Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 09:36 pm BST

PDB ID	:	5NPB
Title	:	Crystal Structure of cjAgd31B (alpha-transglucosylase from Glycoside Hydrolase Family 31) in complex with alpha Cyclophellitol Cyclosulfate probe ME647
Authors	:	Wu, L.; Davies, G.J.
Deposited on	:	2017-04-16
Resolution	:	1.90 Å(reported)

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

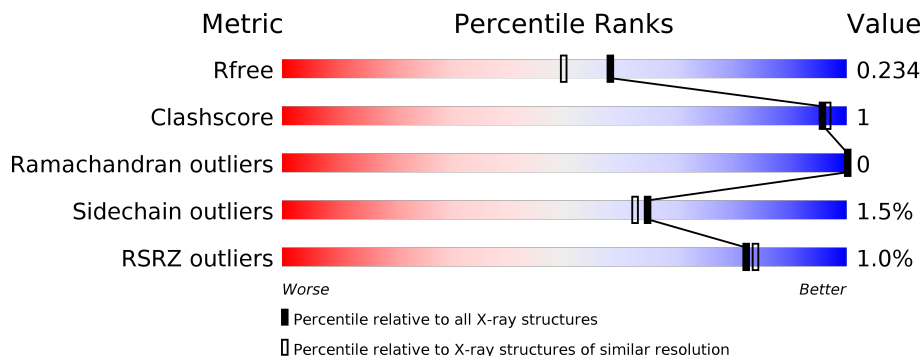|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.90 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	Percentile Ranks	Value
Rfree		0.234
Clashscore		1
Ramachandran outliers		0
Sidechain outliers		1.5%
RSRZ outliers		1.0%

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	836	88% 5% 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6864 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 Oligosaccharide 4-alpha-D-glucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	780	6302	4025	1081	1175	21	0	8	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	initiating methionine	UNP B3PEE6
A	817	LYS	-	expression tag	UNP B3PEE6
A	818	GLY	-	expression tag	UNP B3PEE6
A	819	GLY	-	expression tag	UNP B3PEE6
A	820	ARG	-	expression tag	UNP B3PEE6
A	821	ALA	-	expression tag	UNP B3PEE6
A	822	ASP	-	expression tag	UNP B3PEE6
A	823	PRO	-	expression tag	UNP B3PEE6
A	824	ALA	-	expression tag	UNP B3PEE6
A	825	PHE	-	expression tag	UNP B3PEE6
A	826	LEU	-	expression tag	UNP B3PEE6
A	827	TYR	-	expression tag	UNP B3PEE6
A	828	LYS	-	expression tag	UNP B3PEE6
A	829	VAL	-	expression tag	UNP B3PEE6
A	830	VAL	-	expression tag	UNP B3PEE6
A	831	ILE	-	expression tag	UNP B3PEE6
A	832	ASN	-	expression tag	UNP B3PEE6
A	833	SER	-	expression tag	UNP B3PEE6
A	834	LYS	-	expression tag	UNP B3PEE6
A	835	LEU	-	expression tag	UNP B3PEE6
A	836	GLU	-	expression tag	UNP B3PEE6
A	837	GLY	-	expression tag	UNP B3PEE6
A	838	LYS	-	expression tag	UNP B3PEE6
A	839	PRO	-	expression tag	UNP B3PEE6
A	840	ILE	-	expression tag	UNP B3PEE6
A	841	PRO	-	expression tag	UNP B3PEE6
A	842	ASN	-	expression tag	UNP B3PEE6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	843	PRO	-	expression tag	UNP B3PEE6
A	844	LEU	-	expression tag	UNP B3PEE6
A	845	LEU	-	expression tag	UNP B3PEE6
A	846	GLY	-	expression tag	UNP B3PEE6
A	847	LEU	-	expression tag	UNP B3PEE6
A	848	ASP	-	expression tag	UNP B3PEE6
A	849	SER	-	expression tag	UNP B3PEE6
A	850	THR	-	expression tag	UNP B3PEE6
A	851	ARG	-	expression tag	UNP B3PEE6
A	852	THR	-	expression tag	UNP B3PEE6
A	853	GLY	-	expression tag	UNP B3PEE6
A	854	HIS	-	expression tag	UNP B3PEE6
A	855	HIS	-	expression tag	UNP B3PEE6
A	856	HIS	-	expression tag	UNP B3PEE6
A	857	HIS	-	expression tag	UNP B3PEE6
A	858	HIS	-	expression tag	UNP B3PEE6
A	859	HIS	-	expression tag	UNP B3PEE6

