



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:31 AM UTC

PDB ID : 6SXR / pdb_00006sxr
Title : E221Q mutant of GH54 α -l-arabinofuranosidase soaked with 4-nitrophenyl α -l-arabinofuranoside
Authors : McGregor, N.G.S.; Davies, G.J.; Nin-Hill, A.; Rovira, C.
Deposited on : 2019-09-26
Resolution : 1.64 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

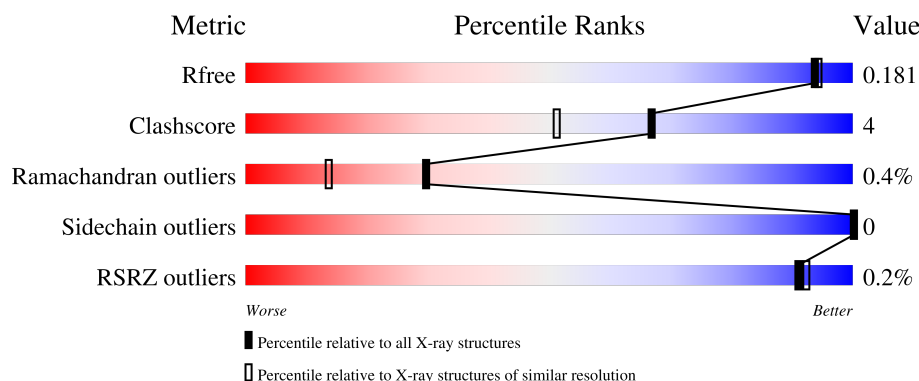
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

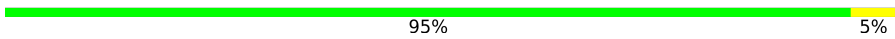
The reported resolution of this entry is 1.64 Å.

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}	180053	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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 $\leq 5\%$. 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	A	482	
2	B	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
5	ACT	A	505	-	-	X	-
8	PEG	A	530	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7728 atoms, of which 3544 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
1	A	481	Total	C	H	N	O	S	226	0	0
			6830	2207	3258	589	760	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP Q8NK89
A	221	GLN	GLU	engineered mutation	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
2	B	2	Total	C	H	N	O		5	0	0
			56	16	28	2	10				

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



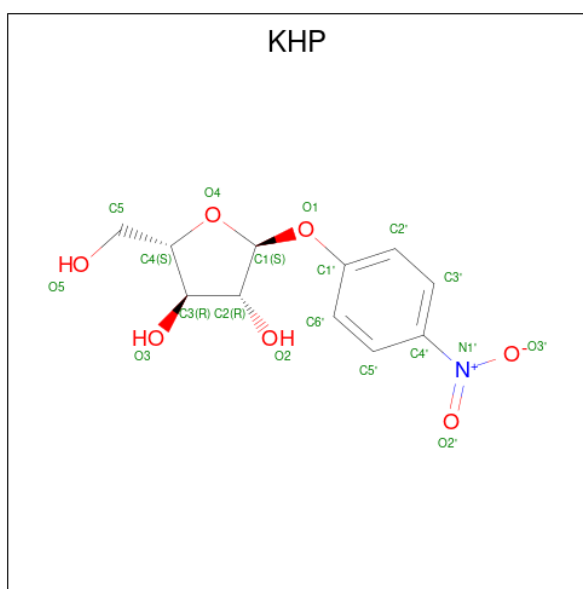
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



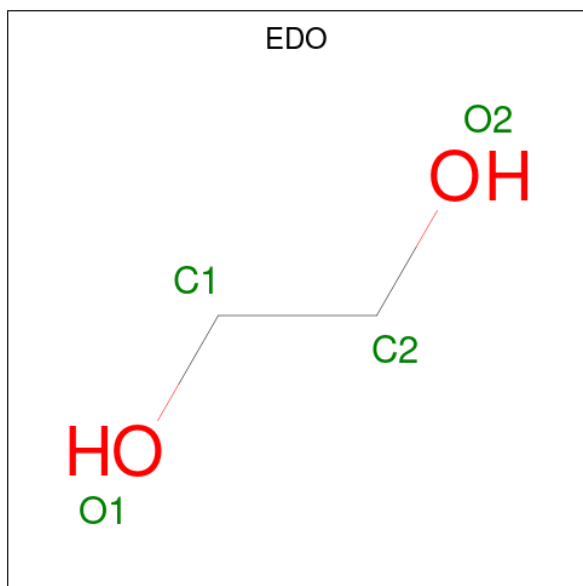
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			7	2	3	2		
5	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 6 is 4-nitrophenyl alpha-L-arabinofuranoside (CCD ID: KHP) (formula: $C_{11}H_{13}NO_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	
			32	11	13	1	7	
6	A	1	Total	C	H	N	O	
			32	11	13	1	7	
6	A	1	Total	C	H	N	O	
			32	11	13	1	7	

