1:B:438:ARG:HD2	1:B:490:GLU:OE1	2.04	0.57
1:A:358:ASP:O	1:A:362:HIS:HD2	1.87	0.57
1:B:247:THR:HB	1:B:249:LEU:HD12	1.86	0.57
1:B:790:LEU:HA	1:B:793:LEU:HD12	1.88	0.56
1:A:210:TRP:HB3	1:A:213:LEU:HD12	1.88	0.55
1:A:259:ASN:HD22	1:A:272:LEU:HD11	1.72	0.54
1:A:633:TYR:OH	1:A:641:ARG:HG2	2.06	0.54
1:A:452:ASN:HD21	1:A:455:ALA:HB3	1.73	0.54
1:A:663:TYR:HA	1:A:670:PRO:HA	1.89	0.54
1:A:643:ARG:NH2	1:A:883:ASP:OD2	2.40	0.54
1:A:695:ASP:HB3	1:A:698:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:LEU:HD22	1:A:806:LEU:HD21	1.90	0.53
1:A:238:THR:OG1	7:A:1011:IJE:O25	2.27	0.53
1:A:605:LEU:HB3	1:A:705:LYS:HA	1.88	0.53
1:A:654:LEU:HB2	1:A:661:THR:HG22	1.91	0.53
1:A:474:LYS:HD3	1:A:491:PRO:HA	1.90	0.52
1:A:192:PRO:HB3	1:A:397:CYS:O	2.09	0.52
1:A:187:ALA:O	1:A:188:GLU:HB2	2.09	0.52
1:A:839:PRO:HG3	1:A:865:HIS:CE1	2.46	0.50
1:B:589:GLU:OE2	1:B:641:ARG:NH2	2.36	0.50
1:B:300:GLY:O	1:B:350:TYR:HA	2.12	0.50
1:A:361:GLY:O	1:A:515:GLY:HA3	2.13	0.49
1:B:793:LEU:HD22	1:B:806:LEU:HD21	1.94	0.49
1:B:412:SER:HB3	1:B:415:LYS:HB2	1.95	0.49
1:B:233:MET:N	1:B:241:ASN:OD1	2.42	0.48
1:A:761:LEU:HG	1:A:771:ILE:HD11	1.96	0.48
1:B:230:MET:HE1	1:B:403:ILE:HD11	1.96	0.48
1:A:816:THR:HG22	1:A:831:LEU:HD22	1.95	0.48
1:A:411:GLY:HA3	1:A:514:SER:O	2.14	0.47
1:B:188:GLU:O	1:B:346:ARG:NH2	2.46	0.47
1:B:435:PRO:HA	1:B:496:LEU:HD13	1.95	0.47
1:B:339:LEU:HD23	1:B:394:LEU:HD13	1.95	0.47
1:A:378:VAL:O	1:A:382:VAL:HG23	2.15	0.47
1:A:434:GLY:HA2	1:A:501:GLN:HE21	1.80	0.47
1:A:771:ILE:HD12	1:A:815:LEU:HD22	1.96	0.47
1:B:470:ARG:HD2	1:B:472:TYR:CE2	2.49	0.47
1:B:517:HIS:HB2	1:B:526:MET:CE	2.45	0.46
1:A:338:TRP:O	1:A:346:ARG:HG3	2.14	0.46
1:A:438:ARG:HB3	1:A:490:GLU:HB2	1.98	0.46
1:A:474:LYS:HG2	1:A:484:ALA:HA	1.98	0.46
1:A:807:ILE:HA	1:A:808:PRO:HD3	1.82	0.46
1:A:884:ARG:HG3	1:A:886:GLU:OE2	2.16	0.46
1:B:669:MET:SD	1:B:779:PHE:HZ	2.38	0.46
