Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:27 AM BST

PDB ID	:	2XWE
Title	:	X-RAY STRUCTURE OF ACID-BETA-GLUCOSIDASE WITH 5N,6S-(N'-(N-OCTYL)IMINO)-6-THIONOJIRIMYCIN IN THE ACTIVE SITE
Authors	:	Brumshtein, B.; Aguilar-Moncayo, M.; Benito, J.M.; Ortiz Mellet, C.; Garcia Fernandez, J.M.; Silman, I.; Shaaltiel, Y.; Sussman, J.L.; Futerman, A.H.
Deposited on	:	2010-11-02
Resolution	:	2.31 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:

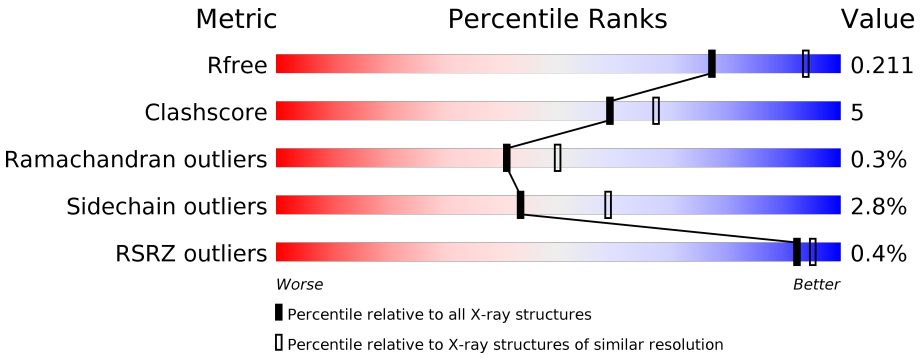
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 on 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 <=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	505	% 86% 11%
1	B	505	86% 12%
2	C	4	100%
2	D	4	50% 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8426 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.

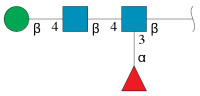
- Molecule 1 is a protein called GLUCOSYLCERAMIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3892	2509	662	705	16			
1	B	498	Total	C	N	O	S	0	0	0
			3911	2518	667	710	16			

There are 18 discrepancies between the modelled and reference sequences:

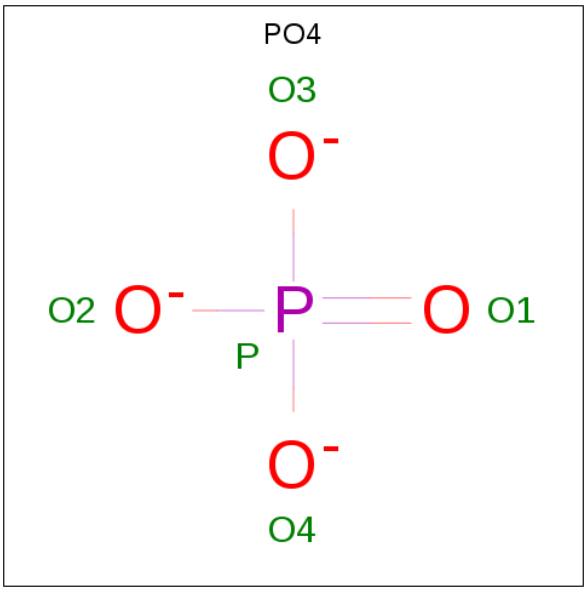
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLU	-	expression tag	UNP P04062
A	0	PHE	-	expression tag	UNP P04062
A	495	HIS	ARG	variant	UNP P04062
A	498	LEU	-	expression tag	UNP P04062
A	499	LEU	-	expression tag	UNP P04062
A	500	VAL	-	expression tag	UNP P04062
A	501	ASP	-	expression tag	UNP P04062
A	502	THR	-	expression tag	UNP P04062
A	503	MET	-	expression tag	UNP P04062
B	-1	GLU	-	expression tag	UNP P04062
B	0	PHE	-	expression tag	UNP P04062
B	495	HIS	ARG	variant	UNP P04062
B	498	LEU	-	expression tag	UNP P04062
B	499	LEU	-	expression tag	UNP P04062
B	500	VAL	-	expression tag	UNP P04062
B	501	ASP	-	expression tag	UNP P04062
B	502	THR	-	expression tag	UNP P04062
B	503	MET	-	expression tag	UNP P04062

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



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

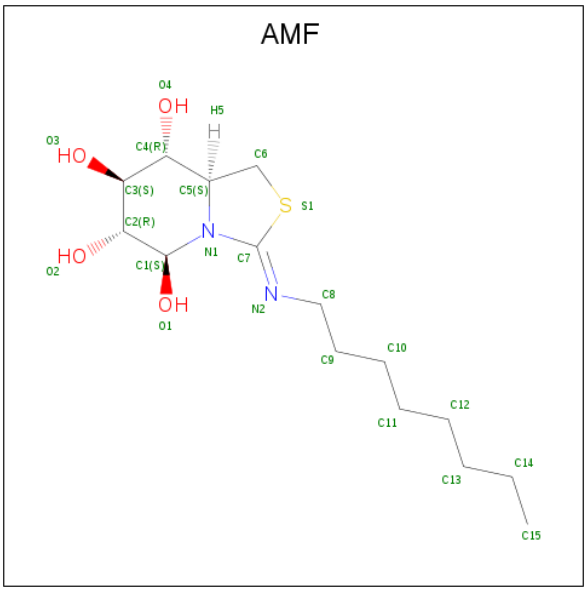


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total K 1 1	0	0
4	A	1	Total K 1 1	0	0

- Molecule 5 is (3Z,5S,6R,7S,8R,8aS)-3-(octylimino)hexahydro[1,3]thiazolo[3,4-a]pyridine-5,6,7,8-tetrol (three-letter code: AMF) (formula: $C_{15}H_{28}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			22	15	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			17	10	2	4	1		

- Molecule 6 is water.