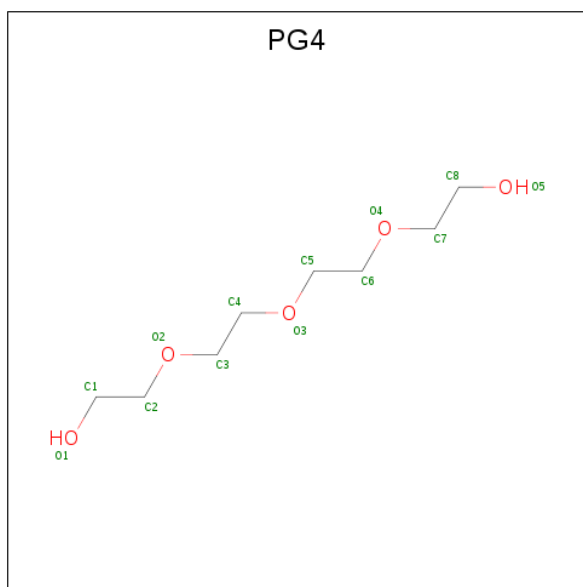- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
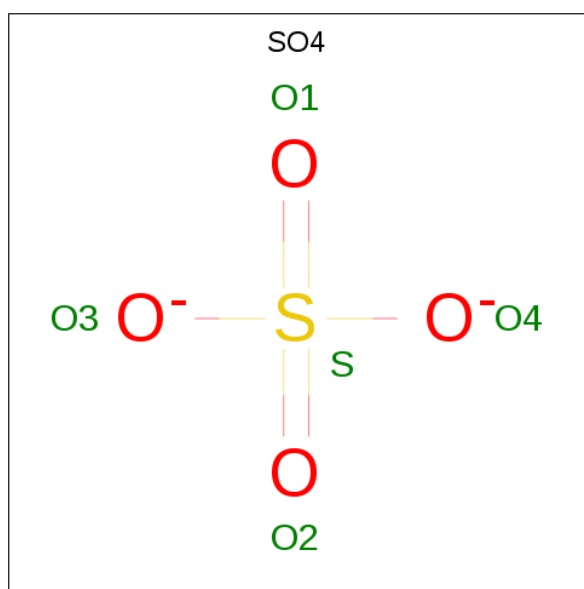
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 13	C 8	O 5	0	0

- Molecule 4 is [(1 {S},2 {R},3 {R},4 {S},5 {R})-2-(hydroxymethyl)-3,4,5,6-tetrakis(oxidanyl)cyclohexyl] hydrogen sulfate (three-letter code: 93Z) (formula: $C_7H_{14}O_9S$).
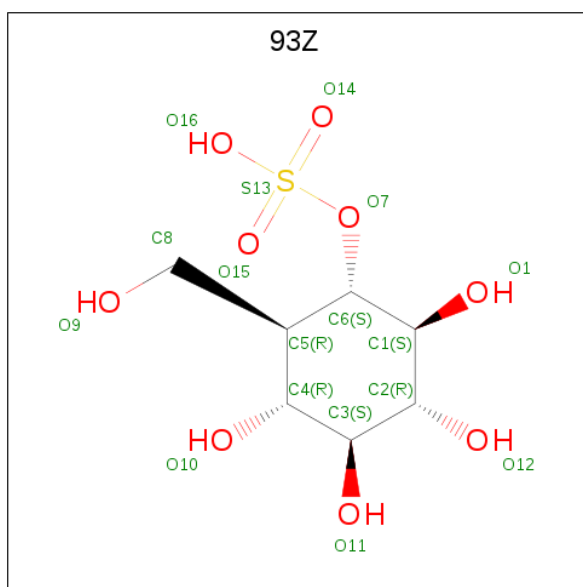
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	A	1	16	7	8	1	0	0