1:A:410:GLN:NE2	1:A:411:GLY:H	2.14	0.45
1:B:596:CYS:HB3	1:B:697:ARG:HB3	1.99	0.45
1:B:838:LEU:HD11	1:B:862:LEU:HD22	1.99	0.45
1:B:543:VAL:HG21	1:B:576:LEU:HD11	1.99	0.45
1:B:316:PRO:HB2	1:B:319:TYR:HB3	1.99	0.45
1:B:641:ARG:HD3	1:B:653:LEU:HD21	1.98	0.45
1:B:474:LYS:HG2	1:B:491:PRO:HA	1.98	0.44
1:B:752:ILE:HG23	1:B:858:VAL:HG13	1.99	0.44
1:B:297:VAL:HG21	1:B:561:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:HD12	1:A:350:TYR:CZ	2.52	0.44
1:A:358:ASP:O	1:A:362:HIS:CD2	2.69	0.44
1:B:214:LEU:HD21	1:B:375:LEU:HB3	2.00	0.44
1:A:364:HIS:CE1	1:A:370:GLU:HG2	2.53	0.43
1:A:452:ASN:HD21	1:A:455:ALA:CB	2.30	0.43
1:B:587:PRO:HG2	1:B:645:LEU:HD11	2.00	0.43
1:B:470:ARG:HD2	1:B:472:TYR:HE2	1.82	0.43
1:B:220:LEU:HB3	1:B:531:ILE:HG21	2.00	0.43
1:B:338:TRP:HA	1:B:341:LEU:HD13	2.00	0.43
1:B:641:ARG:HD2	1:B:642:PRO:O	2.18	0.43
1:A:470:ARG:HD3	1:A:846:GLU:O	2.19	0.42
1:B:470:ARG:HA	1:B:471:PRO:HD3	1.94	0.42
1:B:271:SER:O	1:B:274:SER:HB3	2.20	0.42
1:B:257:ILE:HG13	1:B:483:PHE:HE1	1.84	0.42
1:B:354:LEU:HD23	1:B:378:VAL:HG22	2.01	0.42
1:A:386:MET:CE	1:A:400:LEU:HD22	2.48	0.42
1:B:200:ASP:OD2	1:B:238:THR:HG23	2.19	0.42
1:B:236:THR:OG1	1:B:519:SER:O	2.38	0.42
1:A:366:PRO:O	1:A:371:VAL:HG21	2.19	0.42
1:B:264:PRO:HG3	1:B:448:TYR:CE2	2.55	0.42
1:B:479:LYS:HE3	1:B:810:HIS:CE1	2.55	0.42
1:B:778:VAL:HB	1:B:810:HIS:HB2	2.02	0.42
1:A:596:CYS:HB3	1:A:697:ARG:HB3	2.02	0.41
1:B:225:THR:HG21	1:B:576:LEU:HG	2.02	0.41
1:B:300:GLY:H	1:B:347:PRO:HB3	1.85	0.41
1:B:841:ARG:HH12	1:B:845:ILE:HG22	1.85	0.41
1:A:338:TRP:O	1:A:341:LEU:HB2	2.20	0.41
1:A:669:MET:SD	1:A:779:PHE:HZ	2.43	0.41
1:A:196:LEU:HD22	1:A:555:MET:SD	2.60	0.41
1:A:301:THR:HG21	1:A:307:SER:HB2	2.02	0.41
1:A:530:PHE:CD1	1:A:530:PHE:C	2.95	0.40
1:A:225:THR:HG21	1:A:576:LEU:HG	2.03	0.40
1:A:717:TYR:O	1:A:750:GLN:NE2	2.55	0.40
1:A:298:LYS:HB2	1:A:347:PRO:HA	2.03	0.40
1:A:674:SER:HA	1:A:773:VAL:O	2.22	0.40

