

wwPDB X-ray Structure Validation Summary Report (i)

Sep 26, 2023 – 11:55 AM EDT

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 (i) 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 (i)) were used in the production of this report:

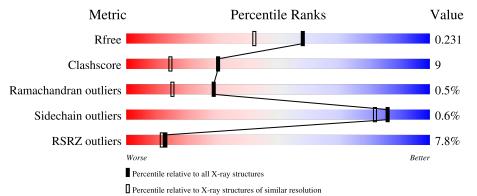
MolProbity		4 021 467
MOIFTODIty	•	4.020-407
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.83 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 <=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	А	431	9% 84%	15%	•			
1	В	431	<u>6%</u> 82%	17%	•			
2	С	4	50% 50%					
3	D	3	100%					



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 7500 atoms, of which 17 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 Hemagglutinin-neuraminidase.

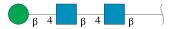
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	431	Total	С	Ν	0	\mathbf{S}	0	2	0
	A	401	3392	2145	583	644	20	0	2	0
1	р	428	Total	С	Ν	0	S	0	2	0
	D	420	3361	2126	579	636	20	0	Δ	0

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



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

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



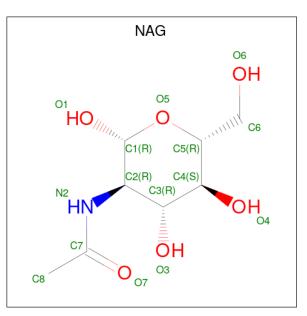
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	Л	2	Total	С	Η	Ν	0	0	0	0
5		5	50	22	11	2	15	0		U

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Ca 1 1	0	0
4	В	1	Total Ca 1 1	0	0

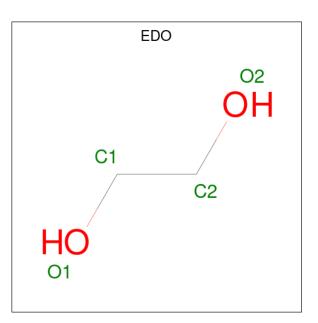
• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



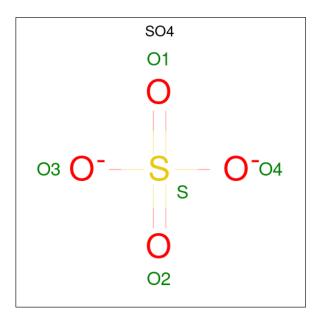
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total C N O 14 8 1 5	0	0
5	В	1	Total C N O 14 8 1 5	0	0

• Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
6	В	1	Total C H O 10 2 6 2	0	0



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
7	А	1	Total 5	0 4	S 1	0	0

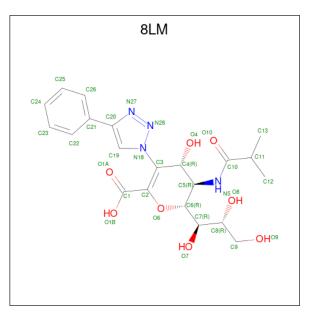
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

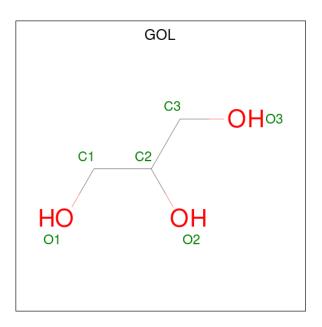
• Molecule 8 is 2,6-anhydro-3,5-dideoxy-5-[(2-methylpropanoyl)amino]-3-(4-phenyl-1H-1,2, 3-triazol-1-yl)-D-glycero-D-galacto-non-2-enoni c acid (three-letter code: 8LM) (formula: $C_{21}H_{26}N_4O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	Total C N O 33 21 4 8	0	0
8	А	1	Total C N O 33 21 4 8	0	0
8	В	1	Total C N O 33 21 4 8	0	0

• Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	В	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 6 & 3 \end{array}$	O 3	0	0