- Molecule 5 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).
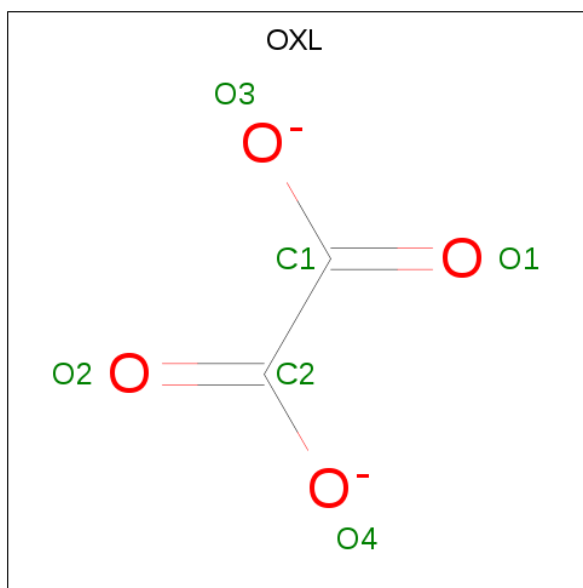
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	2	4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	502	Total 502	O 502	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Oligosaccharide 4-alpha-D-glucosyltransferase
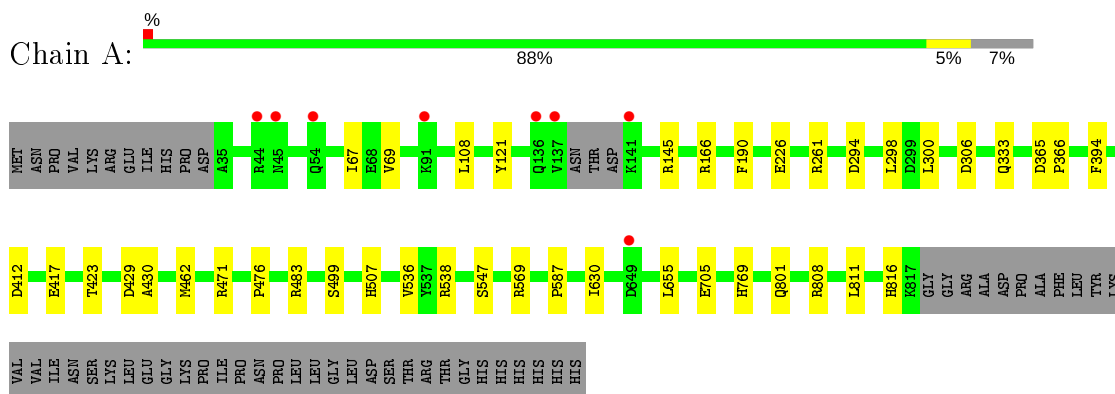
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α, β, γ	197.38Å 197.38Å 102.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.85 – 1.90	Depositor
	49.85 – 1.90	EDS
% Data completeness	99.9 (49.85-1.90)	Depositor
(in resolution range)	100.0 (49.85-1.90)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.90 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.196 , 0.228	Depositor
	0.205 , 0.234	DCC
R_{free} test set	4584 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	26.5	Xtriage
Anisotropy	0.779	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.3	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6864	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OXL, 93Z, PG4, SO4

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	0.74	1/6470 (0.0%)	0.85	9/8772 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	ASP	CG-OD2	6.35	1.40	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	538	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	471	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	471	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	811	LEU	CA-CB-CG	6.07	129.26	115.30
1	A	483	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	412	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	145	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	429	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	261	ARG	NE-CZ-NH1	5.16	122.88	120.30

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	6302	0	6116	14	0
2	A	25	0	0	0	0
3	A	13	0	18	0	0
4	A	16	0	0	0	0
5	A	6	0	0	0	0
6	A	502	0	0	4	2
All	All	6864	0	6134	14	2

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 1.

