Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2024 – 02:47 pm GMT

PDB ID	:	6SXT
Title	:	GH54 a-l-arabinofuranosidase soaked with aziridine inhibitor
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Deposited on	:	2019-09-26
Resolution	:	1.47 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 (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:

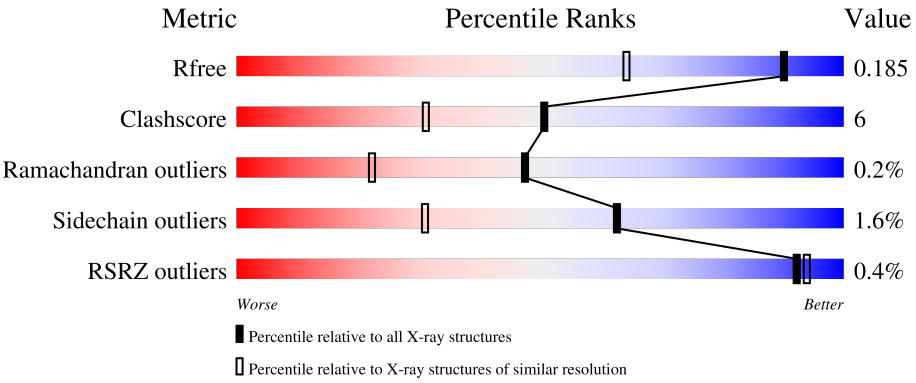
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.47 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	A	483	93% 6%
2	B	2	100%

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
10	EDO	A	516	-	-	X	-
5	SO4	A	512	-	-	X	-
7	ACT	A	508	-	-	X	-
9	PGE	A	531	-	-	X	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7832 atoms, of which 3551 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	A	482	6929	2241	3311	590	771	16	230	8	0

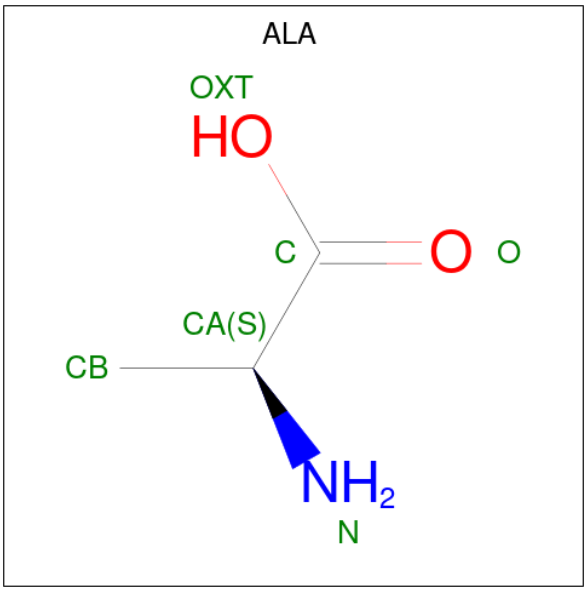
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	SER	-	expression tag	UNP Q8NK89
A	18	MET	-	expression tag	UNP Q8NK89

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

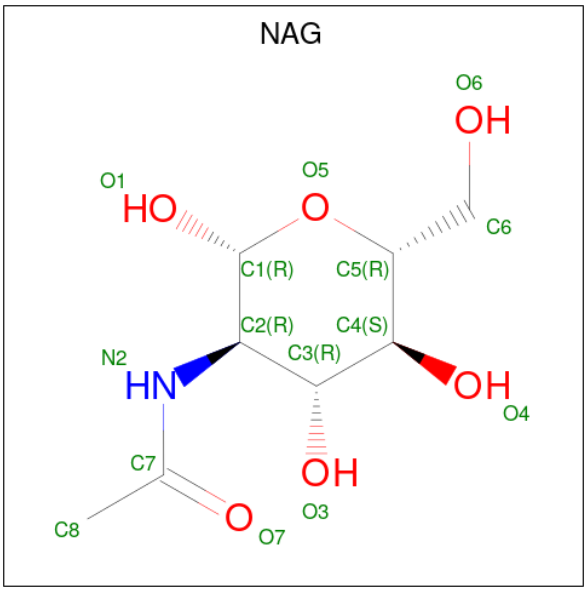
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	B	2	55	16	27	2	10	5	0	0

- Molecule 3 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



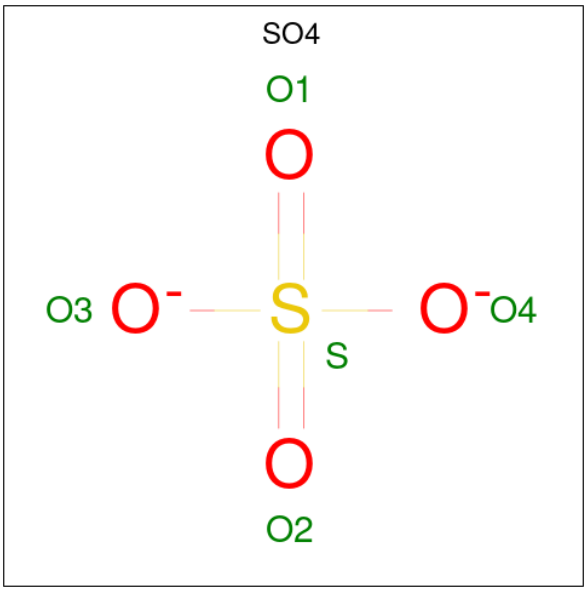
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			12	3	7	1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



