



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 06:57 AM BST

PDB ID : 6SXS  
Title : GH54 α-l-arabinofuranosidase soaked with cyclic sulfate inhibitor  
Authors : McGregor, N.G.S.; Davies, G.J.; Nin-Hill, A.; Rovira, C.  
Deposited on : 2019-09-26  
Resolution : 1.86 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](mailto: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.

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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

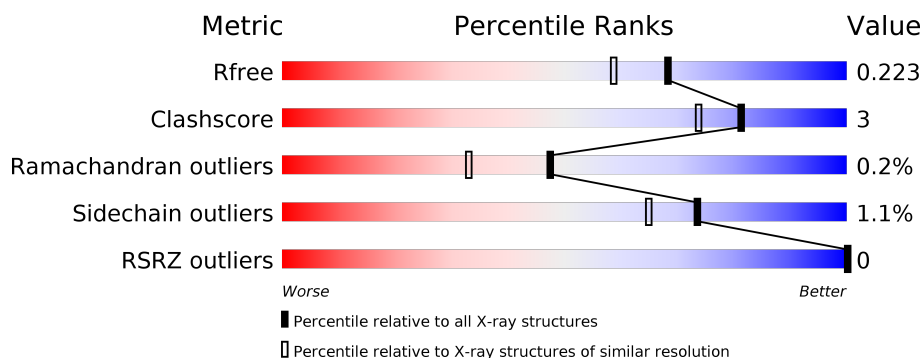
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	AAA	482	
2	A	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ACT	AAA	509	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7329 atoms, of which 3395 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 Alpha-L-arabinofuranosidase B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	481	6822	2205	3254	588	759	16	225	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	18	MET	-	initiating methionine	UNP Q8NK89

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O				
2	A	2	56	16	28	2	10		5	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



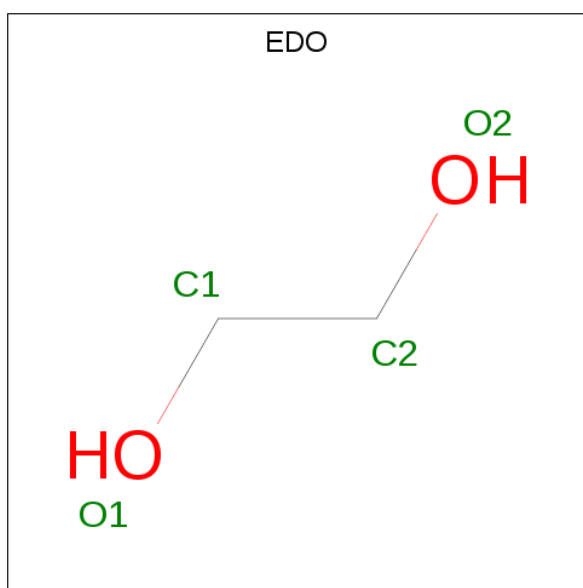
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	O	S	0	0
			5	4	1		
4	AAA	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	H	O	1	0
			24	6	14	4		
5	AAA	1	Total	C	H	O	1	0
			24	6	14	4		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
6	AAA	1	Total	C	H	O	1	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



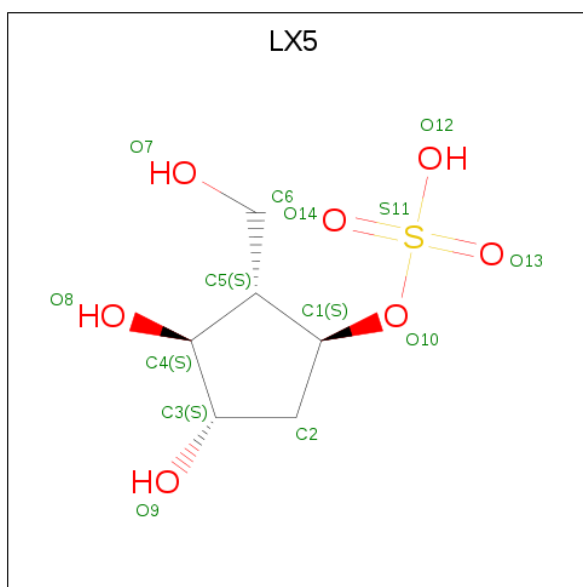
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
7	AAA	1	Total	C	H	O	1	0
			15	4	9	2		
7	AAA	1	Total	C	H	O	1	0
			15	4	9	2		
7	AAA	1	Total	C	H	O	2	0
			15	4	9	2		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	AAA	1	Total	C	H	O	0	0
			7	2	3	2		
8	AAA	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 9 is [(1 {S},2 {S},3 {S},4 {S})-2-(hydroxymethyl)-3,4-bis(oxidanyl)cyclopentyl] hydrogen sulfate (three-letter code: LX5) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>7</sub>S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	AAA	1	Total	C	H	O	S	3	0
			24	6	10	7	1		