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



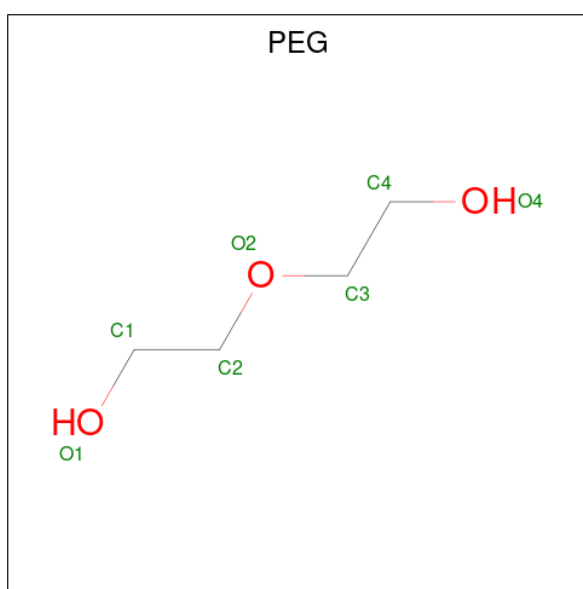
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O		
			10	2	6	2		
7	A	1	Total	C	H	O		
			10	2	6	2		
7	A	1	Total	C	H	O		
			10	2	6	2		
7	A	1	Total	C	H	O		
			10	2	6	2		
7	A	1	Total	C	H	O		
			10	2	6	2		
7	A	1	Total	C	H	O		
			10	2	6	2		
7	A	1	Total	C	H	O		
			10	2	6	2		
7	A	1	Total	C	H	O		
			10	2	6	2		

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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



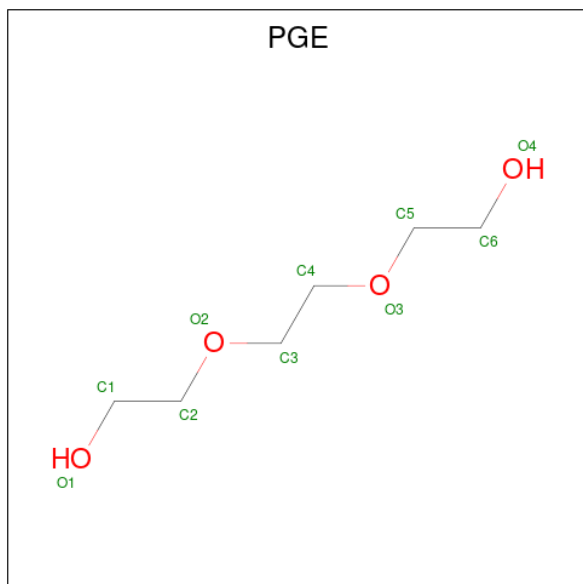
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	2	0
			12	3	7	2		
8	A	1	Total	C	H	O	1	0
			17	4	10	3		
8	A	1	Total	C	H	O	2	0
			12	3	7	2		
8	A	1	Total	C	H	O	1	0
			17	4	10	3		
8	A	1	Total	C	H	O	2	0
			12	3	7	2		
8	A	1	Total	C	H	O	1	1
			12	3	7	2		
8	A	1	Total	C	H	O	1	0
			17	4	10	3		

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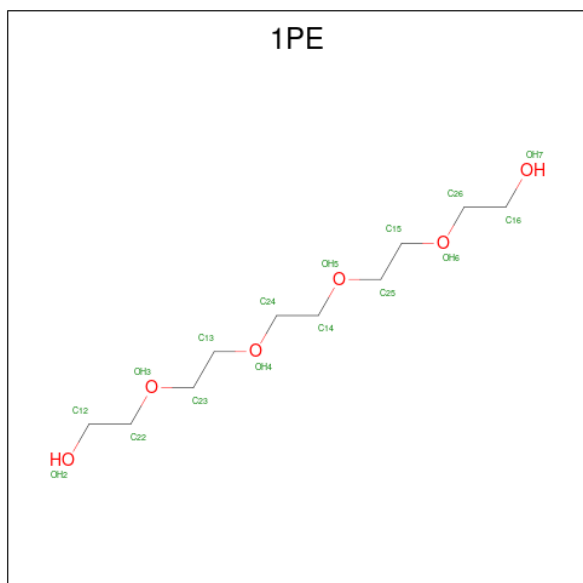
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	1	0
			17	4	10	3		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 10 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	1	0
			36	10	21	5		
10	A	1	Total	C	H	O	2	0
			31	9	18	4		

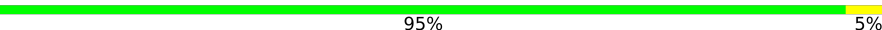
- Molecule 11 is water.