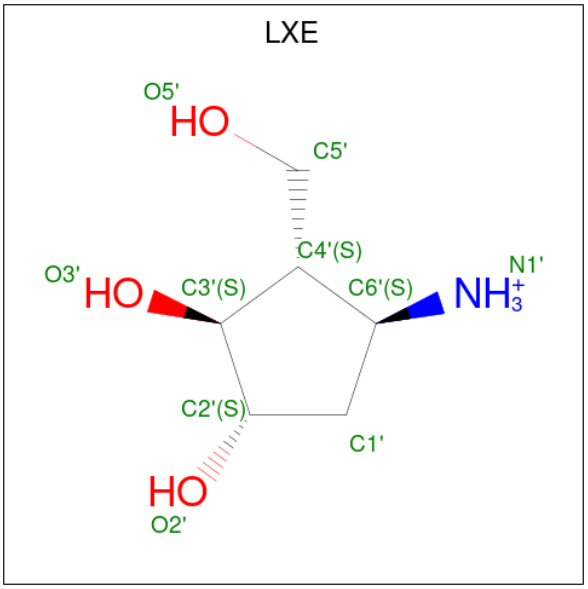
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



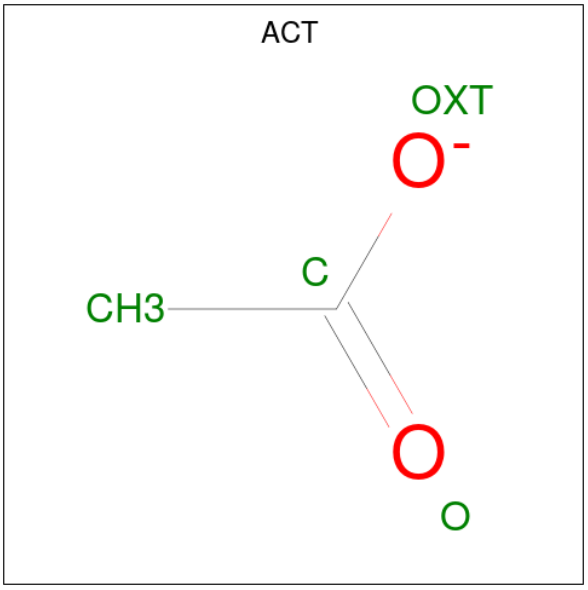
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

- Molecule 6 is [(1 {S},2 {S},3 {S},4 {S})-2-(hydroxymethyl)-3,4-bis(oxidanyl)cyclopentyl] azanium (three-letter code: LXE) (formula: $C_6H_{14}NO_3$) (labeled as "Ligand of Interest" by depositor).



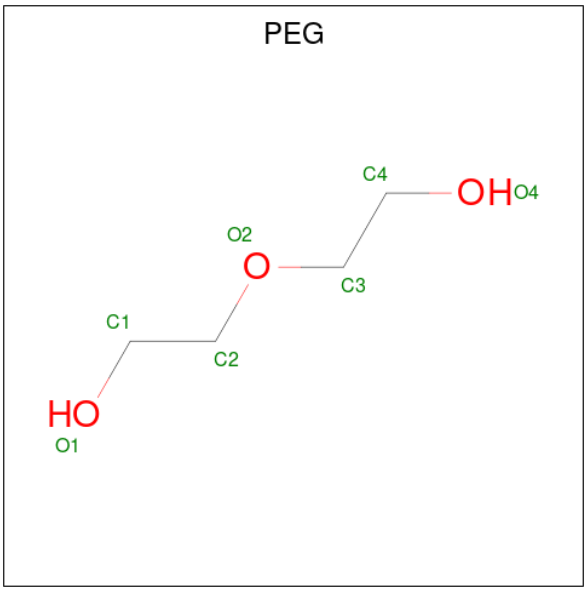
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	2	0
			23	6	13	1	3		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



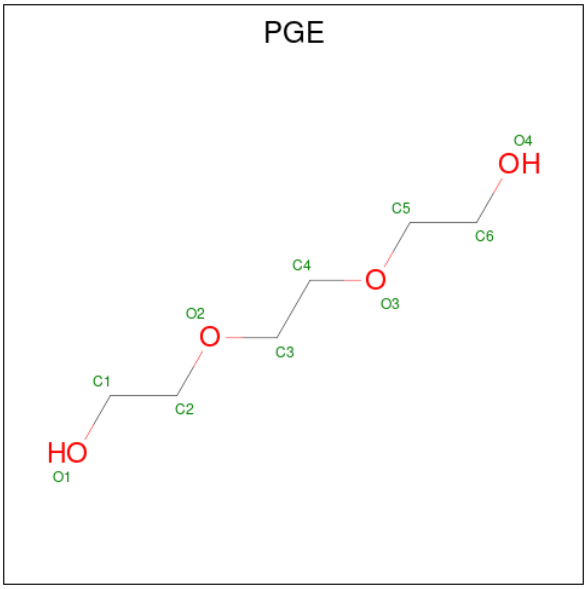
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			7	2	3	2		
7	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