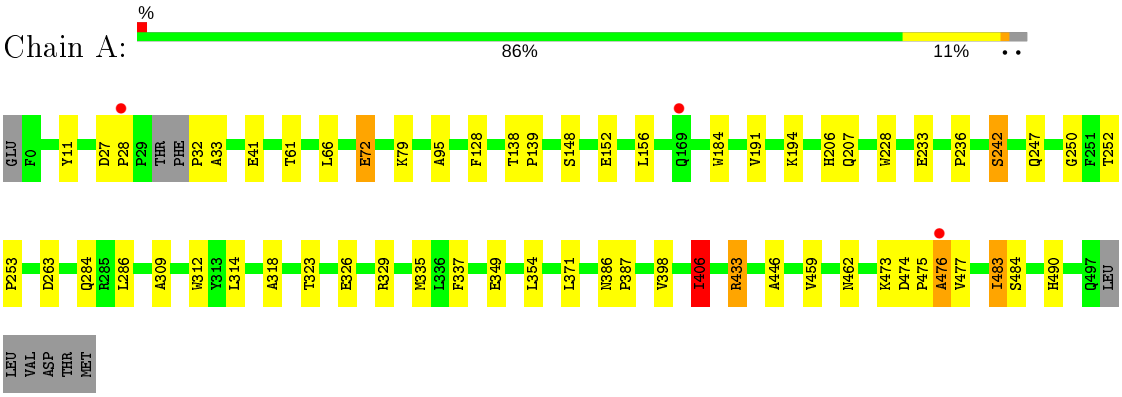
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	253	Total	O	0	0
			253	253		
6	B	221	Total	O	0	0
			221	221		

3 Residue-property plots (i)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

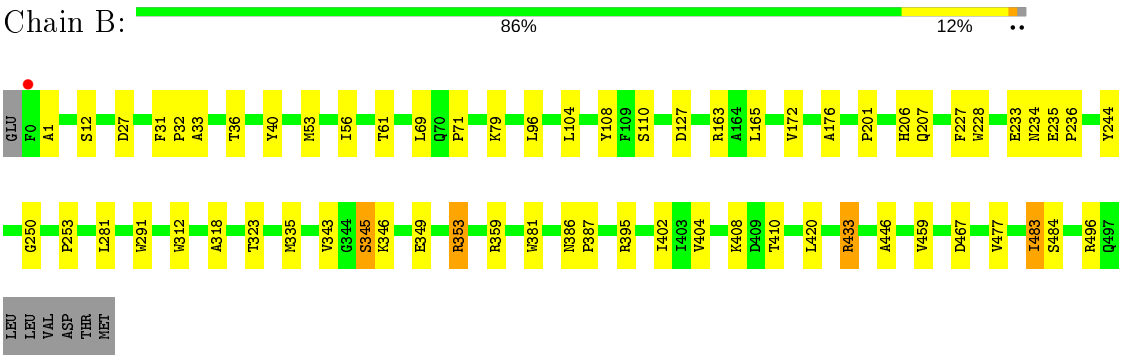
• Molecule 1: GLUCOSYLCERAMIDASE

Chain A:



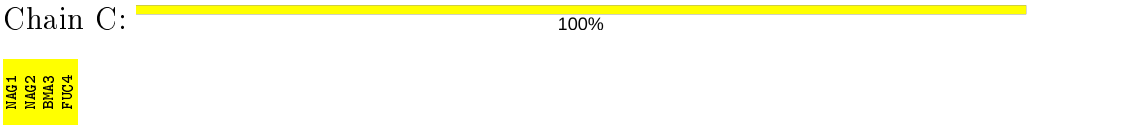
• Molecule 1: GLUCOSYLCERAMIDASE

Chain B:



• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:


NAG1
NAG2
BMA3
FUC4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.14Å 96.69Å 82.97Å 90.00° 102.84° 90.00°	Depositor
Resolution (Å)	19.82 – 2.31 19.82 – 2.31	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.82-2.31) 96.5 (19.82-2.31)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.51 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.150 , 0.213 0.150 , 0.211	Depositor DCC
R_{free} test set	2234 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	22.7	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8426	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, PO4, AMF, FUC, K