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	663/823 (81%)	602 (91%)	58 (9%)	3 (0%)	29	67
1	B	667/823 (81%)	616 (92%)	45 (7%)	6 (1%)	17	56
All	All	1330/1646 (81%)	1218 (92%)	103 (8%)	9 (1%)	22	61

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	GLU
1	A	303	PHE
1	B	465	PRO
1	B	606	GLY
1	B	179	SER
1	B	647	LYS
1	B	341	LEU
1	B	598	ILE
1	A	491	PRO

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	593/755 (78%)	555 (94%)	38 (6%)	17	52
1	B	570/755 (76%)	533 (94%)	37 (6%)	17	51
All	All	1163/1510 (77%)	1088 (94%)	75 (6%)	17	52

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	PHE
1	A	239	PHE
1	A	302	TYR
1	A	345	GLU
1	A	359	SER
1	A	392	LEU
1	A	412	SER
1	A	416	TYR
1	A	427	ASN
1	A	452	ASN
1	A	461	SER
1	A	463	ARG
1	A	474	LYS
1	A	479	LYS
1	A	512	CYS
1	A	551	VAL
1	A	566	ASN
1	A	579	LYS
1	A	585	SER
1	A	593	LEU
1	A	604	ASP
1	A	608	THR
1	A	641	ARG
1	A	645	LEU
1	A	658	GLN
1	A	661	THR
1	A	694	GLN
1	A	716	SER
1	A	751	VAL
1	A	761	LEU
1	A	792	ILE
1	A	805	ILE
1	A	807	ILE
1	A	816	THR
1	A	818	CYS
1	A	834	SER
1	A	847	SER
1	A	874	LEU
1	B	182	THR
1	B	197	PHE
1	B	202	PHE
1	B	236	THR

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Mol	Chain	Res	Type
1	B	239	PHE
1	B	253	SER
1	B	258	ASP
1	B	274	SER
1	B	302	TYR
1	B	308	ASP
1	B	333	LEU
1	B	354	LEU
1	B	367	VAL
1	B	369	SER
1	B	378	VAL
1	B	416	TYR
1	B	452	ASN
1	B	473	LEU
1	B	493	THR
1	B	496	LEU
1	B	514	SER
1	B	519	SER
1	B	607	CYS
1	B	643	ARG
1	B	645	LEU
1	B	652	CYS
1	B	656	GLN
1	B	658	GLN
1	B	704	HIS
1	B	706	CYS
1	B	738	LEU
1	B	792	ILE
1	B	819	LYS
1	B	832	GLU
1	B	841	ARG
1	B	842	PRO
1	B	874	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	452	ASN
1	A	501	GLN
1	A	885	GLN
1	B	452	ASN
1	B	482	HIS

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Mol	Chain	Res	Type
1	B	583	ASN
1	B	810	HIS

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 ⓘ

8 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	C	1	1,2	14,14,15	0.59	0	17,19,21	1.43	3 (17%)
2	NAG	C	2	2	14,14,15	0.40	0	17,19,21	1.32	1 (5%)
2	BMA	C	3	2	11,11,12	0.57	0	15,15,17	1.40	1 (6%)
2	MAN	C	4	2	11,11,12	0.76	0	15,15,17	1.52	3 (20%)
2	NAG	D	1	1,2	14,14,15	0.45	0	17,19,21	1.60	4 (23%)
2	NAG	D	2	2	14,14,15	0.56	0	17,19,21	1.39	2 (11%)
2	BMA	D	3	2	11,11,12	0.93	1 (9%)	15,15,17	1.11	1 (6%)
2	MAN	D	4	2	11,11,12	0.76	0	15,15,17	1.48	2 (13%)

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	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	BMA	C2-C3	2.09	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	4.56	118.37	112.19
2	C	2	NAG	C1-O5-C5	4.53	118.33	112.19
2	D	1	NAG	C1-O5-C5	3.99	117.59	112.19
2	D	4	MAN	C1-C2-C3	3.93	114.49	109.67
2	C	3	BMA	C3-C4-C5	3.62	116.70	110.24
2	C	4	MAN	C1-O5-C5	3.40	116.81	112.19
2	C	4	MAN	O5-C5-C6	3.39	112.52	107.20
2	C	1	NAG	O5-C1-C2	-3.35	106.00	111.29
2	D	1	NAG	O5-C1-C2	-3.24	106.17	111.29
2	C	1	NAG	C4-C3-C2	3.14	115.61	111.02
2	D	4	MAN	C1-O5-C5	2.68	115.82	112.19
2	D	1	NAG	C4-C3-C2	2.56	114.77	111.02
2	C	4	MAN	C1-C2-C3	2.46	112.69	109.67
2	D	3	BMA	O5-C5-C6	2.30	110.81	107.20
2	D	2	NAG	O4-C4-C5	2.22	114.80	109.30
2	D	1	NAG	C1-C2-N2	2.07	114.03	110.49
2	C	1	NAG	C3-C4-C5	2.03	113.85	110.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	MAN	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6