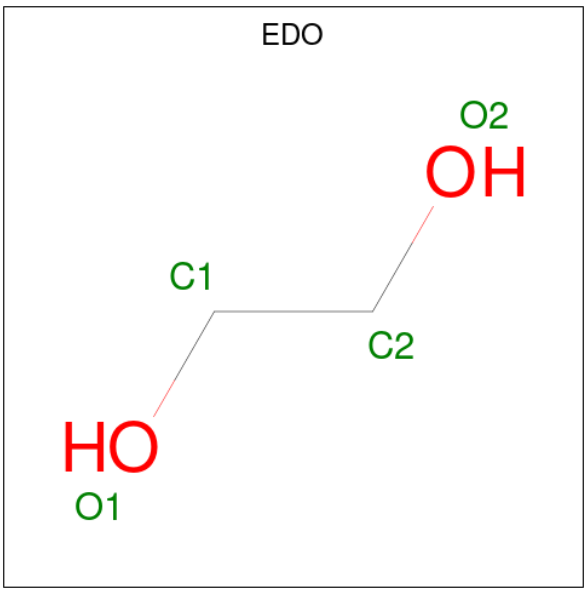
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H O 17 4 10 3	1	0
8	A	1	Total C H O 17 4 10 3	1	0
8	A	1	Total C H O 17 4 10 3	1	0
8	A	1	Total C H O 11 3 6 2	2	0
8	A	1	Total C H O 14 4 8 2	0	0
8	A	1	Total C H O 17 4 10 3	1	0
8	A	1	Total C H O 14 4 8 2	0	0
8	A	1	Total C H O 13 4 7 2	1	0
8	A	1	Total C H O 15 4 9 2	1	1

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C H O 10 2 6 2	1	0
10	A	1	Total C H O 10 2 6 2	1	0
10	A	1	Total C H O 10 2 6 2	1	0
10	A	1	Total C H O 10 2 6 2	1	0
10	A	1	Total C H O 8 2 5 1	2	0
10	A	1	Total C H O 10 2 6 2	1	0
10	A	1	Total C H O 10 2 6 2	1	0
10	A	1	Total C H O 10 2 6 2	1	0
10	A	1	Total C H O 10 2 6 2	1	0

- Molecule 11 is water.

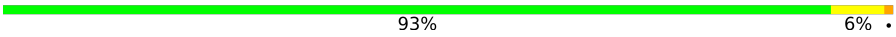
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	456	Total O 456 456	0	0

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.

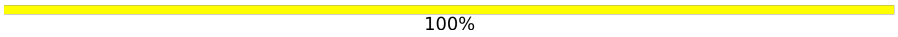
• Molecule 1: Alpha-L-arabinofuranosidase B

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	112.23Å 112.23Å 342.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.69 – 1.47 84.54 – 1.47	Depositor EDS
% Data completeness (in resolution range)	99.3 (84.69-1.47) 99.3 (84.54-1.47)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.157 , 0.179 0.165 , 0.185	Depositor DCC
R_{free} test set	6980 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 61.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	7832	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: NAG, PEG, ACT, PGE, EDO, LXE, 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	0.83	1/3723 (0.0%)	0.96	4/5081 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	GLU	CD-OE2	13.04	1.40	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	241	TYR	CB-CG-CD2	-7.46	116.53	121.00
1	A	271	TYR	CB-CG-CD1	-6.90	116.86	121.00
1	A	275	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	A	73	ASP	CB-CG-OD2	-5.26	113.57	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3618	3311	3306	26	1
2	B	28	27	25	0	0
3	A	5	7	4	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	14	13	0	0
5	A	20	0	0	3	0
6	A	10	13	0	0	0
7	A	8	6	6	4	0
8	A	57	78	66	4	0
9	A	30	42	42	16	1
10	A	35	53	50	6	0
11	A	456	0	0	11	1
All	All	4281	3551	3512	41	3

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 6.

All (41) 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)
10:A:516:EDO:H21	11:A:637:HOH:O	1.59	1.00
1:A:63:ILE:HA	9:A:531:PGE:H1	1.46	0.94
5:A:505:SO4:O1	11:A:601:HOH:O	1.88	0.91
1:A:498:ALA:C	3:A:501:ALA:N	2.29	0.86
1:A:459:ARG:HH22	1:A:477:GLN:HE22	1.20	0.85
9:A:531:PGE:H22	11:A:605:HOH:O	1.75	0.84
9:A:531:PGE:H12	11:A:731:HOH:O	1.77	0.82
9:A:531:PGE:O3	11:A:602:HOH:O	2.00	0.78
10:A:516:EDO:C2	11:A:637:HOH:O	2.24	0.78
1:A:235:GLY:HA3	10:A:516:EDO:H12	1.73	0.68
9:A:531:PGE:C2	11:A:605:HOH:O	2.34	0.68
1:A:459:ARG:NH2	1:A:477:GLN:HE22	1.94	0.65
1:A:459:ARG:HH22	1:A:477:GLN:NE2	1.91	0.65
1:A:68:ALA:H	10:A:530:EDO:H22	1.62	0.64
9:A:531:PGE:C2	9:A:531:PGE:H5	2.28	0.64
1:A:398:ASN:HD21	7:A:508:ACT:H2	1.63	0.62
1:A:372:ASN:HD21	1:A:374:GLN:HE21	1.47	0.62
9:A:531:PGE:H22	9:A:531:PGE:H5	1.81	0.61
1:A:335[A]:VAL:HG11	7:A:508:ACT:H3	1.87	0.57
5:A:512:SO4:O3	11:A:603:HOH:O	2.15	0.56
1:A:62:THR:O	9:A:531:PGE:C1	2.53	0.56
1:A:157:GLY:HA2	8:A:513:PEG:H31	1.88	0.56
1:A:477:GLN:NE2	1:A:480:ASP:OD2	2.41	0.53
9:A:531:PGE:H5	9:A:531:PGE:O2	2.08	0.53
9:A:531:PGE:C6	11:A:880:HOH:O	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:531:PGE:C4	11:A:602:HOH:O	2.58	0.51
1:A:235:GLY:CA	10:A:516:EDO:H12	2.39	0.51
1:A:399:SER:H	8:A:509:PEG:H32	1.77	0.50
1:A:400:GLN:HE21	7:A:508:ACT:H3	1.76	0.50
9:A:531:PGE:H62	11:A:880:HOH:O	2.12	0.49
1:A:421:LEU:HD12	1:A:468:LEU:HB3	1.96	0.47
3:A:501:ALA:O	9:A:517:PGE:O4	2.32	0.46
1:A:478[A]:THR:OG1	10:A:523:EDO:H21	2.16	0.46
1:A:179:ASP:HA	1:A:198:ILE:O	2.16	0.46
1:A:194:HIS:NE2	5:A:512:SO4:O2	2.47	0.45
1:A:62:THR:O	9:A:531:PGE:C2	2.65	0.44
1:A:398:ASN:HD21	7:A:508:ACT:CH3	2.31	0.43
1:A:63:ILE:HA	9:A:531:PGE:C1	2.34	0.43
1:A:399:SER:N	8:A:509:PEG:H32	2.34	0.42
1:A:62:THR:O	9:A:531:PGE:H1	2.21	0.41
1:A:44:SER:OG	8:A:511:PEG:H41	2.22	0.40