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	1.05	2/4011 (0.0%)	0.88	2/5472 (0.0%)
1	B	1.01	2/4031 (0.0%)	0.88	6/5502 (0.1%)
All	All	1.03	4/8042 (0.0%)	0.88	8/10974 (0.1%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	ALA	CA-CB	6.21	1.65	1.52
1	A	72	GLU	CG-CD	5.36	1.59	1.51
1	B	244	TYR	CD2-CE2	5.20	1.47	1.39
1	B	40	TYR	CD2-CE2	5.02	1.46	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	433	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	B	433	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	420	LEU	CB-CG-CD1	-6.20	100.46	111.00
1	B	163	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	395	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	B	353	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	406	ILE	CB-CA-C	-5.13	101.34	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	433	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	476	ALA	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	3892	0	3769	29	0
1	B	3911	0	3791	31	0
2	C	49	0	43	0	0
2	D	49	0	43	1	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	22	0	28	8	0
5	B	17	0	15	5	0
6	A	253	0	0	1	0
6	B	221	0	0	0	0
All	All	8426	0	7689	73	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 (73) 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)
5:B:607:AMF:H82C	5:B:607:AMF:O1	1.45	1.12
5:A:607:AMF:O1	5:A:607:AMF:H82C	1.53	1.06
5:B:607:AMF:O1	5:B:607:AMF:C8	2.11	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:607:AMF:O1	5:A:607:AMF:C8	2.10	0.97
5:A:607:AMF:C1	5:A:607:AMF:H81C	2.08	0.83
1:A:406:ILE:HG13	6:A:709:HOH:O	1.87	0.75
1:B:1:ALA:N	1:B:27:ASP:OD1	2.23	0.72
5:A:607:AMF:C1	5:A:607:AMF:C8	2.68	0.72
1:B:346:LYS:HE2	1:B:349:GLU:CD	2.14	0.68
1:B:236:PRO:O	1:B:250:GLY:HA2	1.97	0.65
1:B:343:VAL:HG21	1:B:359:ARG:HG2	1.77	0.65
1:B:165:LEU:HD22	1:B:172:VAL:HB	1.79	0.64
1:B:33:ALA:O	1:B:36:THR:HB	1.99	0.62
1:B:467:ASP:HB3	1:B:483:ILE:HD11	1.83	0.60
1:A:27:ASP:HB3	1:A:28:PRO:HD2	1.84	0.60
1:B:346:LYS:HG2	1:B:349:GLU:OE1	2.03	0.58
1:B:345:SER:HB3	5:B:607:AMF:S1	2.43	0.57
1:A:446:ALA:HA	1:A:459:VAL:O	2.06	0.55
1:B:104:LEU:HD23	1:B:104:LEU:C	2.26	0.55
1:B:79:LYS:HE2	1:B:228:TRP:CE2	2.42	0.55
1:A:95:ALA:HB1	1:A:406:ILE:HG23	1.90	0.54
1:B:408:LYS:O	1:B:410:THR:HG23	2.10	0.52
5:A:607:AMF:H82C	5:A:607:AMF:H154	1.71	0.51
1:A:66:LEU:HD11	1:A:473:LYS:HB2	1.91	0.51
5:B:607:AMF:H82C	5:B:607:AMF:H154	1.67	0.51
1:B:346:LYS:HE2	1:B:349:GLU:OE2	2.10	0.51
1:A:318:ALA:HB1	1:A:323:THR:HG21	1.94	0.50
5:A:607:AMF:O1	5:A:607:AMF:H81C	1.94	0.50
1:B:386:ASN:HB2	1:B:387:PRO:CD	2.42	0.49
1:A:284:GLN:HG3	1:A:314:LEU:HD12	1.93	0.49
1:A:309:ALA:HA	1:A:337:PHE:O	2.13	0.49
1:A:286:LEU:C	1:A:286:LEU:HD12	2.33	0.48
1:B:343:VAL:HG21	1:B:359:ARG:CG	2.40	0.48
1:B:56:ILE:HG21	1:B:477:VAL:HG23	1.95	0.48
1:B:12:SER:OG	3:B:605:PO4:O3	2.25	0.48
5:B:607:AMF:C8	5:B:607:AMF:C1	2.91	0.48
1:A:462:ASN:HB2	1:A:484:SER:OG	2.15	0.47
1:A:371:LEU:O	1:A:433:ARG:HD2	2.14	0.47
1:A:79:LYS:HE2	1:A:228:TRP:CE2	2.51	0.46
1:B:165:LEU:CD2	1:B:172:VAL:HB	2.46	0.46
1:B:108:TYR:CE2	1:B:402:ILE:HD12	2.51	0.46
5:A:607:AMF:H154	5:A:607:AMF:C8	2.26	0.45
1:B:201:PRO:HA	1:B:206:HIS:CG	2.51	0.45
1:A:138:THR:HA	1:A:139:PRO:HD3	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LYS:HB2	1:A:242:SER:HA	1.98	0.45
1:B:253:PRO:HB3	1:B:291:TRP:CD2	2.52	0.45
1:A:483:ILE:HG12	1:A:484:SER:N	2.31	0.45
1:A:11:TYR:HD2	1:A:354:LEU:O	2.01	0.44
1:B:176:ALA:HB2	1:B:227:PHE:CE2	2.53	0.44
1:B:234:ASN:O	1:B:235:GLU:C	2.56	0.44
1:A:386:ASN:HB2	1:A:387:PRO:CD	2.48	0.44
1:B:71:PRO:HG3	1:B:496:ARG:NH2	2.33	0.44
5:A:607:AMF:H81C	5:A:607:AMF:H155	1.95	0.43
1:A:206:HIS:HB3	1:A:263:ASP:OD2	2.19	0.43
1:B:318:ALA:HB1	1:B:323:THR:HG21	2.00	0.43
1:A:152:GLU:O	1:A:156:LEU:HB2	2.19	0.43
1:A:27:ASP:HB3	1:A:28:PRO:CD	2.47	0.42
1:A:32:PRO:HB2	1:A:33:ALA:H	1.52	0.42
1:A:139:PRO:HA	1:A:184:TRP:CD1	2.54	0.42
1:A:474:ASP:HA	1:A:475:PRO:HD2	1.93	0.42
1:A:41:GLU:HG3	1:A:490:HIS:CD2	2.55	0.41
1:B:346:LYS:HG2	1:B:349:GLU:CD	2.41	0.41
1:B:483:ILE:HG13	1:B:484:SER:N	2.34	0.41
1:B:96:LEU:HD21	1:B:404:VAL:HG13	2.02	0.41
1:A:191:VAL:O	1:A:247:GLN:HA	2.21	0.41
1:A:128:PHE:CZ	1:A:398:VAL:HG22	2.55	0.41
1:B:446:ALA:HA	1:B:459:VAL:O	2.21	0.41
1:A:326:GLU:OE2	1:A:329:ARG:NH2	2.45	0.40
1:A:236:PRO:O	1:A:250:GLY:HA2	2.20	0.40
1:B:127:ASP:N	1:B:127:ASP:OD1	2.54	0.40
1:B:31:PHE:HA	1:B:32:PRO:HD2	1.93	0.40
1:A:252:THR:HB	1:A:253:PRO:HD2	2.04	0.40
2:D:1:NAG:H61	2:D:2:NAG:C1	2.52	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 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	492/505 (97%)	466 (95%)	25 (5%)	1 (0%)	47 58
1	B	496/505 (98%)	474 (96%)	20 (4%)	2 (0%)	34 41
All	All	988/1010 (98%)	940 (95%)	45 (5%)	3 (0%)	41 50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	GLU
1	B	281	LEU
1	B	233	GLU