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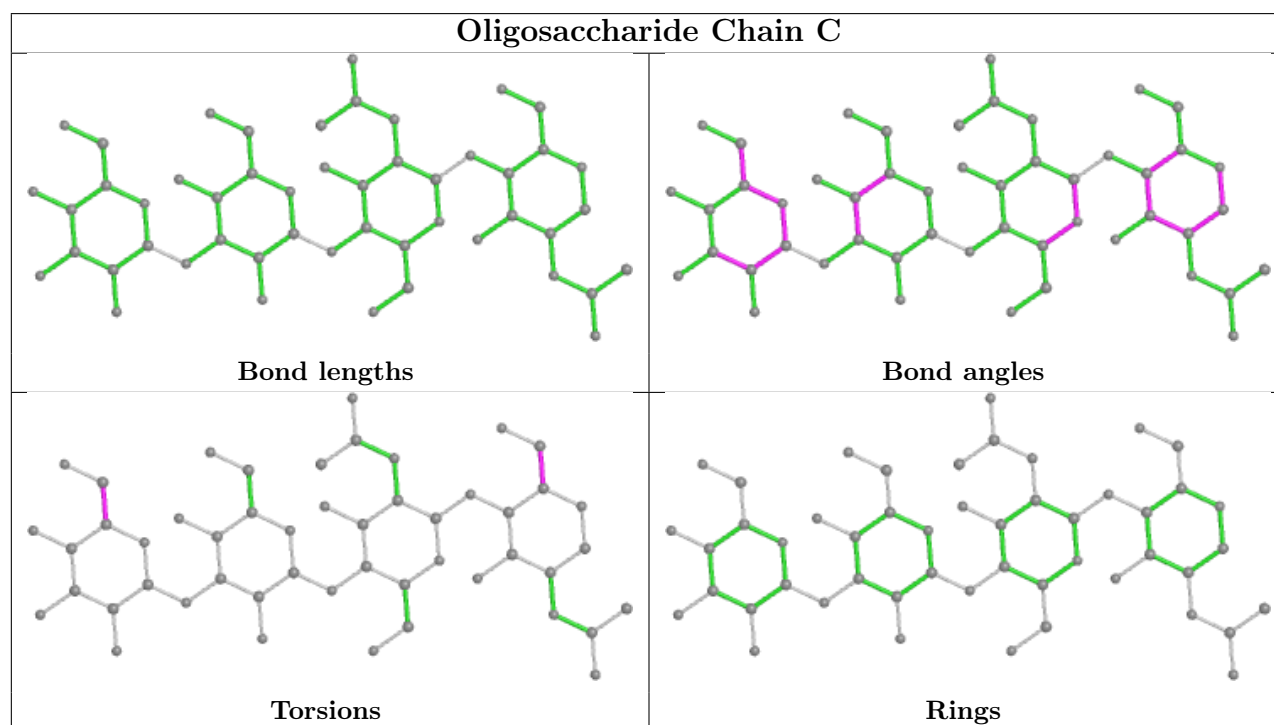
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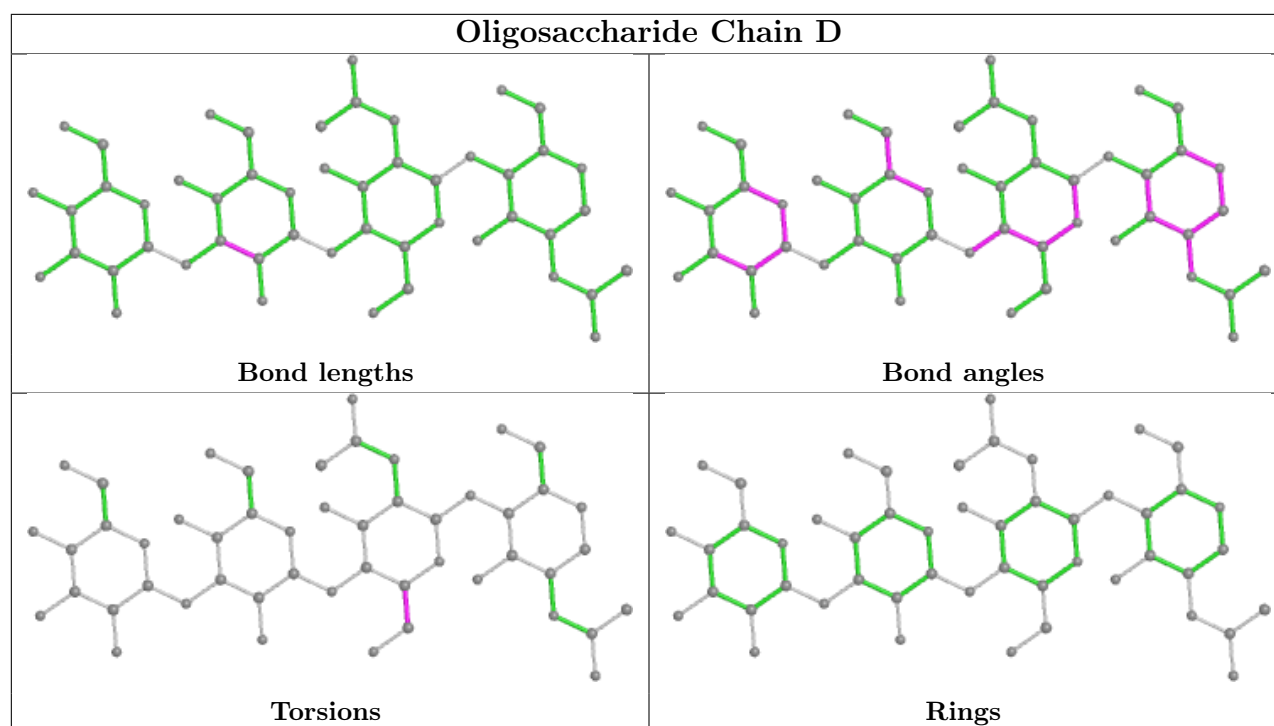
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