All (3) 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)
1:A:383:THR:HG21	1:A:409:THR:HG1[6_555]	1.27	0.33
11:A:814:HOH:O	11:A:893:HOH:O[10_455]	2.10	0.10
3:A:501:ALA:O	9:A:517:PGE:HO1[6_555]	1.52	0.08

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	488/483 (101%)	477 (98%)	10 (2%)	1 (0%)	47 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	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	385/378 (102%)	379 (98%)	6 (2%)	62 31

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	372	ASN
1	A	415	ARG
1	A	462	ARG
1	A	473	ASN
1	A	477	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	325	GLN
1	A	372	ASN
1	A	477	GLN

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)

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	B	1	2,1	14,14,15	1.21	2 (14%)	17,19,21	1.60	5 (29%)
2	NAG	B	2	2	14,14,15	1.22	1 (7%)	17,19,21	1.21	2 (11%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C2-N2	-2.66	1.41	1.46
2	B	1	NAG	C1-C2	2.54	1.56	1.52
2	B	1	NAG	O3-C3	2.21	1.48	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	C1-O5-C5	-3.16	107.92	112.19
2	B	1	NAG	O5-C1-C2	-2.93	106.66	111.29
2	B	1	NAG	O3-C3-C2	-2.72	103.84	109.47
2	B	2	NAG	O7-C7-N2	-2.38	117.57	121.95
2	B	2	NAG	O7-C7-C8	2.37	126.45	122.06
2	B	1	NAG	C3-C4-C5	-2.36	106.02	110.24
2	B	1	NAG	O4-C4-C5	-2.18	103.87	109.30

There are no chirality outliers.

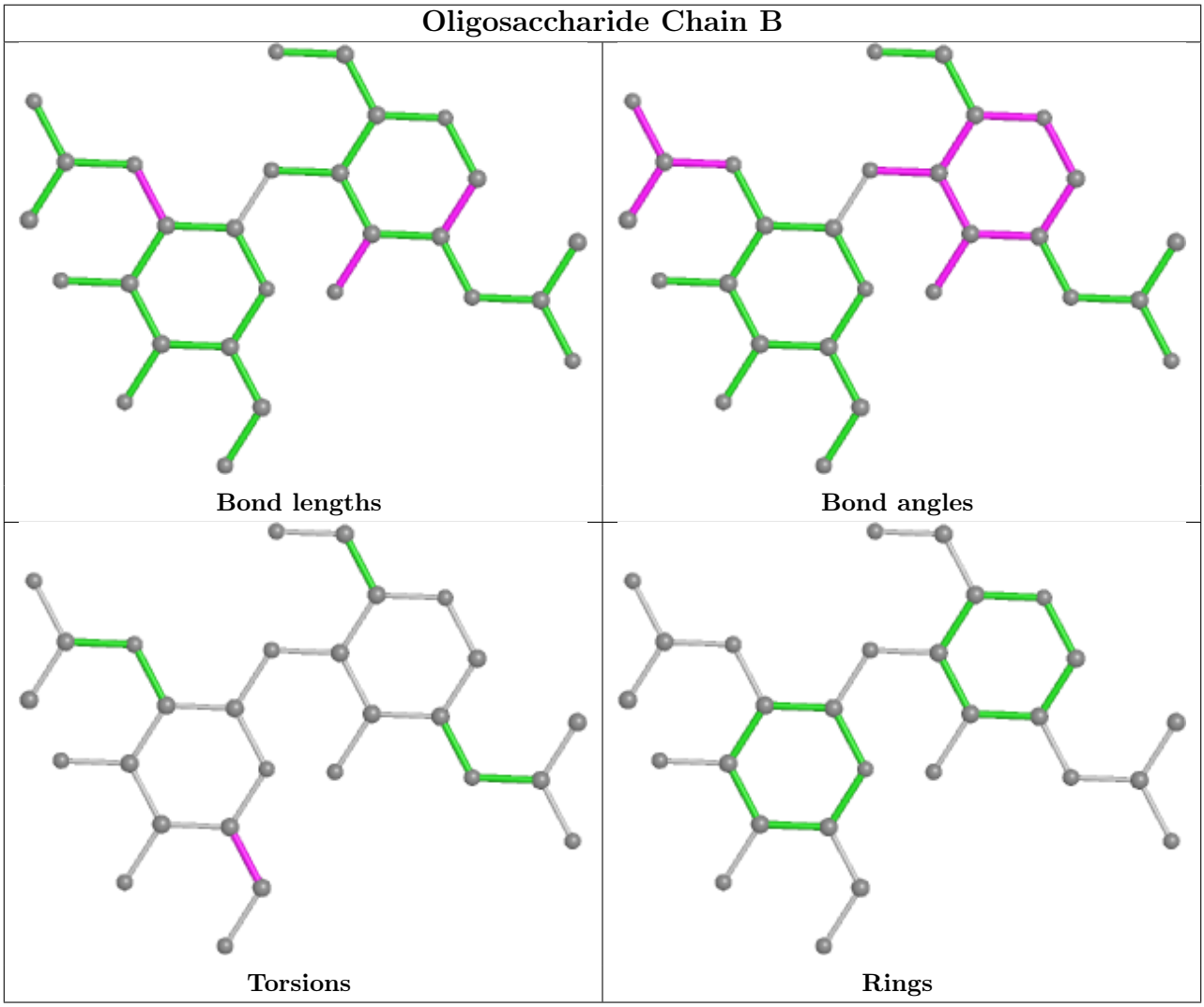
All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