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 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	413/432 (96%)	402 (97%)	11 (3%)	44 60
1	B	417/432 (96%)	405 (97%)	12 (3%)	42 57
All	All	830/864 (96%)	807 (97%)	23 (3%)	43 59

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	THR
1	A	72	GLU
1	A	148	SER
1	A	207	GLN
1	A	242	SER
1	A	312	TRP
1	A	335	MET
1	A	349	GLU
1	A	406	ILE
1	A	477	VAL
1	A	483	ILE
1	B	53	MET
1	B	61	THR

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Mol	Chain	Res	Type
1	B	69	LEU
1	B	110	SER
1	B	207	GLN
1	B	312	TRP
1	B	335	MET
1	B	345	SER
1	B	353	ARG
1	B	381	TRP
1	B	433	ARG
1	B	483	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN

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	0.64	0	17,19,21	2.16	6 (35%)
2	NAG	C	2	2	14,14,15	0.72	0	17,19,21	1.65	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BMA	C	3	2	11,11,12	1.02	0	15,15,17	2.56	5 (33%)
2	FUC	C	4	2	10,10,11	0.96	0	14,14,16	1.16	1 (7%)
2	NAG	D	1	1,2	14,14,15	0.55	0	17,19,21	1.36	2 (11%)
2	NAG	D	2	2	14,14,15	0.71	0	17,19,21	1.36	3 (17%)
2	BMA	D	3	2	11,11,12	0.76	0	15,15,17	1.16	2 (13%)
2	FUC	D	4	2	10,10,11	0.76	0	14,14,16	1.92	5 (35%)

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

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	BMA	C1-O5-C5	7.15	121.88	112.19
2	C	1	NAG	C2-N2-C7	-5.92	114.47	122.90
2	D	4	FUC	O5-C1-C2	-4.08	104.47	110.77
2	C	1	NAG	O5-C5-C6	3.81	113.17	107.20
2	C	3	BMA	O3-C3-C2	3.66	117.00	109.99
2	C	2	NAG	O5-C5-C6	3.48	112.65	107.20
2	D	1	NAG	O5-C5-C6	3.35	112.45	107.20
2	C	3	BMA	O5-C1-C2	3.33	115.91	110.77
2	D	4	FUC	C1-O5-C5	-2.77	106.51	112.78
2	C	2	NAG	C3-C4-C5	-2.62	105.57	110.24
2	D	3	BMA	C1-O5-C5	2.61	115.72	112.19
2	C	2	NAG	O4-C4-C5	2.47	115.43	109.30
2	C	1	NAG	O7-C7-C8	-2.46	117.49	122.06
2	C	2	NAG	C2-N2-C7	-2.42	119.45	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	NAG	C1-C2-N2	-2.41	106.36	110.49
2	C	3	BMA	O2-C2-C3	2.37	114.88	110.14
2	C	1	NAG	O5-C1-C2	-2.35	107.58	111.29
2	D	2	NAG	C4-C3-C2	-2.28	107.68	111.02
2	D	4	FUC	O2-C2-C3	2.27	114.69	110.14
2	D	4	FUC	C1-C2-C3	-2.25	106.89	109.67
2	D	4	FUC	O5-C5-C6	2.22	112.12	107.33
2	C	4	FUC	O5-C5-C6	2.22	112.11	107.33
2	C	1	NAG	C1-C2-N2	2.10	114.07	110.49
2	D	3	BMA	C3-C4-C5	2.09	113.97	110.24
2	D	1	NAG	O7-C7-C8	-2.08	118.20	122.06
2	C	3	BMA	O4-C4-C5	2.06	114.41	109.30
2	D	2	NAG	O4-C4-C5	2.03	114.35	109.30
2	C	1	NAG	C8-C7-N2	2.03	119.54	116.10

There are no chirality outliers.

All (7) torsion outliers are listed below:

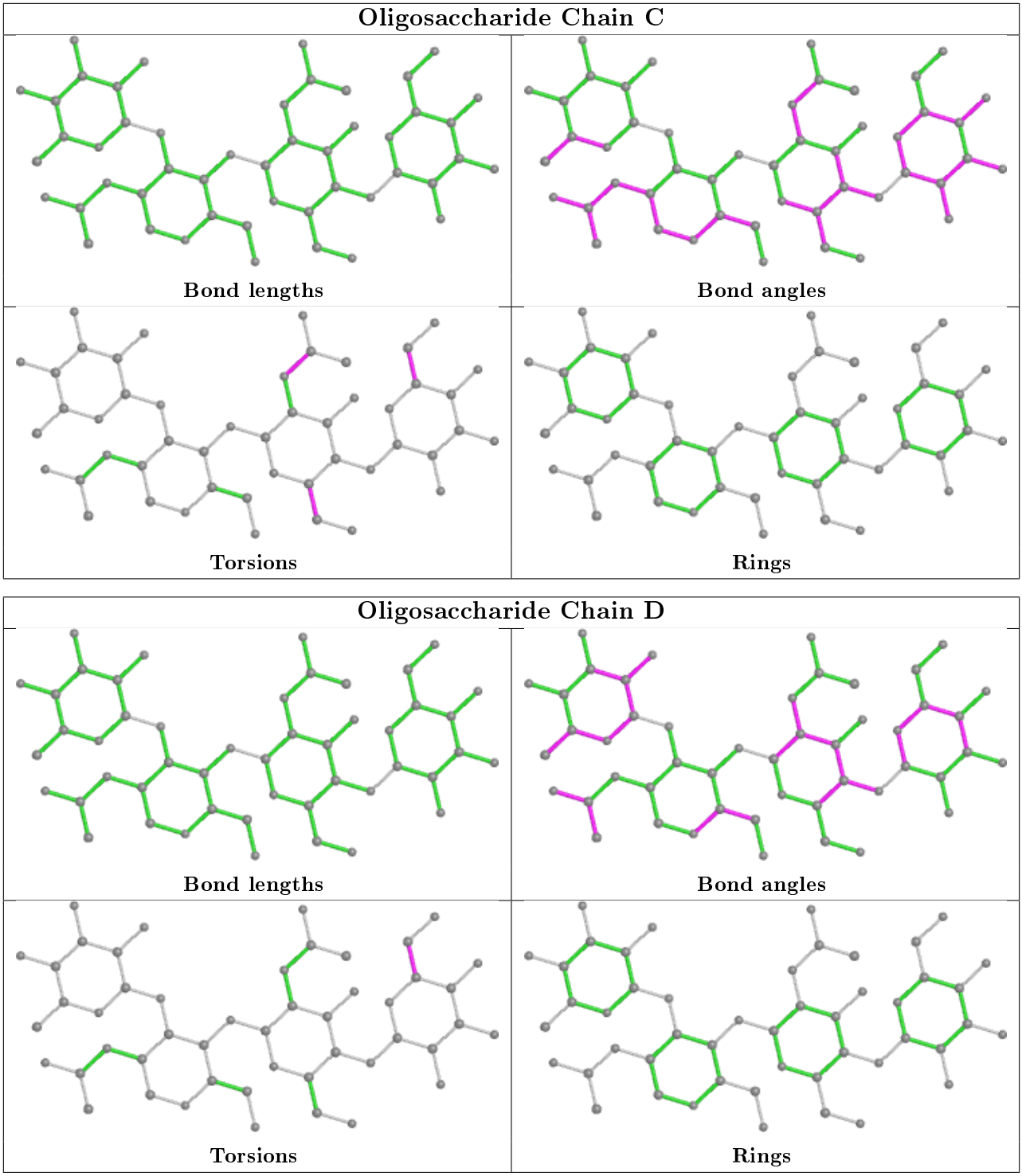
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	C	3	BMA	O5-C5-C6-O6
2	C	2	NAG	O7-C7-N2-C2
2	D	3	BMA	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
2	D	1	NAG	1	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)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	PO4	A	605	-	4,4,4	1.37	0	6,6,6	1.81	1 (16%)
3	PO4	B	605	-	4,4,4	1.13	0	6,6,6	1.52	1 (16%)
5	AMF	B	607	-	16,18,23	1.88	3 (18%)	16,26,31	3.77	8 (50%)
5	AMF	A	607	-	21,23,23	1.48	3 (14%)	21,31,31	2.73	8 (38%)

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	AMF	B	607	-	-	3/4/37/42	0/2/2/2
5	AMF	A	607	-	-	5/9/42/42	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	607	AMF	C7-N2	5.17	1.35	1.26
5	A	607	AMF	C2-C1	4.30	1.57	1.52
5	B	607	AMF	C2-C1	3.41	1.56	1.52
5	B	607	AMF	C7-S1	-2.65	1.71	1.75
5	A	607	AMF	C7-N2	2.37	1.30	1.26
5	A	607	AMF	C5-N1	2.16	1.50	1.47

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	607	AMF	O1-C1-N1	-10.17	95.72	111.90
5	A	607	AMF	C6-C5-C4	-7.01	105.11	115.72
5	B	607	AMF	C6-C5-C4	-6.13	106.44	115.72
5	A	607	AMF	O1-C1-N1	-6.11	102.18	111.90
5	B	607	AMF	C9-C8-N2	4.75	119.50	111.33
5	B	607	AMF	N1-C7-N2	4.58	129.90	124.04
5	A	607	AMF	C3-C2-C1	4.47	116.03	109.05
5	B	607	AMF	C3-C2-C1	4.11	115.47	109.05
5	A	607	AMF	C9-C8-N2	3.43	116.91	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	605	PO4	O3-P-O2	3.31	118.59	107.97
5	A	607	AMF	C8-N2-C7	-2.99	112.97	117.84
5	A	607	AMF	C5-C6-S1	-2.98	101.96	105.75
5	B	607	AMF	O2-C2-C3	-2.59	104.37	110.35
5	B	607	AMF	C5-C6-S1	-2.55	102.51	105.75
5	B	607	AMF	C3-C4-C5	-2.47	107.20	111.37
5	A	607	AMF	C3-C4-C5	-2.24	107.58	111.37
3	B	605	PO4	O4-P-O1	-2.22	102.77	110.89
5	A	607	AMF	O3-C3-C2	-2.08	105.54	110.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	607	AMF	S1-C7-N2-C8
5	A	607	AMF	N1-C7-N2-C8
5	B	607	AMF	S1-C7-N2-C8
5	B	607	AMF	N1-C7-N2-C8
5	A	607	AMF	C11-C12-C13-C14
5	A	607	AMF	C9-C10-C11-C12
5	A	607	AMF	C11-C10-C9-C8
5	B	607	AMF	N2-C8-C9-C10