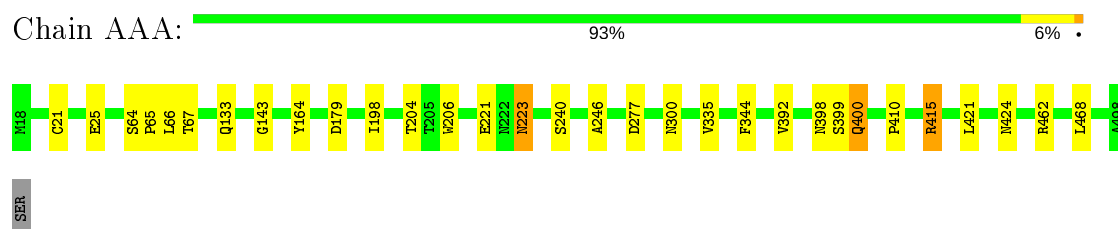
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	AAA	235	Total 235	O 235	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Alpha-L-arabinofuranosidase B



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.14Å 111.14Å 342.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.06 – 1.86 83.92 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.7 (84.06-1.86) 99.8 (83.92-1.86)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.182 , 0.215 0.190 , 0.223	Depositor DCC
$R_{free}$ test set	3338 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7329	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: LX5, PGE, NAG, EDO, SO4, ACT, PEG

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	AAA	0.82	2/3651 (0.1%)	0.90	2/4982 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	221	GLU	CD-OE2	17.08	1.44	1.25
1	AAA	221	GLU	CD-OE1	-5.34	1.19	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	277	ASP	CB-CA-C	6.31	123.03	110.40
1	AAA	400	GLN	CB-CA-C	-5.26	99.88	110.40

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	AAA	3568	3254	3241	17	0
2	A	28	28	25	1	0
3	AAA	14	14	13	0	0
4	AAA	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	20	28	28	1	0
6	AAA	12	18	18	0	0
7	AAA	25	37	31	1	0
8	AAA	8	6	6	3	0
9	AAA	14	10	0	0	0
10	AAA	235	0	0	1	0
All	All	3934	3395	3362	18	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 3.

All (18) 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:AAA:415:ARG:HH11	1:AAA:424:ASN:HD22	1.23	0.82
1:AAA:143:GLY:HA2	1:AAA:300:ASN:HD22	1.67	0.59
1:AAA:204:THR:OG1	2:A:1:NAG:H81	2.05	0.57
1:AAA:421:LEU:HD12	1:AAA:468:LEU:HB3	1.86	0.56
1:AAA:400:GLN:HE21	8:AAA:509:ACT:H3	1.71	0.55
1:AAA:398:ASN:HD21	8:AAA:509:ACT:H2	1.72	0.54
1:AAA:66:LEU:HD12	1:AAA:133:GLN:OE1	2.09	0.53
1:AAA:21:CYS:O	1:AAA:25:GLU:HB2	2.11	0.51
1:AAA:179:ASP:HA	1:AAA:198:ILE:O	2.12	0.50
1:AAA:399:SER:N	7:AAA:512:PEG:H32	2.27	0.49
1:AAA:164:TYR:HA	1:AAA:246:ALA:O	2.13	0.48
1:AAA:335:VAL:HG11	8:AAA:509:ACT:H3	1.98	0.45
1:AAA:344:PHE:CB	1:AAA:392:VAL:HG11	2.48	0.44
1:AAA:65:PRO:HB2	1:AAA:67:THR:O	2.18	0.43
1:AAA:415:ARG:HH11	1:AAA:424:ASN:ND2	2.03	0.41
1:AAA:206:TRP:HB3	1:AAA:223:ASN:HD22	1.85	0.41
1:AAA:64:SER:HB3	1:AAA:65:PRO:HD2	2.03	0.41
5:AAA:505:PGE:H6	10:AAA:820:HOH:O	2.20	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	AAA	479/482 (99%)	464 (97%)	14 (3%)	1 (0%)	47	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	223	ASN

### 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	AAA	375/377 (100%)	371 (99%)	4 (1%)	73	65

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	240	SER
1	AAA	410	PRO
1	AAA	415	ARG
1	AAA	462	ARG