31 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	$\#\|Z\| > 2$
10	EDO	A	528	-	3,3,3	0.85	0	2,2,2	0.43	0
8	PEG	A	519	-	4,4,6	0.25	0	3,3,5	0.30	0
5	SO4	A	512	-	4,4,4	0.61	0	6,6,6	0.69	0
10	EDO	A	514	-	3,3,3	0.32	0	2,2,2	0.09	0
10	EDO	A	529	-	3,3,3	0.17	0	2,2,2	0.09	0
8	PEG	A	525	-	5,5,6	0.22	0	4,4,5	0.44	0
10	EDO	A	530	-	3,3,3	0.72	0	2,2,2	0.32	0
10	EDO	A	527	-	2,2,3	0.38	0	1,1,2	0.33	0
7	ACT	A	508	-	3,3,3	2.63	1 (33%)	3,3,3	1.58	1 (33%)
10	EDO	A	516	-	3,3,3	1.06	0	2,2,2	1.40	0
9	PGE	A	531	-	9,9,9	0.64	0	8,8,8	0.78	0
5	SO4	A	505	-	4,4,4	0.36	0	6,6,6	0.05	0
10	EDO	A	515	-	3,3,3	0.54	0	2,2,2	0.65	0
8	PEG	A	521	-	5,5,6	0.49	0	4,4,5	0.19	0
8	PEG	A	511	-	6,6,6	0.45	0	5,5,5	0.36	0
8	PEG	A	524	-	5,5,6	0.33	0	4,4,5	0.18	0
8	PEG	A	513	-	6,6,6	0.18	0	5,5,5	0.28	0
10	EDO	A	532	-	3,3,3	0.15	0	2,2,2	0.21	0
5	SO4	A	518	-	4,4,4	0.22	0	6,6,6	0.17	0
5	SO4	A	506	-	4,4,4	0.62	0	6,6,6	0.42	0
8	PEG	A	522	-	6,6,6	0.19	0	5,5,5	0.08	0
6	LXE	A	507	1	10,10,10	1.94	4 (40%)	8,14,14	1.10	0
8	PEG	A	509	-	6,6,6	0.29	0	5,5,5	0.16	0
4	NAG	A	504	1	14,14,15	0.72	0	17,19,21	0.75	0
3	ALA	A	501	-	3,4,5	0.66	0	2,4,6	1.72	1 (50%)
10	EDO	A	523	-	3,3,3	0.32	0	2,2,2	0.67	0
7	ACT	A	520	-	3,3,3	1.20	0	3,3,3	0.79	0
9	PGE	A	517	-	9,9,9	0.15	0	8,8,8	0.13	0
9	PGE	A	510	-	9,9,9	0.25	0	8,8,8	0.24	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
10	EDO	A	528	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	A	519	-	-	2/2/2/4	-
10	EDO	A	514	-	-	0/1/1/1	-
10	EDO	A	529	-	-	0/1/1/1	-
8	PEG	A	525	-	-	2/3/3/4	-
10	EDO	A	530	-	-	1/1/1/1	-
10	EDO	A	516	-	-	1/1/1/1	-
9	PGE	A	531	-	-	4/7/7/7	-
10	EDO	A	515	-	-	1/1/1/1	-
8	PEG	A	521	-	-	0/3/3/4	-
8	PEG	A	511	-	-	1/4/4/4	-
8	PEG	A	524	-	-	0/3/3/4	-
8	PEG	A	513	-	-	3/4/4/4	-
10	EDO	A	532	-	-	1/1/1/1	-
8	PEG	A	522	-	-	3/4/4/4	-
6	LXE	A	507	1	-	0/2/18/18	0/1/1/1
8	PEG	A	509	-	-	3/4/4/4	-
4	NAG	A	504	1	-	0/6/23/26	0/1/1/1
3	ALA	A	501	-	-	0/0/2/4	-
10	EDO	A	523	-	-	1/1/1/1	-
9	PGE	A	517	-	-	3/7/7/7	-
9	PGE	A	510	-	-	1/7/7/7	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	507	LXE	C2'-C3'	-4.07	1.47	1.53
7	A	508	ACT	O-C	3.89	1.40	1.22
6	A	507	LXE	O3'-C3'	2.68	1.49	1.43
6	A	507	LXE	C4'-C6'	2.35	1.58	1.53
6	A	507	LXE	O2'-C2'	-2.25	1.38	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	ALA	O-C-CA	-2.43	116.60	124.28
7	A	508	ACT	O-C-CH3	-2.01	114.50	122.33