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.





5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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	$\# Z > 2$
3	NAG	A	1005	1	14,14,15	0.65	0	17,19,21	1.61	3 (17%)
3	NAG	A	1006	1	14,14,15	0.72	0	17,19,21	0.99	1 (5%)
7	IJE	A	1011	4	28,28,28	1.74	7 (25%)	39,40,40	2.50	13 (33%)

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	NAG	A	1005	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
7	IJE	A	1011	4	-	8/14/24/24	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1011	IJE	C6-C5	4.14	1.49	1.40
7	A	1011	IJE	P24-C23	3.69	1.82	1.78
7	A	1011	IJE	C2-C3	3.56	1.48	1.42
7	A	1011	IJE	P24-O26	2.97	1.56	1.50
7	A	1011	IJE	C4-C3	-2.89	1.37	1.41
7	A	1011	IJE	C3-N14	-2.08	1.33	1.37
7	A	1011	IJE	C11-C2	2.06	1.48	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1011	IJE	O9-C5-C4	-7.94	114.97	125.24
7	A	1011	IJE	O9-C5-C6	6.13	123.95	115.41
7	A	1011	IJE	O7-C6-C1	-4.73	119.13	125.24
3	A	1005	NAG	C4-C3-C2	4.19	117.17	111.02
7	A	1011	IJE	C10-O9-C5	-3.99	111.50	117.53
7	A	1011	IJE	O7-C6-C5	3.93	120.89	115.41
3	A	1006	NAG	C1-O5-C5	3.16	116.48	112.19
7	A	1011	IJE	C21-N16-C17	3.09	118.34	111.52
7	A	1011	IJE	C18-C17-N16	-2.95	105.02	111.10
7	A	1011	IJE	C13-N14-C3	2.93	119.43	115.40
3	A	1005	NAG	C2-N2-C7	2.82	126.92	122.90
7	A	1011	IJE	C2-C11-N12	-2.65	116.48	122.64
3	A	1005	NAG	C1-O5-C5	2.63	115.76	112.19
7	A	1011	IJE	N14-C13-N12	-2.60	124.62	128.68
7	A	1011	IJE	C2-C3-N14	-2.48	120.19	122.83
7	A	1011	IJE	C1-C2-C11	-2.39	122.43	124.94
7	A	1011	IJE	O25-P24-O27	-2.12	101.90	108.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1011	IJE	C22-C23-P24-O25
7	A	1011	IJE	C22-C23-P24-O26