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	1	1,2	14,14,15	1.24	1 (7%)	17,19,21	1.68	2 (11%)
2	NAG	A	2	2	14,14,15	0.42	0	17,19,21	1.59	4 (23%)

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	A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAG	O4-C4	-4.20	1.33	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	O5-C5-C6	3.93	113.37	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	NAG	O3-C3-C4	-2.96	103.51	110.35
2	A	1	NAG	C1-C2-N2	2.62	114.97	110.49
2	A	2	NAG	O7-C7-N2	-2.23	117.85	121.95
2	A	2	NAG	O7-C7-C8	2.21	126.16	122.06
2	A	2	NAG	O4-C4-C5	2.01	114.30	109.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2	NAG	O5-C5-C6-O6
2	A	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	1	0

## 5.6 Ligand geometry ⓘ

15 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	$\# Z  > 2$
7	PEG	AAA	512	-	5,5,6	0.48	0	4,4,5	0.47	0
8	ACT	AAA	509	-	1,3,3	3.11	1 (100%)	0,3,3	0.00	-
4	SO4	AAA	504	-	4,4,4	0.28	0	6,6,6	0.31	0
8	ACT	AAA	517	-	1,3,3	4.58	1 (100%)	0,3,3	0.00	-
7	PEG	AAA	513	-	5,5,6	0.27	0	4,4,5	0.35	0
4	SO4	AAA	506	-	4,4,4	0.45	0	6,6,6	0.15	0
6	EDO	AAA	514	-	3,3,3	0.13	0	2,2,2	0.25	0
5	PGE	AAA	505	-	9,9,9	0.31	0	8,8,8	0.32	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	PEG	AAA	508	-	6,6,6	0.29	0	5,5,5	0.17	0
6	EDO	AAA	507	-	3,3,3	0.33	0	2,2,2	0.30	0
3	NAG	AAA	503	1	14,14,15	0.91	0	17,19,21	1.32	3 (17%)
5	PGE	AAA	515	-	9,9,9	0.34	0	8,8,8	0.17	0
9	LX5	AAA	510	1	14,14,14	1.13	2 (14%)	15,21,21	1.09	2 (13%)
7	PEG	AAA	511	-	5,5,6	0.44	0	4,4,5	0.21	0
6	EDO	AAA	516	-	3,3,3	0.16	0	2,2,2	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
7	PEG	AAA	512	-	-	2/3/3/4	-
7	PEG	AAA	513	-	-	1/3/3/4	-
9	LX5	AAA	510	1	-	0/7/23/23	0/1/1/1
6	EDO	AAA	514	-	-	1/1/1/1	-
5	PGE	AAA	505	-	-	2/7/7/7	-
7	PEG	AAA	508	-	-	2/4/4/4	-
6	EDO	AAA	507	-	-	1/1/1/1	-
3	NAG	AAA	503	1	-	0/6/23/26	0/1/1/1
5	PGE	AAA	515	-	-	4/7/7/7	-
7	PEG	AAA	511	-	-	1/3/3/4	-
6	EDO	AAA	516	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	AAA	517	ACT	CH3-C	4.58	1.54	1.48
8	AAA	509	ACT	CH3-C	3.11	1.52	1.48
9	AAA	510	LX5	O10-C1	-2.71	1.43	1.47
9	AAA	510	LX5	C5-C4	2.03	1.56	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AAA	510	LX5	O12-S11-O14	2.39	116.81	108.49
3	AAA	503	NAG	C3-C4-C5	2.18	114.13	110.24
3	AAA	503	NAG	C8-C7-N2	2.16	119.75	116.10
9	AAA	510	LX5	O9-C3-C2	2.10	118.42	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	503	NAG	C2-N2-C7	2.10	125.89	122.90

There are no chirality outliers.

All (15) torsion outliers are listed below:

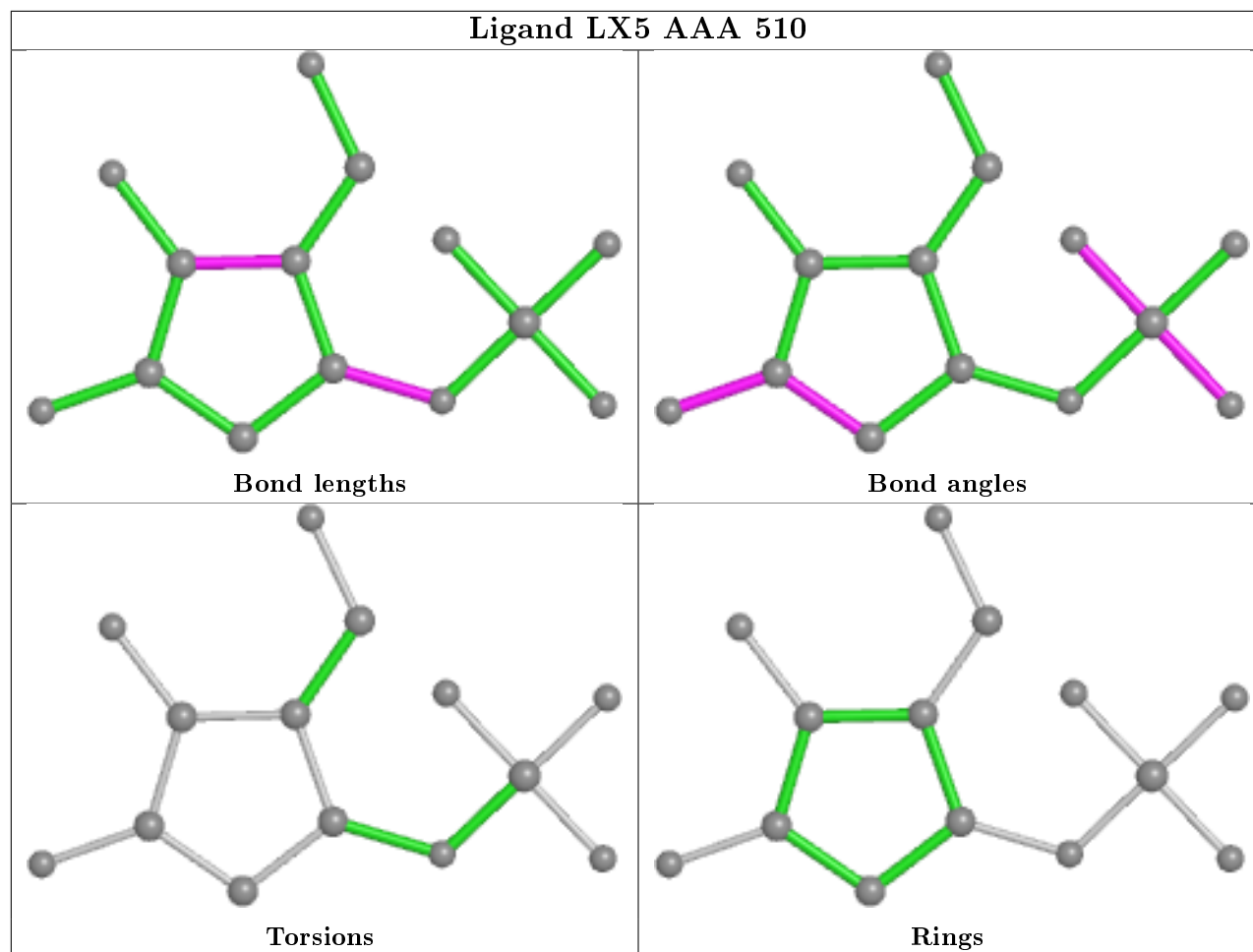
Mol	Chain	Res	Type	Atoms
5	AAA	515	PGE	O2-C3-C4-O3
7	AAA	508	PEG	O2-C3-C4-O4
7	AAA	513	PEG	O2-C3-C4-O4
6	AAA	507	EDO	O1-C1-C2-O2
5	AAA	515	PGE	O1-C1-C2-O2
7	AAA	512	PEG	C1-C2-O2-C3
7	AAA	511	PEG	O2-C3-C4-O4
5	AAA	505	PGE	O2-C3-C4-O3
6	AAA	516	EDO	O1-C1-C2-O2
7	AAA	508	PEG	C4-C3-O2-C2
5	AAA	515	PGE	C4-C3-O2-C2
5	AAA	515	PGE	C3-C4-O3-C5
5	AAA	505	PGE	C3-C4-O3-C5
7	AAA	512	PEG	O2-C3-C4-O4
6	AAA	514	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	AAA	512	PEG	1	0
8	AAA	509	ACT	3	0
5	AAA	505	PGE	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 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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AAA	481/482 (99%)	-0.07	0 <a href="#">100</a> <a href="#">100</a>	35, 43, 55, 73	0

There are no RSRZ outliers to report.