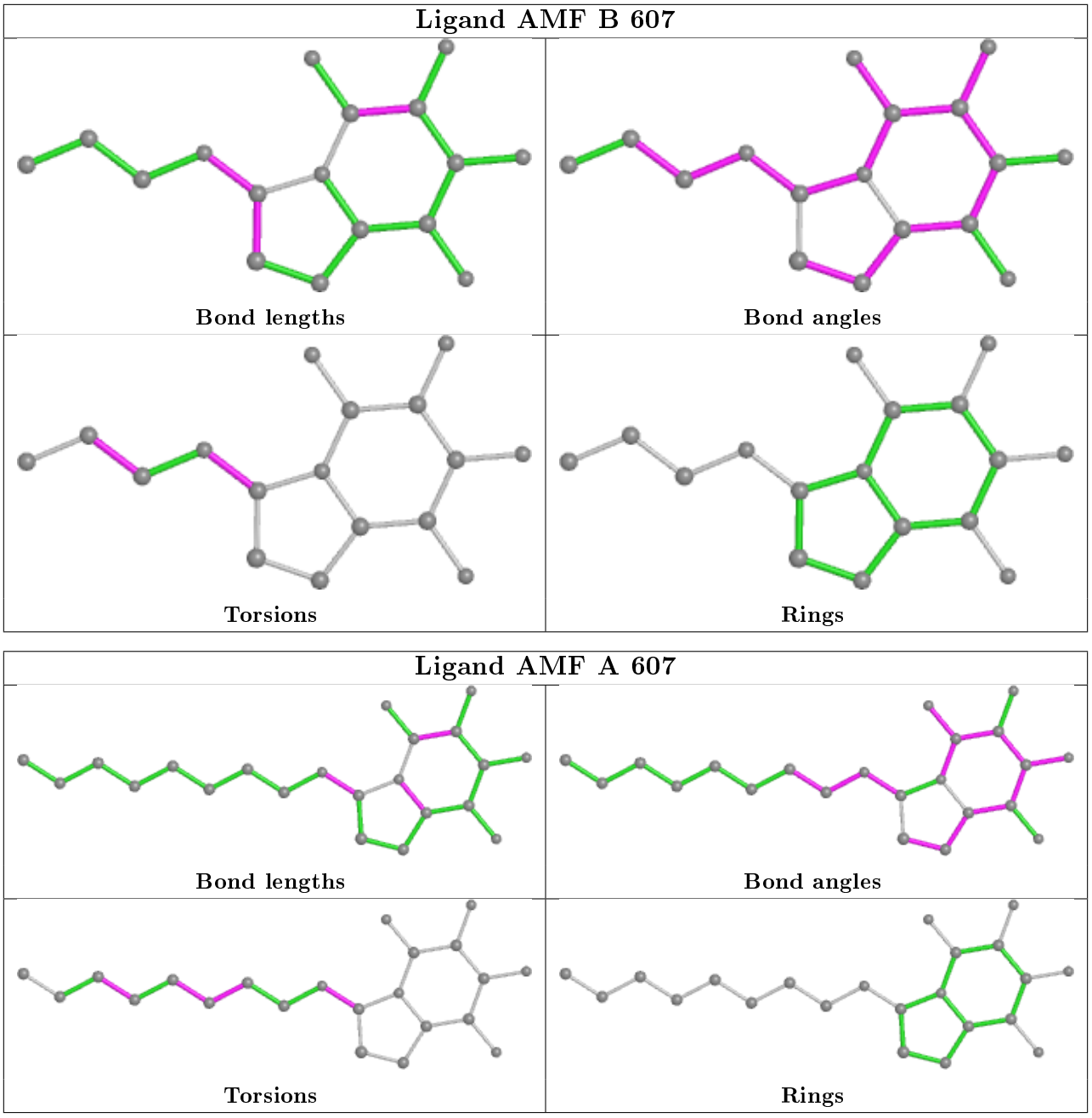
There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	605	PO4	1	0
5	B	607	AMF	5	0
5	A	607	AMF	8	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 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.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	496/505 (98%)	-0.67	3 (0%)	89	92	7, 18, 34, 55	0
1	B	498/505 (98%)	-0.59	1 (0%)	95	97	10, 21, 36, 49	0
All	All	994/1010 (98%)	-0.63	4 (0%)	92	95	7, 19, 35, 55	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	PHE	3.3
1	A	28	PRO	3.2
1	A	476	ALA	2.6
1	A	169	GLN	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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, 95^{th} 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	C	3	11/12	0.75	0.26	66,70,72,72	0
2	FUC	C	4	10/11	0.81	0.26	60,63,64,65	0
2	BMA	D	3	11/12	0.81	0.30	68,70,70,71	0
2	NAG	C	2	14/15	0.92	0.21	49,52,59,60	0
2	FUC	D	4	10/11	0.92	0.26	45,47,49,51	0