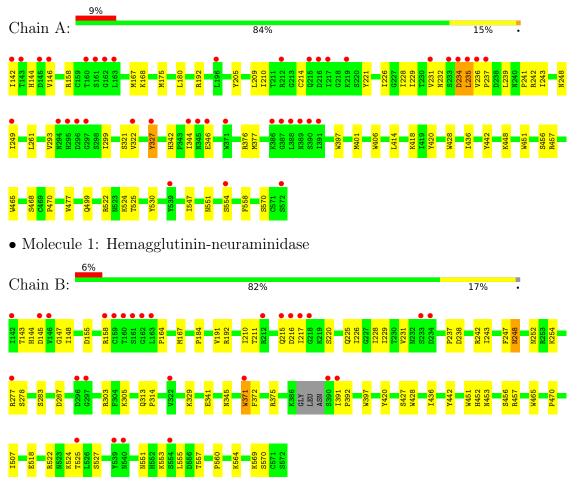
• Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	254	Total O 254 254	0	0
10	В	225	Total O 225 225	0	0



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: Hemagglutinin-neuraminidase

50%

 $\bullet \ Molecule \ 2: \ alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose \\ eta-D-glucopyranose \ (1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose \ (1-4)-2-acetamido-2-deoxy-beta-D-glucopyra$

50%

Chain C:

NAG1 NAG2 BMA3 MAN4

• Molecule 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%

NAG1 NAG2 BMA3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	83.90Å 95.99Å 105.61Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 - 1.83	Depositor
Resolution (A)	29.90 - 1.83	EDS
% Data completeness	91.5 (29.90-1.83)	Depositor
(in resolution range)	91.5(29.90-1.83)	EDS
R _{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.95 (at 1.83 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
B B.	0.181 , 0.228	Depositor
R, R_{free}	0.182 , 0.231	DCC
R_{free} test set	3411 reflections $(4.92%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	25.1	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36 , 49.4	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7500	wwPDB-VP
Average B, all atoms $(Å^2)$	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: MAN, 8LM, BMA, NAG, EDO, CA, SO4, GOL

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	Bond lengths		nd angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.42	0/3474	0.61	2/4735~(0.0%)
1	В	0.41	0/3445	0.59	0/4694
All	All	0.42	0/6919	0.60	2/9429~(0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	327	TYR	N-CA-C	-5.90	95.06	111.00
1	А	234	ASP	N-CA-C	-5.31	96.66	111.00

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	А	3392	0	3346	65	0
1	В	3361	0	3319	59	0
2	С	50	0	43	1	0
3	D	39	11	34	1	0
4	А	1	0	0	0	0
4	В	1	0	0	0	0
5	А	14	0	13	5	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	В	14	0	13	0	0
6	А	8	0	12	3	0
6	В	4	6	6	2	0
7	А	5	0	0	0	0
7	В	10	0	0	0	0
8	А	66	0	0	4	0
8	В	33	0	0	1	0
9	В	6	0	8	1	0
10	А	254	0	0	7	0
10	В	225	0	0	8	0
All	All	7483	17	6794	128	0

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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 9.

The worst 5 of 128 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:234:ASP:O	1:A:234:ASP:OD1	1.85	0.95
1:A:221[A]:TYR:CE2	1:A:249:ILE:HD12	2.13	0.83
1:A:231:VAL:HG12	1:A:235:LEU:HA	1.59	0.83
1:B:277:ARG:HD3	1:B:371:TRP:CH2	2.14	0.82
1:A:499:GLN:H	6:A:607:EDO:H12	1.45	0.81

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	А	431/431 (100%)	407 (94%)	21 (5%)	3~(1%)	22 9
1	В	425/431~(99%)	399~(94%)	25~(6%)	1 (0%)	47 33



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	856/862~(99%)	806 (94%)	46 (5%)	4 (0%)	29 15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	235	LEU
1	В	248	ASN
1	А	248	ASN
1	А	522	ARG

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	Analysed Rotameric Outliers		Percentiles		
1	А	391/389~(100%)	389~(100%)	2~(0%)	88 85		
1	В	388/389~(100%)	385~(99%)	3~(1%)	81 75		
All	All	779/778~(100%)	774 (99%)	5 (1%)	86 82		

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	158	ARG
1	А	457	ARG
1	В	303	ARG
1	В	371	TRP
1	В	457	ARG