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	A	2	14/15	0.96	0.10	20,61,80,88	3
2	NAG	A	1	14/15	0.97	0.09	43,47,53,60	2

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	PEG	AAA	512	6/7	0.76	0.16	56,62,69,72	1
6	EDO	AAA	507	4/4	0.80	0.14	56,59,63,63	1

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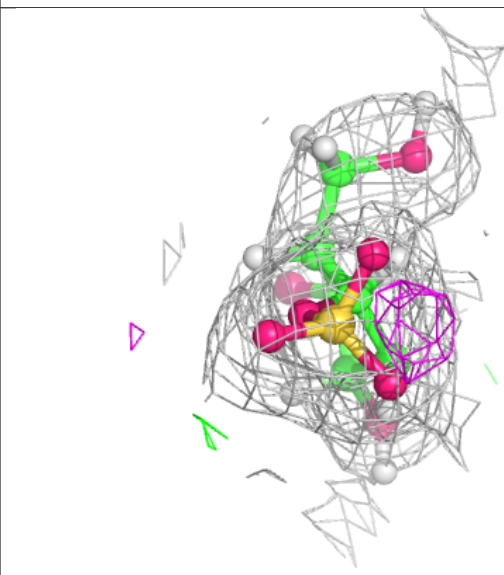
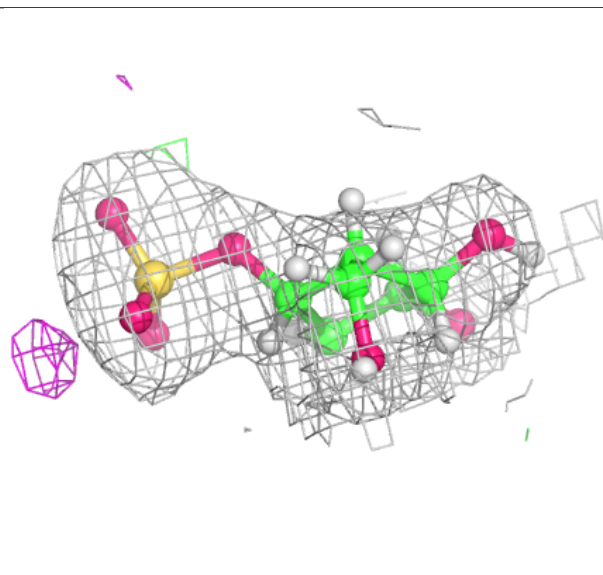
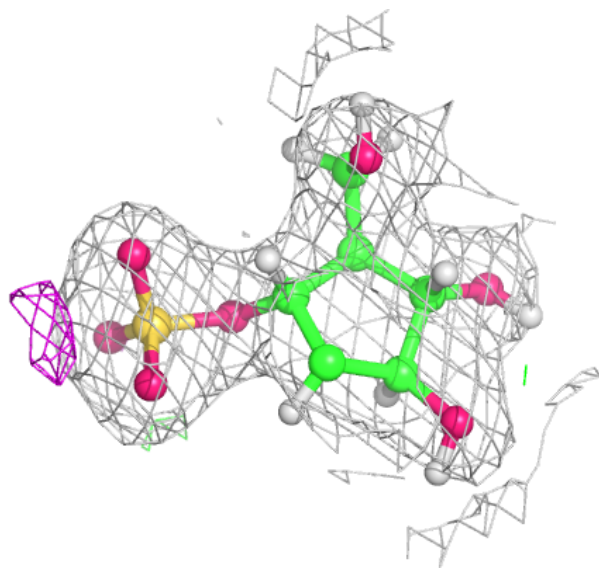
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PGE	AAA	515	10/10	0.83	0.13	54,67,79,80	24
8	ACT	AAA	517	4/4	0.87	0.16	60,66,72,75	0
6	EDO	AAA	516	4/4	0.88	0.09	54,58,63,68	1
8	ACT	AAA	509	4/4	0.91	0.10	47,52,54,58	0
5	PGE	AAA	505	10/10	0.91	0.16	53,74,78,80	1
7	PEG	AAA	511	6/7	0.93	0.09	42,54,63,64	1
7	PEG	AAA	513	6/7	0.93	0.07	0,66,71,73	2
6	EDO	AAA	514	4/4	0.94	0.09	50,55,60,60	1
7	PEG	AAA	508	7/7	0.95	0.14	49,59,63,63	1
4	SO4	AAA	506	5/5	0.95	0.16	36,46,46,47	5
3	NAG	AAA	503	14/15	0.96	0.12	44,48,51,53	3
9	LX5	AAA	510	14/14	0.98	0.12	42,47,49,53	3
4	SO4	AAA	504	5/5	0.98	0.10	52,55,59,60	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 LX5 AAA 510:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.