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	513	PEG	O2-C3-C4-O4
9	A	531	PGE	O1-C1-C2-O2
8	A	522	PEG	O2-C3-C4-O4
8	A	509	PEG	O2-C3-C4-O4
10	A	515	EDO	O1-C1-C2-O2
10	A	516	EDO	O1-C1-C2-O2
10	A	523	EDO	O1-C1-C2-O2
10	A	530	EDO	O1-C1-C2-O2
10	A	532	EDO	O1-C1-C2-O2
9	A	517	PGE	O2-C3-C4-O3
8	A	509	PEG	O1-C1-C2-O2
8	A	513	PEG	O1-C1-C2-O2
10	A	528	EDO	O1-C1-C2-O2
8	A	519	PEG	C4-C3-O2-C2
9	A	531	PGE	O2-C3-C4-O3
9	A	531	PGE	O3-C5-C6-O4
8	A	513	PEG	C1-C2-O2-C3
9	A	531	PGE	C1-C2-O2-C3
8	A	522	PEG	C1-C2-O2-C3
8	A	525	PEG	C4-C3-O2-C2
8	A	519	PEG	O2-C3-C4-O4
8	A	511	PEG	O2-C3-C4-O4
9	A	517	PGE	C3-C4-O3-C5
8	A	509	PEG	C1-C2-O2-C3
8	A	525	PEG	O2-C3-C4-O4
8	A	522	PEG	C4-C3-O2-C2
9	A	510	PGE	O3-C5-C6-O4
9	A	517	PGE	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	512	SO4	2	0
10	A	530	EDO	1	0
7	A	508	ACT	4	0
10	A	516	EDO	4	0
9	A	531	PGE	15	0
5	A	505	SO4	1	0
8	A	511	PEG	1	0
8	A	513	PEG	1	0
8	A	509	PEG	2	0
3	A	501	ALA	2	1

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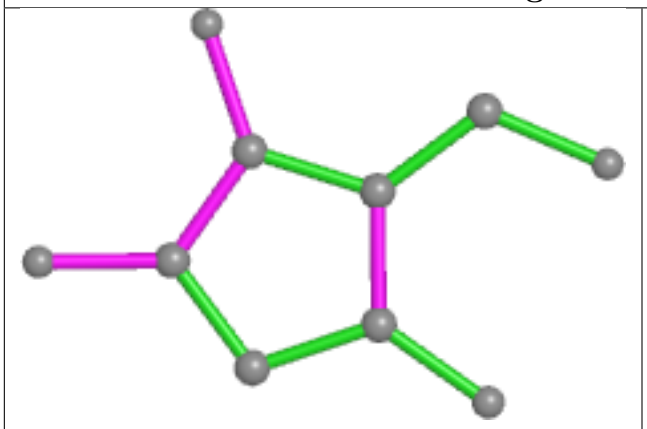
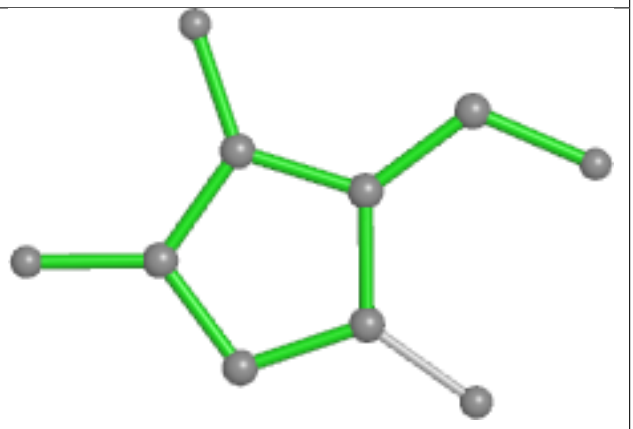
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	523	EDO	1	0
9	A	517	PGE	1	1

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.

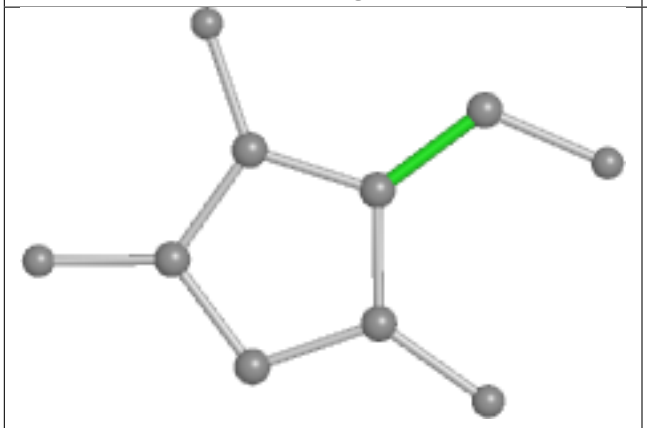
Ligand LXE A 507



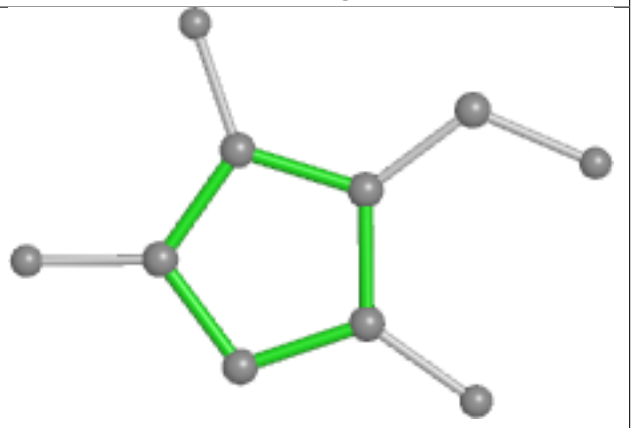
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	482/483 (99%)	-0.07	2 (0%)	92	94	14, 20, 30, 54	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	SER	2.8
1	A	240[A]	SER	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