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

Mol	Chain	Res	Type
1	А	144	HIS



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

7 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	Turne	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
10101	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	NAG	С	1	1,2	14,14,15	0.37	0	17,19,21	0.67	0
2	NAG	С	2	2	14,14,15	0.21	0	17,19,21	0.60	0
2	BMA	С	3	2	11,11,12	0.80	0	$15,\!15,\!17$	0.97	0
2	MAN	С	4	2	11,11,12	1.25	1 (9%)	$15,\!15,\!17$	1.25	3 (20%)
3	NAG	D	1	1,3	14,14,15	0.57	1 (7%)	17,19,21	0.49	0
3	NAG	D	2	3	14,14,15	0.17	0	17,19,21	0.46	0
3	BMA	D	3	3	11,11,12	0.88	0	$15,\!15,\!17$	1.09	1 (6%)

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



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	С	4	MAN	C2-C3	2.36	1.56	1.52
3	D	1	NAG	O5-C1	-2.05	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	С	4	MAN	C1-O5-C5	2.58	115.68	112.19
2	С	4	MAN	C2-C3-C4	2.21	114.72	110.89
3	D	3	BMA	O5-C5-C4	-2.07	105.79	110.83
2	С	4	MAN	O2-C2-C1	2.06	113.36	109.15

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	С	4	MAN	C4-C5-C6-O6
2	С	4	MAN	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6

There are no ring outliers.

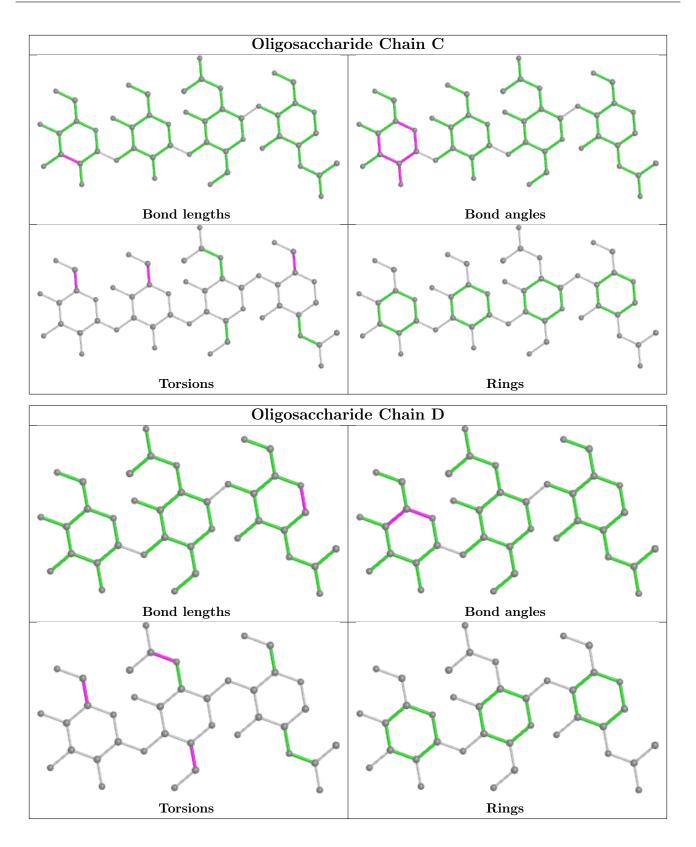
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	2	NAG	1	0
3	D	2	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 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis. In the following table, the Counts columns list the number of bonds (or angles) for which Mogul



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

Mol	Turne	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	А	606	1	$14,\!14,\!15$	0.36	0	17,19,21	0.97	0
6	EDO	В	607	-	3,3,3	0.55	0	2,2,2	0.69	0
9	GOL	В	608	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.18	0
5	NAG	В	605	1	$14,\!14,\!15$	0.20	0	17,19,21	0.67	0
8	8LM	А	611	-	$33,\!35,\!35$	2.25	8 (24%)	$30,\!50,\!50$	1.70	4 (13%)
7	SO4	А	609	-	4,4,4	0.21	0	6,6,6	0.32	0
7	SO4	В	609	-	4,4,4	0.10	0	6,6,6	0.12	0
7	SO4	В	606	-	4,4,4	0.13	0	6,6,6	0.11	0
8	8LM	А	610	-	$33,\!35,\!35$	2.20	8 (24%)	$30,\!50,\!50$	2.47	7 (23%)
8	8LM	В	610	-	$33,\!35,\!35$	2.08	8 (24%)	$30,\!50,\!50$	2.26	7 (23%)
6	EDO	А	607	-	3,3,3	0.52	0	2,2,2	0.26	0
6	EDO	А	608	_	3,3,3	0.52	0	2,2,2	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	А	606	1	-	3/6/23/26	0/1/1/1
6	EDO	В	607	-	-	1/1/1/1	-
9	GOL	В	608	-	-	0/4/4/4	-
5	NAG	В	605	1	-	0/6/23/26	0/1/1/1
8	8LM	А	611	-	-	9/25/50/50	0/3/3/3
8	8LM	А	610	-	-	5/25/50/50	0/3/3/3
8	8LM	В	610	-	-	2/25/50/50	0/3/3/3
6	EDO	А	607	-	-	1/1/1/1	-
6	EDO	А	608	-	-	0/1/1/1	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	А	611	8LM	O6-C6	7.45	1.58	1.46
8	А	610	8LM	O6-C6	7.27	1.58	1.46