All (14) 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:333[A]:GLN:NE2	6:A:1006:HOH:O	2.41	0.53
1:A:769:HIS:CE1	1:A:816[B]:HIS:CD2	3.02	0.48
1:A:630:ILE:HD12	1:A:655:LEU:HD13	1.96	0.47
1:A:67:ILE:HG22	1:A:108:LEU:HD21	1.97	0.47
1:A:69:VAL:HG21	1:A:121:TYR:OH	2.14	0.47
1:A:801:GLN:NE2	6:A:1021:HOH:O	2.50	0.44
1:A:462:MET:O	1:A:476:PRO:HA	2.17	0.44
1:A:365:ASP:HB2	1:A:366:PRO:CD	2.47	0.44
1:A:499:SER:HB3	1:A:587:PRO:CB	2.49	0.43
1:A:808:ARG:NE	6:A:1031:HOH:O	2.52	0.42
1:A:569:ARG:HD2	6:A:1260:HOH:O	2.20	0.41
1:A:423:THR:HB	1:A:430:ALA:HB2	2.03	0.41
1:A:298[B]:LEU:HD12	1:A:298[B]:LEU:N	2.36	0.40
1:A:507:HIS:CG	1:A:536:VAL:HB	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1472:HOH:O	6:A:1472:HOH:O[8_556]	2.08	0.12
6:A:1046:HOH:O	6:A:1046:HOH:O[8_556]	2.17	0.03

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	784/836 (94%)	757 (97%)	27 (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 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	665/706 (94%)	655 (98%)	10 (2%)	65	62

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	ARG
1	A	190	PHE
1	A	226	GLU
1	A	294	ASP
1	A	300	LEU
1	A	306	ASP
1	A	394	PHE
1	A	417	GLU
1	A	547	SER
1	A	705	GLU

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	240	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	#$|Z| > 2$
2	SO4	A	904	-	4,4,4	0.45	0	6,6,6	0.35	0
4	93Z	A	907	1	16,16,17	0.81	0	18,24,26	1.47	3 (16%)
5	OXL	A	908	-	0,5,5	0.00	-	0,6,6	0.00	-
2	SO4	A	905	-	4,4,4	0.38	0	6,6,6	0.30	0
3	PG4	A	906	-	12,12,12	0.65	0	11,11,11	0.91	0
2	SO4	A	901	-	4,4,4	0.33	0	6,6,6	0.51	0
2	SO4	A	902	-	4,4,4	0.34	0	6,6,6	0.50	0
2	SO4	A	903	-	4,4,4	0.42	0	6,6,6	0.33	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
3	PG4	A	906	-	-	8/10/10/10	-
4	93Z	A	907	1	-	4/7/27/31	0/1/1/1
5	OXL	A	908	-	-	0/0/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	907	93Z	C1-C2-C3	3.28	115.46	110.69
4	A	907	93Z	C2-C1-C6	2.91	117.98	111.21
4	A	907	93Z	C1-C6-C5	2.77	116.31	112.47

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	907	93Z	C6-O7-S13-O16
3	A	906	PG4	O2-C3-C4-O3
3	A	906	PG4	C3-C4-O3-C5
3	A	906	PG4	O1-C1-C2-O2
3	A	906	PG4	O4-C7-C8-O5
4	A	907	93Z	C6-O7-S13-O14
4	A	907	93Z	C6-O7-S13-O15
3	A	906	PG4	O3-C5-C6-O4
3	A	906	PG4	C5-C6-O4-C7
3	A	906	PG4	C6-C5-O3-C4
4	A	907	93Z	C5-C6-O7-S13
3	A	906	PG4	C8-C7-O4-C6

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 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.