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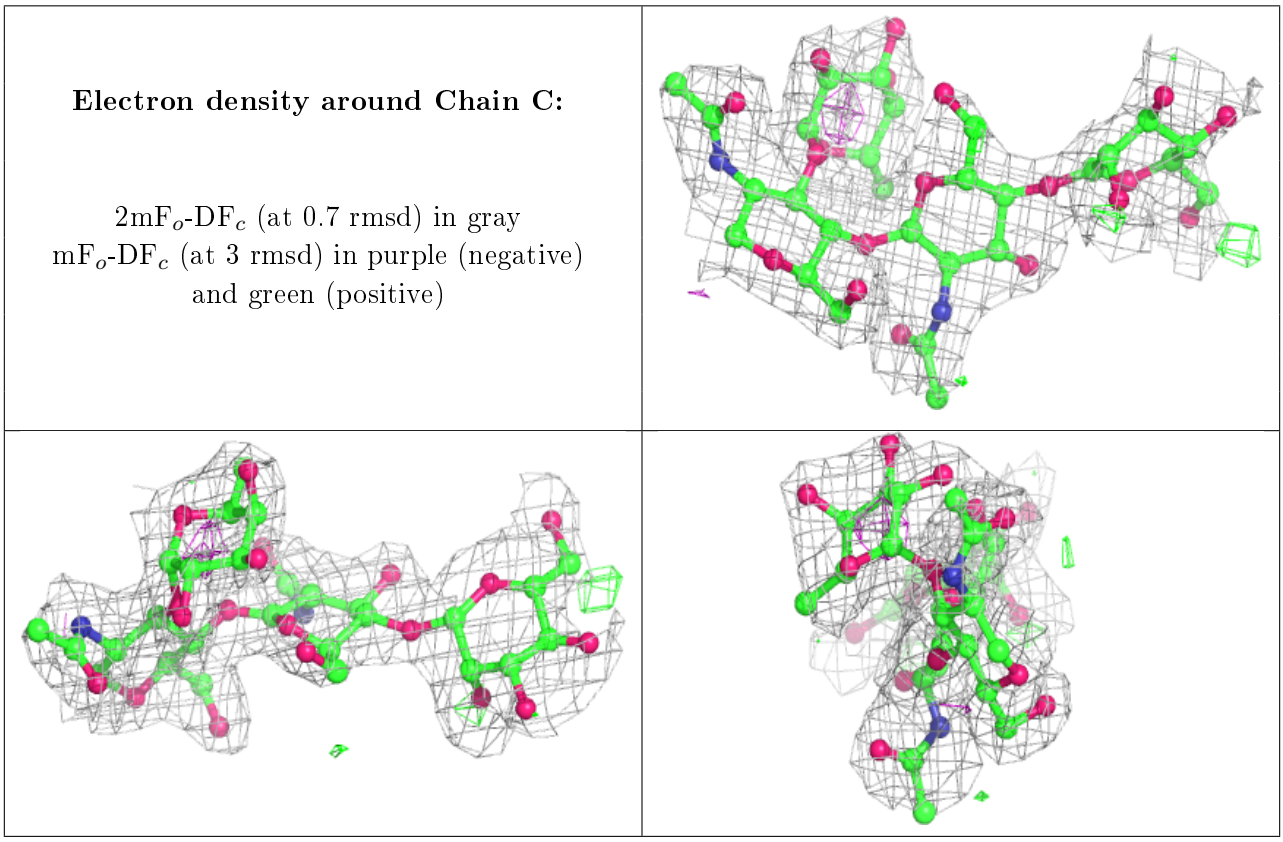
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	D	2	14/15	0.94	0.16	46,50,53,58	0
2	NAG	C	1	14/15	0.95	0.12	30,33,39,46	0
2	NAG	D	1	14/15	0.95	0.10	26,33,37,39	0

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.

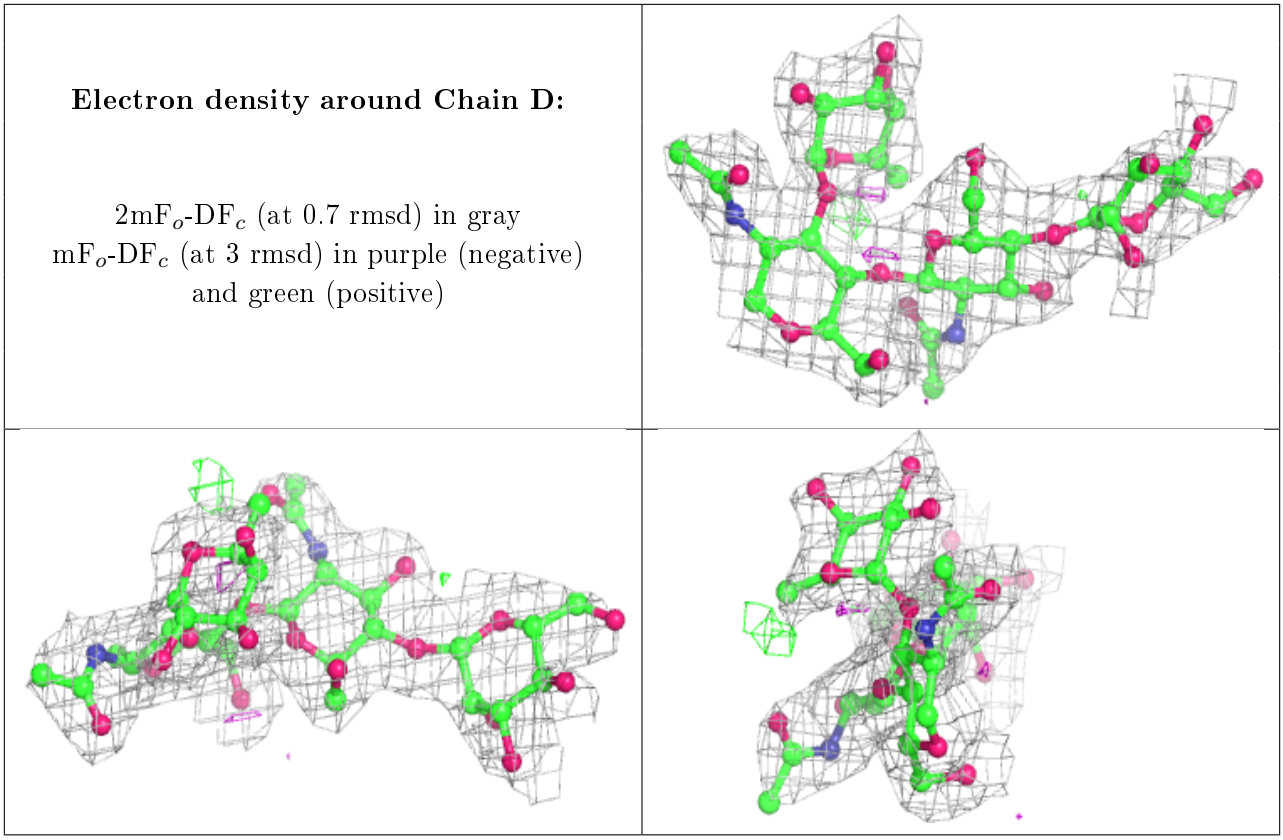
Electron density around Chain C:

$2mF_o$-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

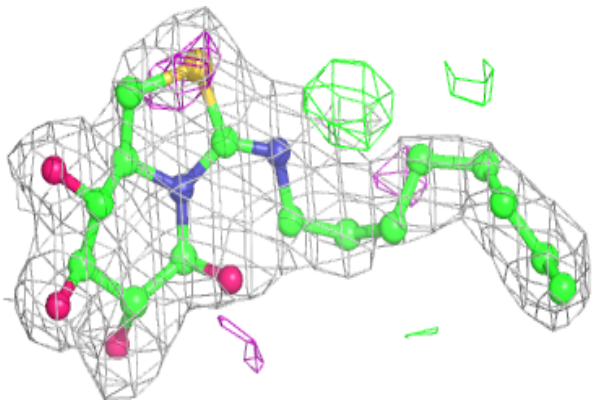
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

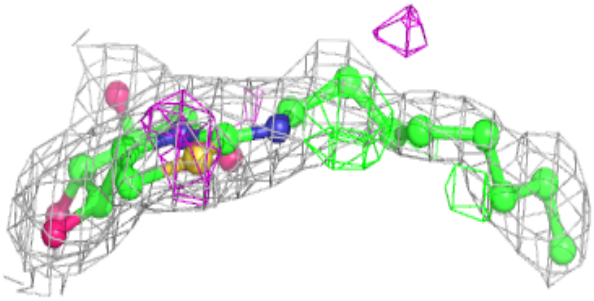
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	AMF	A	607	22/22	0.95	0.13	10,22,47,48	0
5	AMF	B	607	17/22	0.97	0.10	16,24,33,35	0
4	K	B	606	1/1	0.98	0.04	35,35,35,35	0
3	PO4	A	605	5/5	0.99	0.08	26,27,28,29	0
3	PO4	B	605	5/5	0.99	0.06	25,28,29,31	0
4	K	A	606	1/1	0.99	0.04	29,29,29,29	0

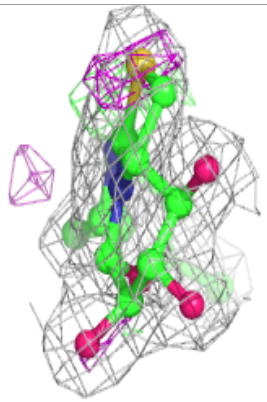
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AMF A 607:

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

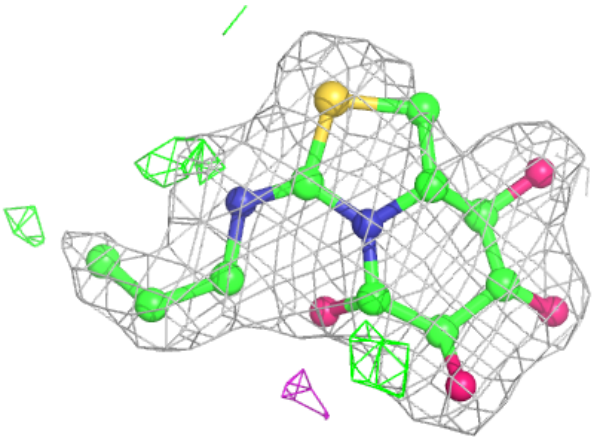


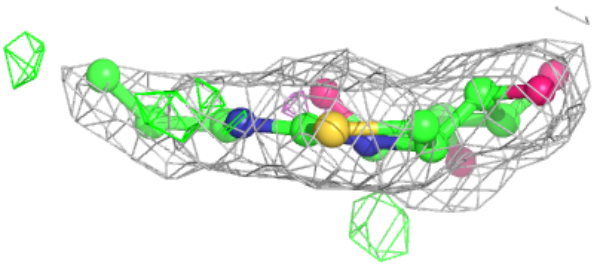


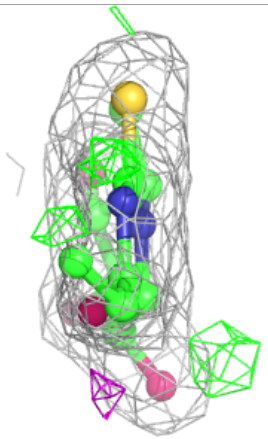


Electron density around AMF B 607:

$2mF_o$-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.