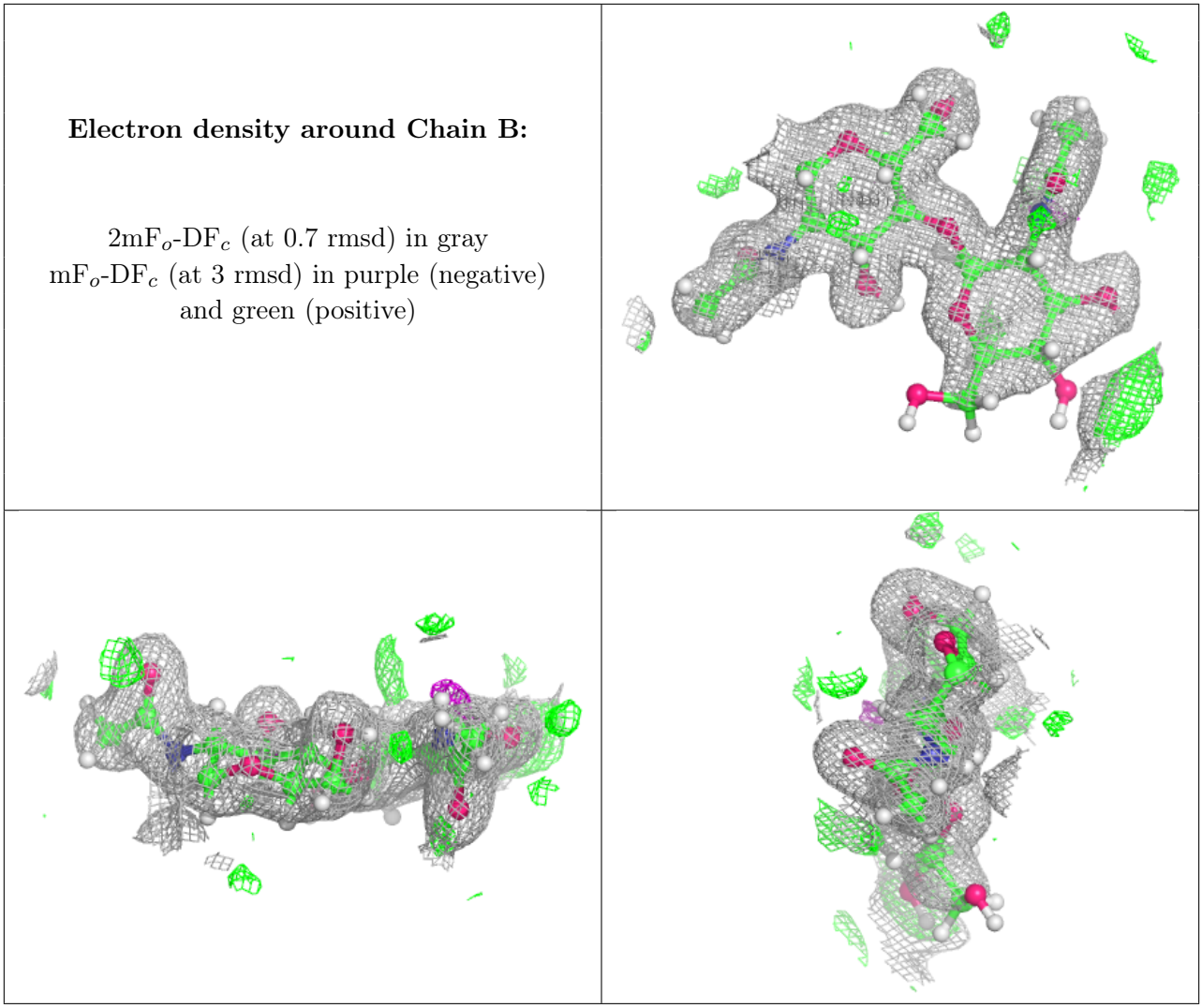
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	NAG	B	2	14/15	0.91	0.13	28,42,70,72	3
2	NAG	B	1	14/15	0.94	0.08	21,26,30,31	2

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 B:

$2mF_o$-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
10	EDO	A	523	4/4	0.64	0.12	50,51,56,56	1
10	EDO	A	527	3/4	0.64	0.22	0,39,47,47	2
8	PEG	A	525	6/7	0.66	0.18	0,55,68,68	1
10	EDO	A	515	4/4	0.68	0.20	47,48,53,53	1
8	PEG	A	513	7/7	0.72	0.17	50,55,68,68	1
3	ALA	A	501	5/6	0.73	0.24	59,71,83,83	0
9	PGE	A	531	10/10	0.74	0.53	22,40,50,52	1
7	ACT	A	508	4/4	0.75	0.15	24,33,33,34	0