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Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(Å)	Ideal(Å)					
8	В	610	8LM	O6-C6	6.46	1.57	1.46					
8	А	611	8LM	C10-N5	5.61	1.46	1.34					
8	А	610	8LM	C10-N5	5.55	1.46	1.34					

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The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
8	В	610	8LM	C5-N5-C10	-7.86	111.36	123.21
8	А	610	8LM	C11-C10-N5	7.24	123.07	115.95
8	А	610	8LM	C5-N5-C10	-5.68	114.65	123.21
8	В	610	8LM	C11-C10-N5	5.27	121.13	115.95
8	А	610	8LM	O6-C2-C3	-4.96	117.44	123.76

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	А	610	8LM	O1B-C1-C2-O6
8	А	611	8LM	O8-C8-C9-O9
8	А	611	8LM	C6-C7-C8-C9
8	А	611	8LM	07-C7-C8-08
8	А	611	8LM	C6-C7-C8-O8

There are no ring outliers.

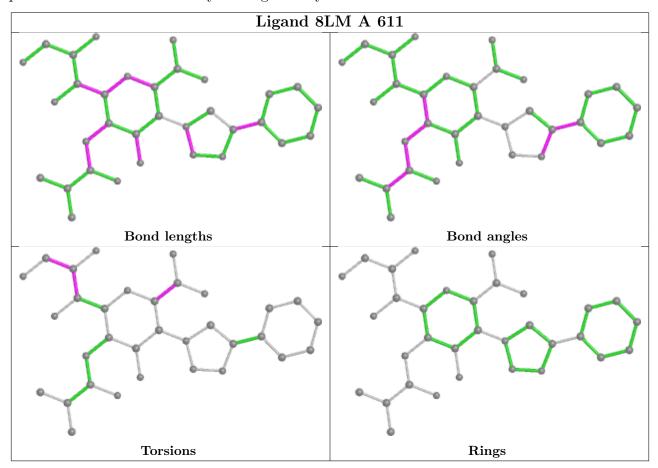
8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	606	NAG	5	0
6	В	607	EDO	2	0
9	В	608	GOL	1	0
8	А	611	8LM	1	0
8	А	610	8LM	3	0
8	В	610	8LM	1	0
6	А	607	EDO	2	0
6	А	608	EDO	1	0

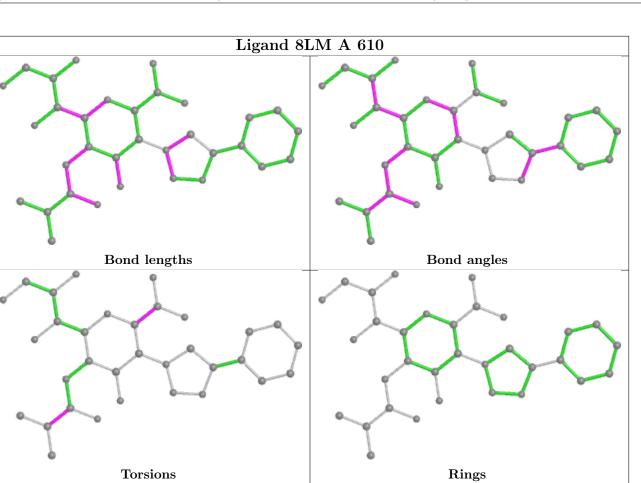
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