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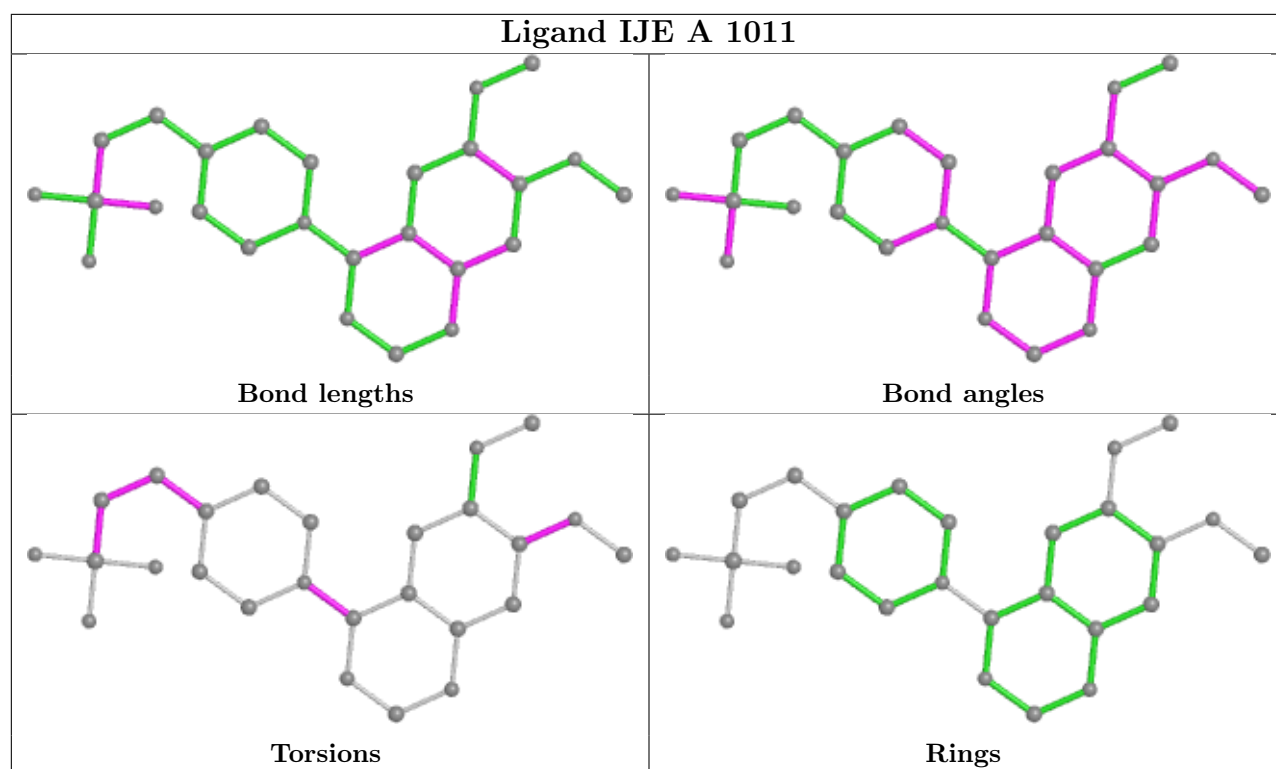
Mol	Chain	Res	Type	Atoms
7	A	1011	IJE	C19-C22-C23-P24
7	A	1011	IJE	C2-C11-N16-C21
7	A	1011	IJE	N12-C11-N16-C21
7	A	1011	IJE	C6-C5-O9-C10
7	A	1011	IJE	C4-C5-O9-C10
7	A	1011	IJE	C18-C19-C22-C23

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1011	IJE	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.



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, 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	679/823 (82%)	0.12	24 (3%)	44 28	36, 64, 100, 132	0
1	B	681/823 (82%)	0.01	18 (2%)	56 40	36, 64, 96, 123	0
All	All	1360/1646 (82%)	0.06	42 (3%)	49 32	36, 64, 98, 132	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	600	SER	3.9
1	A	609	CYS	3.8
1	A	602	SER	3.7
1	B	467	GLN	3.5
1	A	442	THR	3.5
1	A	596	CYS	3.5
1	B	456	LEU	3.4
1	B	600	SER	3.3
1	A	426	VAL	3.0
1	B	423	LEU	3.0
1	A	598	ILE	3.0
1	B	428	ASN	2.9
1	B	429	VAL	2.9
1	A	696	LEU	2.8
1	B	692	LEU	2.8
1	A	737	LEU	2.8
1	A	607	CYS	2.7
1	B	465	PRO	2.7
1	A	441	PRO	2.7
1	B	460	LEU	2.6
1	A	429	VAL	2.5
1	B	707	SER	2.5
1	A	443	ASP	2.4
1	B	424	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	439	LEU	2.4
1	A	425	ASP	2.4
1	B	455	ALA	2.4
1	B	419	LEU	2.4
1	A	460	LEU	2.3
1	A	384	MET	2.3
1	A	422	TYR	2.3
1	A	503	ALA	2.2
1	A	691	CYS	2.1
1	A	457	ALA	2.1
1	B	441	PRO	2.1
1	B	704	HIS	2.1
1	A	427	ASN	2.1
1	B	597	PRO	2.1
1	B	462	CYS	2.1
1	A	389	LEU	2.1
1	A	260	LYS	2.0
1	A	700	LEU	2.0

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.