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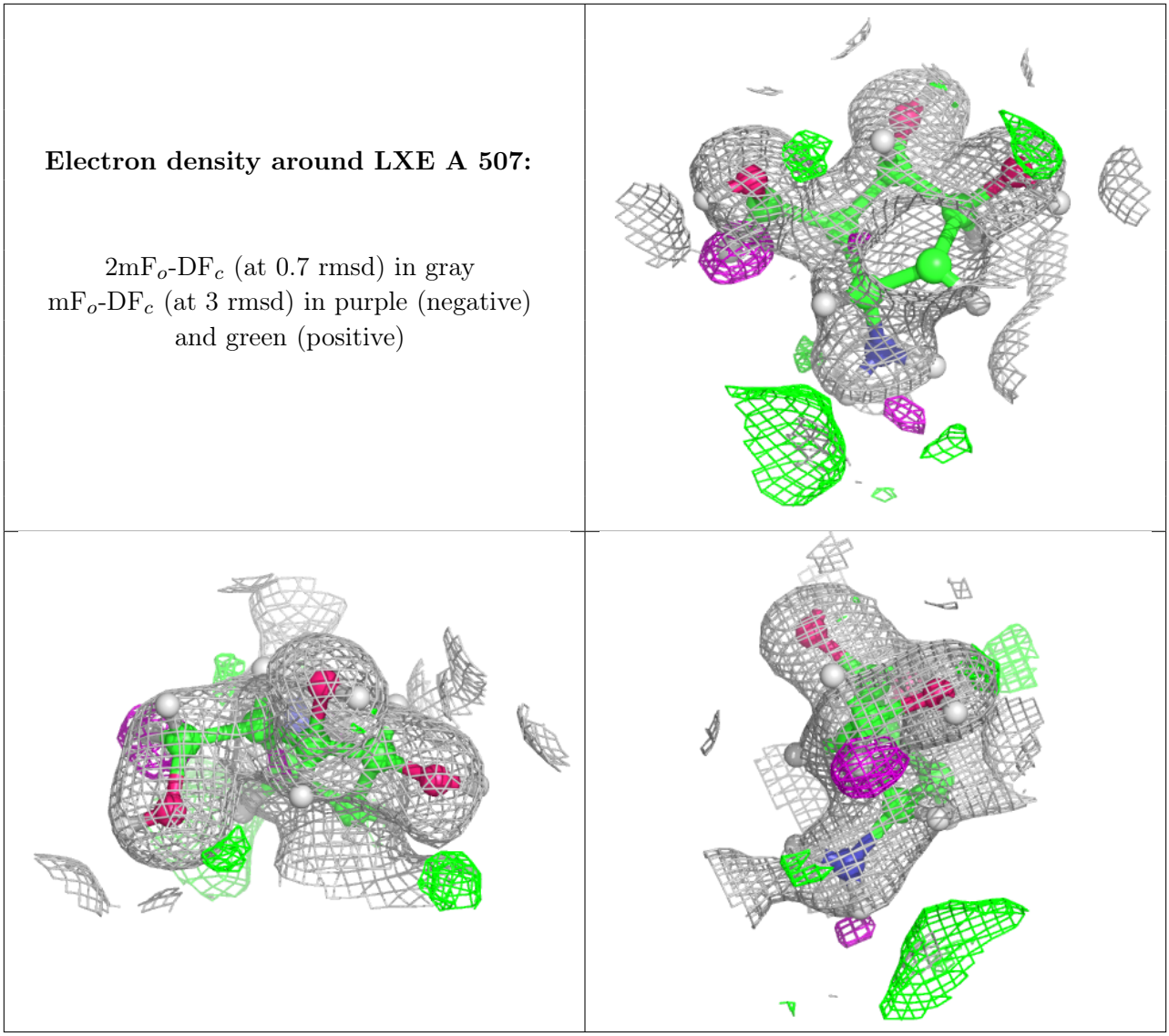
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	EDO	A	530	4/4	0.77	0.17	37,41,55,55	1
8	PEG	A	519	5/7	0.79	0.13	0,49,56,56	2
10	EDO	A	514	4/4	0.79	0.11	47,51,60,60	1
10	EDO	A	529	4/4	0.81	0.14	52,54,62,62	1
8	PEG	A	526[B]	6/7	0.85	0.12	54,54,60,60	0
8	PEG	A	526[A]	6/7	0.85	0.12	54,54,60,60	1
10	EDO	A	516	4/4	0.87	0.21	25,38,38,38	1
8	PEG	A	509	7/7	0.89	0.18	40,45,57,57	1
8	PEG	A	511	7/7	0.89	0.12	36,42,58,58	1
5	SO4	A	518	5/5	0.89	0.28	57,58,78,82	0
5	SO4	A	505	5/5	0.92	0.13	57,58,58,62	5
9	PGE	A	517	10/10	0.92	0.20	41,44,47,48	24
10	EDO	A	532	4/4	0.92	0.12	53,55,62,62	1
5	SO4	A	512	5/5	0.93	0.21	30,34,36,37	5
9	PGE	A	510	10/10	0.93	0.12	32,40,48,58	1
8	PEG	A	524	6/7	0.93	0.11	39,41,50,50	0
10	EDO	A	528	4/4	0.94	0.19	39,40,48,48	1
7	ACT	A	520	4/4	0.94	0.15	31,43,46,46	0
8	PEG	A	521	6/7	0.94	0.09	22,35,44,44	0
8	PEG	A	522	7/7	0.94	0.16	25,33,49,49	1
6	LXE	A	507	10/10	0.96	0.08	0,23,29,29	2
5	SO4	A	506	5/5	0.98	0.12	22,24,26,28	5
4	NAG	A	504	14/15	0.98	0.09	19,22,28,28	3

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 LXE A 507:

$2mF_o$-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.