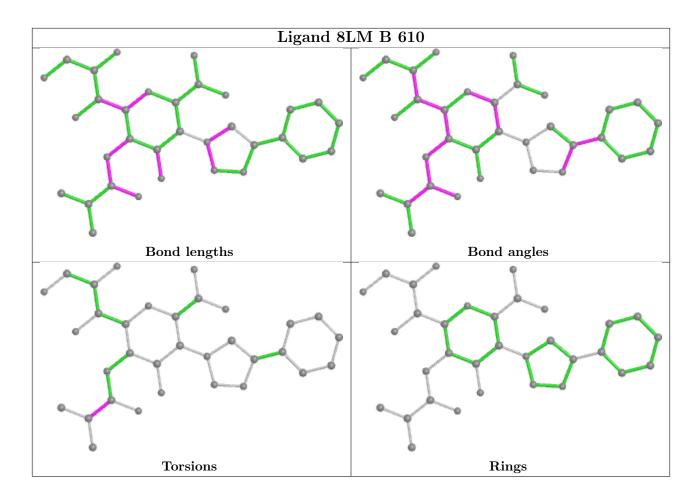












5.7 Other polymers (i)

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, 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	$\langle RSRZ \rangle$	$\#RSRZ{>}2$		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	431/431 (100%)	0.30	40 (9%) 8	7	16, 28, 69, 92	0
1	В	428/431 (99%)	0.23	27 (6%) 20	17	18, 30, 61, 110	0
All	All	859/862~(99%)	0.26	67 (7%) 13	12	16, 29, 66, 110	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	146	VAL	10.4
1	В	145	ASP	9.0
1	А	388	LEU	8.8
1	А	146	VAL	8.4
1	В	217	ILE	8.4

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, 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.

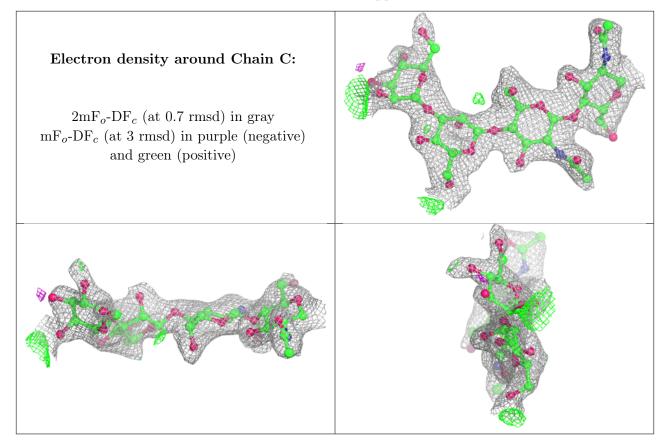
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
3	BMA	D	3	11/12	0.57	0.27	82,99,115,123	0
2	MAN	С	4	11/12	0.76	0.24	58,67,72,78	0
2	BMA	С	3	11/12	0.76	0.18	54,65,73,76	0
3	NAG	D	2	14/15	0.87	0.20	53,59,67,74	0
2	NAG	С	2	14/15	0.90	0.10	47,52,57,61	0



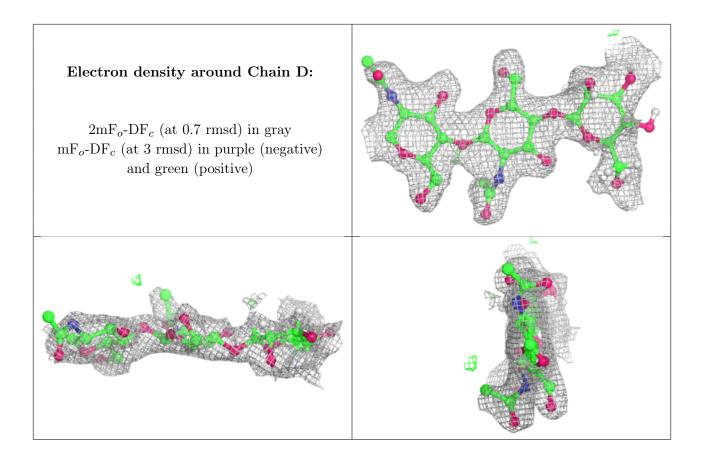
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
3	NAG	D	1	14/15	0.90	0.17	$51,\!58,\!77,\!80$	0
2	NAG	С	1	14/15	0.92	0.12	37,47,58,64	0

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.