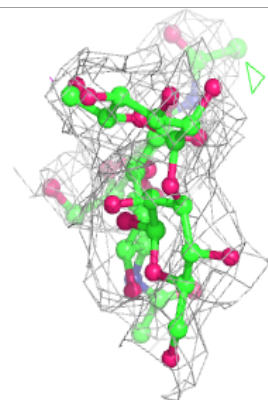
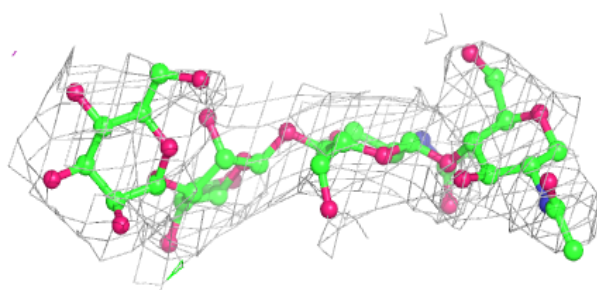
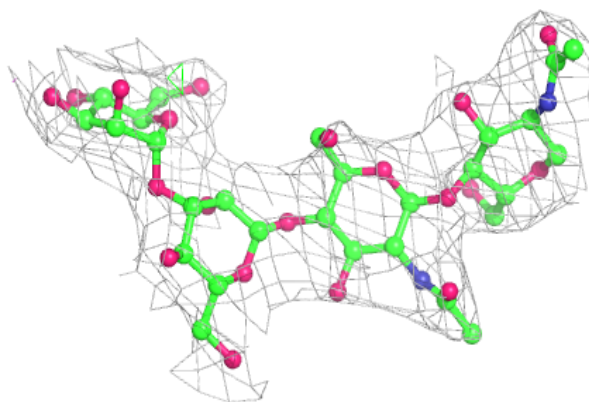
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	D	3	11/12	0.73	0.23	103,109,117,117	0
2	MAN	D	4	11/12	0.73	0.30	110,118,120,129	0
2	MAN	C	4	11/12	0.89	0.15	94,95,97,97	0
2	NAG	D	2	14/15	0.90	0.18	65,77,87,96	0
2	BMA	C	3	11/12	0.91	0.15	85,91,95,95	0
2	NAG	C	2	14/15	0.92	0.20	73,80,86,87	0
2	NAG	D	1	14/15	0.96	0.18	47,55,60,67	0
2	NAG	C	1	14/15	0.97	0.19	52,56,59,68	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

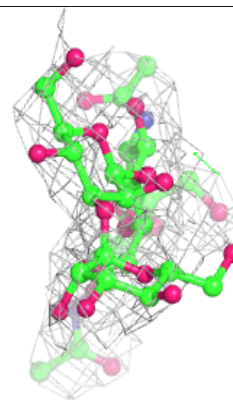
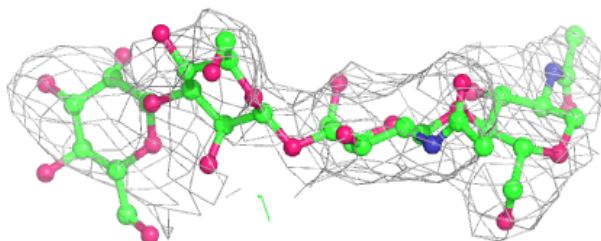
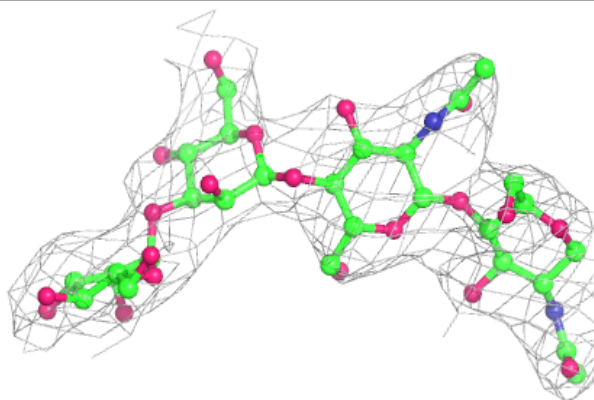
Electron density around Chain C:

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



Electron density around Chain D:

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

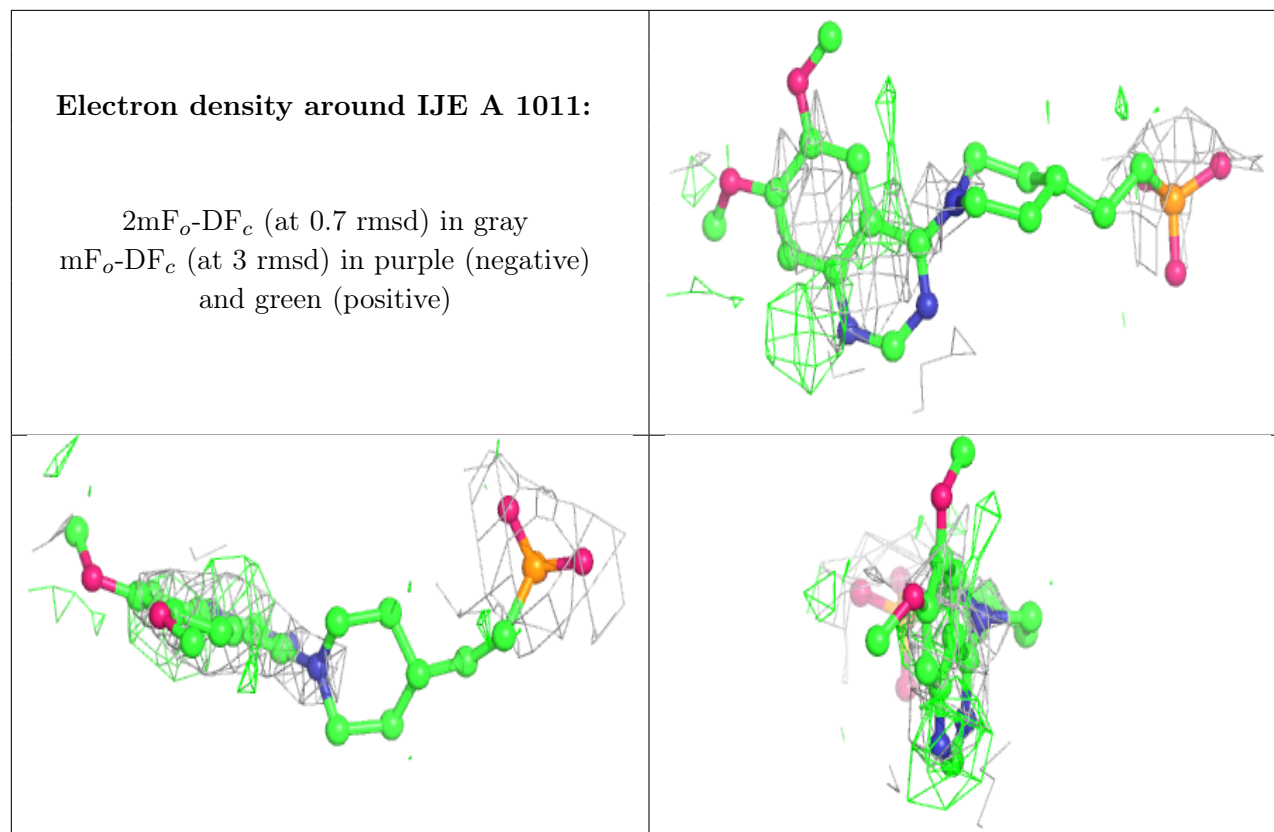


6.4 Ligands ⓘ

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(Å ²)	Q<0.9
3	NAG	A	1006	14/15	0.77	0.34	85,97,106,112	0
3	NAG	A	1005	14/15	0.81	0.31	89,103,114,117	0
6	CL	A	1010	1/1	0.93	0.15	43,43,43,43	0
5	CA	B	1003	1/1	0.96	0.14	64,64,64,64	0
5	CA	A	1009	1/1	0.97	0.12	70,70,70,70	0
7	IJE	A	1011	26/26	0.97	0.27	59,66,68,70	26
4	ZN	B	1002	1/1	0.98	0.19	61,61,61,61	0
4	ZN	A	1008	1/1	0.99	0.16	54,54,54,54	0
4	ZN	A	1007	1/1	0.99	0.17	57,57,57,57	0
4	ZN	B	1001	1/1	1.00	0.17	45,45,45,45	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.