Ligand 93Z A 907

Bond lengths

Bond angles

Torsions

Rings
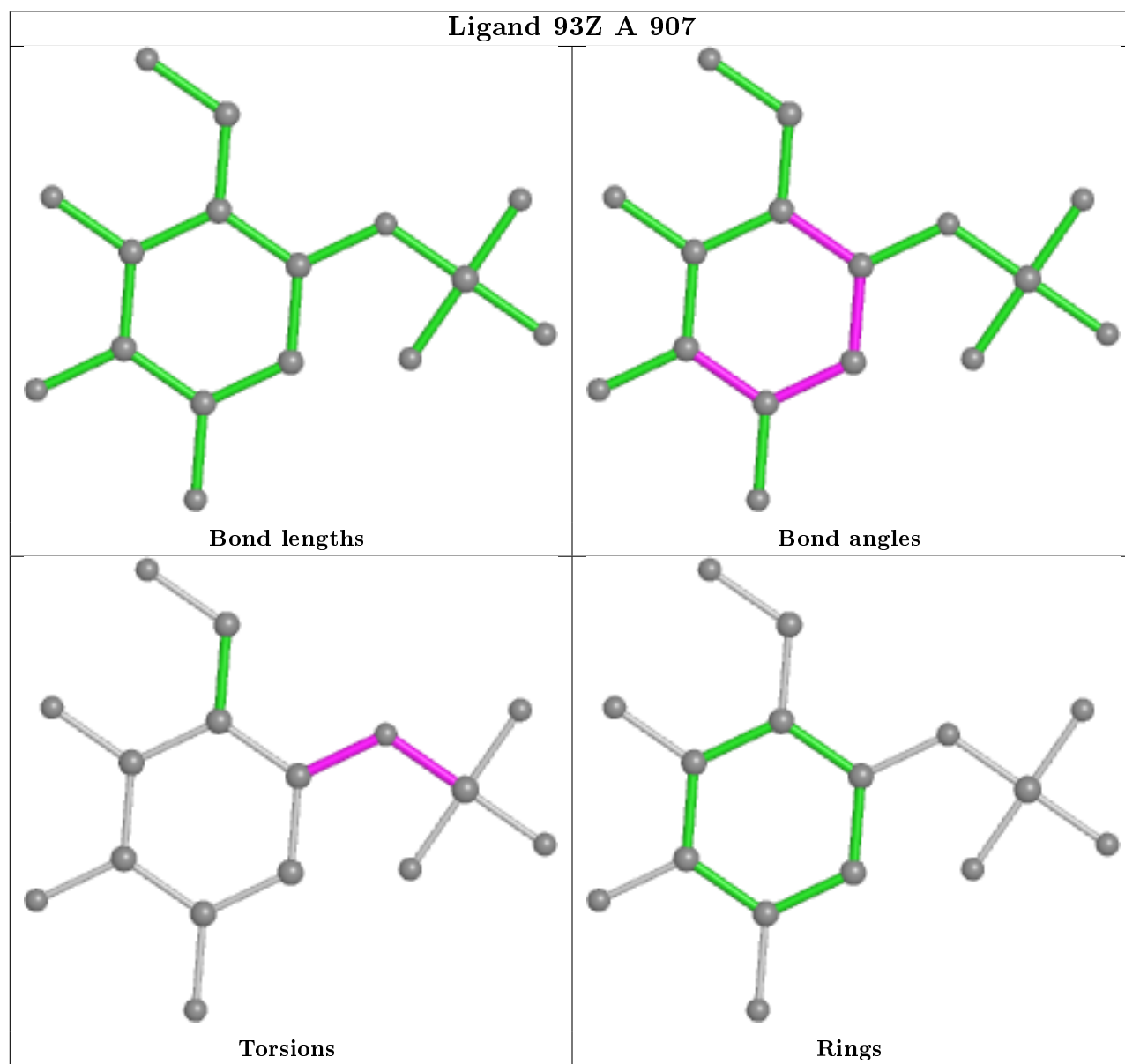
5.7 Other polymers ⓘ

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	780/836 (93%)	-0.17	8 (1%)	82	84	17, 29, 55, 95	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	ARG	4.2
1	A	137	VAL	3.3
1	A	54	GLN	2.8
1	A	136	GLN	2.8
1	A	649	ASP	2.7
1	A	91	LYS	2.7
1	A	45	ASN	2.3
1	A	141	LYS	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.
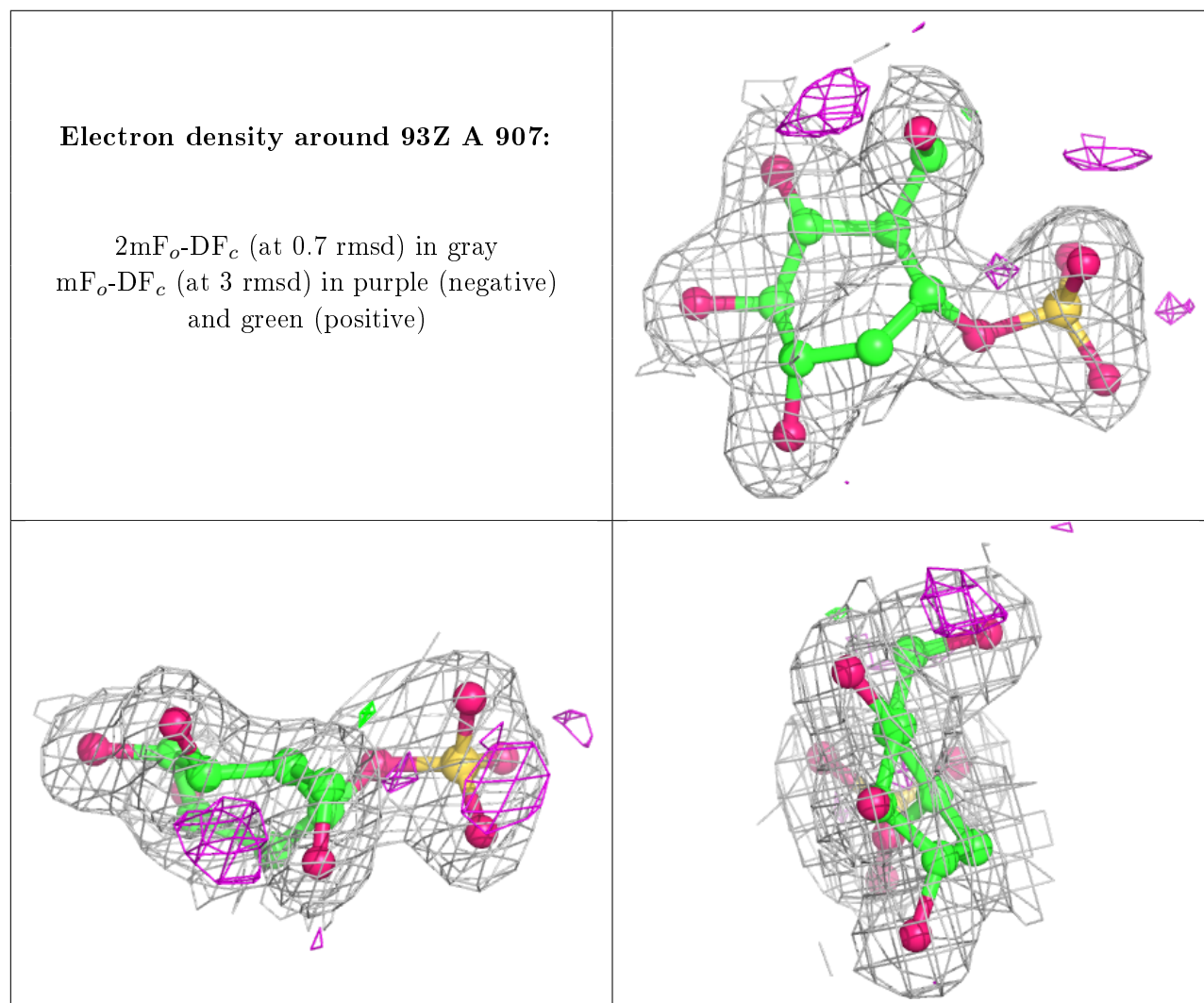
6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

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, 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
5	OXL	A	908	6/6	0.85	0.11	36,44,46,49	0
3	PG4	A	906	13/13	0.86	0.15	41,46,51,54	0
2	SO4	A	905	5/5	0.88	0.23	85,92,95,103	0
2	SO4	A	904	5/5	0.94	0.12	66,73,74,76	0
2	SO4	A	903	5/5	0.94	0.18	66,71,76,80	0
2	SO4	A	901	5/5	0.97	0.12	50,51,54,62	0
4	93Z	A	907	16/17	0.97	0.07	20,24,34,41	0
2	SO4	A	902	5/5	0.99	0.15	47,48,49,55	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 93Z A 907:

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

6.5 Other polymers (i)

There are no such residues in this entry.