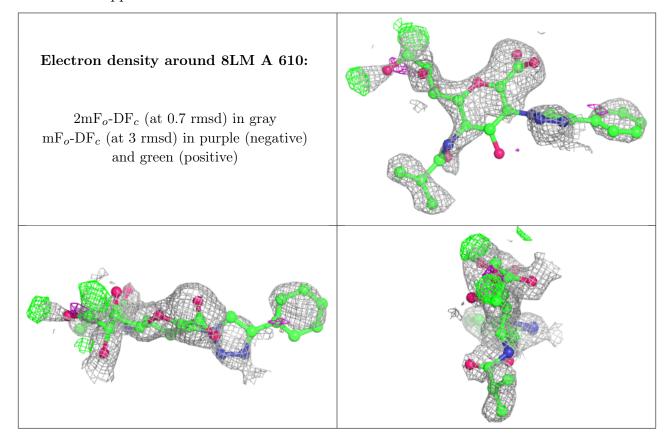
6.4 Ligands (i)

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, 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.

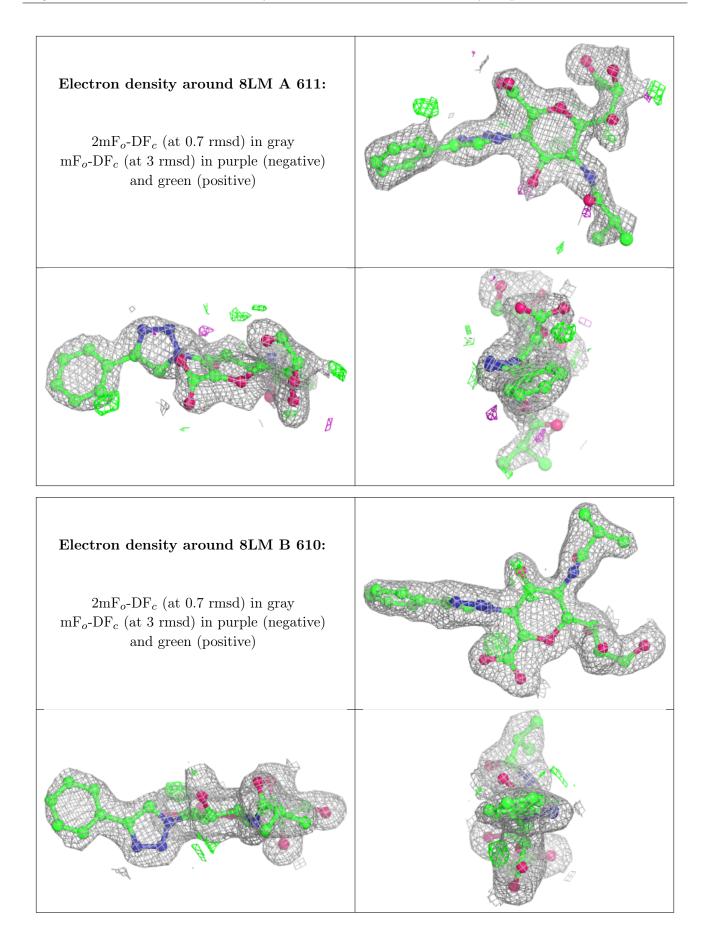
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
5	NAG	В	605	14/15	0.66	0.27	$63,\!75,\!86,\!91$	0
8	8LM	А	610	33/33	0.69	0.29	43,74,87,87	0
8	8LM	А	611	33/33	0.74	0.25	48,62,71,75	0
9	GOL	В	608	6/6	0.74	0.27	43,54,56,59	0
6	EDO	А	608	4/4	0.78	0.14	$53,\!57,\!57,\!61$	0
5	NAG	А	606	14/15	0.80	0.27	41,53,60,64	0
6	EDO	А	607	4/4	0.83	0.12	36,40,42,52	0
6	EDO	В	607	4/4	0.84	0.14	27,36,44,44	0
8	8LM	В	610	33/33	0.92	0.11	$24,\!40,\!58,\!59$	0
7	SO4	В	609	5/5	0.95	0.10	43,49,56,57	0
7	SO4	В	606	5/5	0.98	0.07	50,50,52,56	0
4	CA	В	601	1/1	0.99	0.04	32,32,32,32	0
4	CA	А	601	1/1	0.99	0.05	29,29,29,29	0
7	SO4	А	609	5/5	0.99	0.11	28,31,36,40	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.









6.5 Other polymers (i)

There are no such residues in this entry.