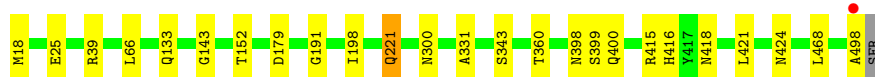
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	352	Total	O	0	0
			352	352		

3 Residue-property plots

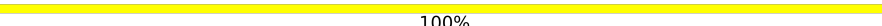
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A:  95% 5%



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

Chain B:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	111.97Å 111.97Å 341.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	93.28 – 1.64 93.28 – 1.64	Depositor EDS
% Data completeness (in resolution range)	98.1 (93.28-1.64) 98.1 (93.28-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.160 , 0.181 0.160 , 0.181	Depositor DCC
R_{free} test set	5141 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7728	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: ACT, PGE, 1PE, SO4, PEG, KHP, NAG, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.07	1/3655 (0.0%)	1.17	3/4987 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	GLY	C-O	7.06	1.30	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	THR	CA-CB-OG1	-7.11	98.94	109.60
1	A	498	ALA	CA-C-O	-5.24	111.89	120.80
1	A	416	HIS	CB-CA-C	5.04	117.84	109.53

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	3572	3258	3249	23	0
2	B	28	28	25	0	0
3	A	14	14	13	0	0
4	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	8	6	6	4	0
6	A	57	39	12	1	0
7	A	52	78	78	3	0
8	A	48	68	55	7	0
9	A	10	14	14	0	0
10	A	28	39	33	2	0
11	A	352	0	0	5	2
All	All	4184	3544	3485	26	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 4.

All (26) 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:400:GLN:HE21	5:A:505:ACT:H3	1.34	0.92
1:A:398:ASN:HD21	5:A:505:ACT:H2	1.43	0.83
1:A:415:ARG:HH11	1:A:424:ASN:HD22	1.29	0.81
10:A:533:1PE:H232	11:A:726:HOH:O	1.90	0.71
1:A:66:LEU:HD12	1:A:133:GLN:OE1	1.99	0.62
1:A:399:SER:H	8:A:515:PEG:H32	1.64	0.61
1:A:360:THR:OG1	7:A:529:EDO:H12	2.01	0.60
1:A:143:GLY:HA2	1:A:300:ASN:HD22	1.67	0.60
1:A:399:SER:N	8:A:515:PEG:H32	2.18	0.59
8:A:530:PEG:H41	11:A:894:HOH:O	2.06	0.55
1:A:18:MET:N	11:A:606:HOH:O	2.44	0.51
1:A:39:ARG:HH11	8:A:530:PEG:H41	1.75	0.51
1:A:221:GLN:HE22	6:A:513:KHP:C1	2.25	0.50
1:A:421:LEU:HD12	1:A:468:LEU:HB3	1.95	0.48
1:A:179:ASP:HA	1:A:198:ILE:O	2.15	0.47
1:A:398:ASN:ND2	5:A:505:ACT:H2	2.20	0.47
1:A:25:GLU:HG3	11:A:947:HOH:O	2.18	0.44
1:A:39:ARG:HH11	8:A:530:PEG:C4	2.31	0.43
7:A:532:EDO:H21	10:A:533:1PE:C12	2.48	0.43
1:A:398:ASN:HD21	5:A:505:ACT:CH3	2.22	0.42
1:A:360:THR:H	7:A:529:EDO:H11	1.84	0.42
1:A:133:GLN:HG2	11:A:631:HOH:O	2.19	0.42
1:A:331:ALA:HA	8:A:530:PEG:H22	2.02	0.41
1:A:39:ARG:HH11	8:A:530:PEG:H32	1.86	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:605:HOH:O	11:A:605:HOH:O[11_565]	1.75	0.45
11:A:659:HOH:O	11:A:839:HOH:O[10_455]	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	479/482 (99%)	471 (98%)	6 (1%)	2 (0%)	30 14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	SER
1	A	221	GLN

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	376/377 (100%)	376 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	221	GLN
1	A	222	ASN
1	A	223	ASN
1	A	298	ASN
1	A	300	ASN
1	A	325	GLN
1	A	372	ASN
1	A	374	GLN
1	A	398	ASN
1	A	418	ASN
1	A	424	ASN
1	A	486	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 ⓘ

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	1,2	14,14,15	1.09	1 (7%)	17,19,21	1.32	3 (17%)
2	NAG	B	2	2	14,14,15	0.93	0	17,19,21	1.65	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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C8-C7	-2.43	1.45	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	-3.70	107.23	112.19
2	B	1	NAG	C1-C2-N2	2.96	115.09	110.43
2	B	2	NAG	C3-C4-C5	-2.48	105.73	110.23
2	B	1	NAG	C1-O5-C5	-2.38	108.99	112.19
2	B	2	NAG	C1-C2-N2	2.26	114.00	110.43
2	B	2	NAG	O4-C4-C5	2.25	114.87	109.32
2	B	1	NAG	O5-C5-C4	-2.14	105.62	110.83

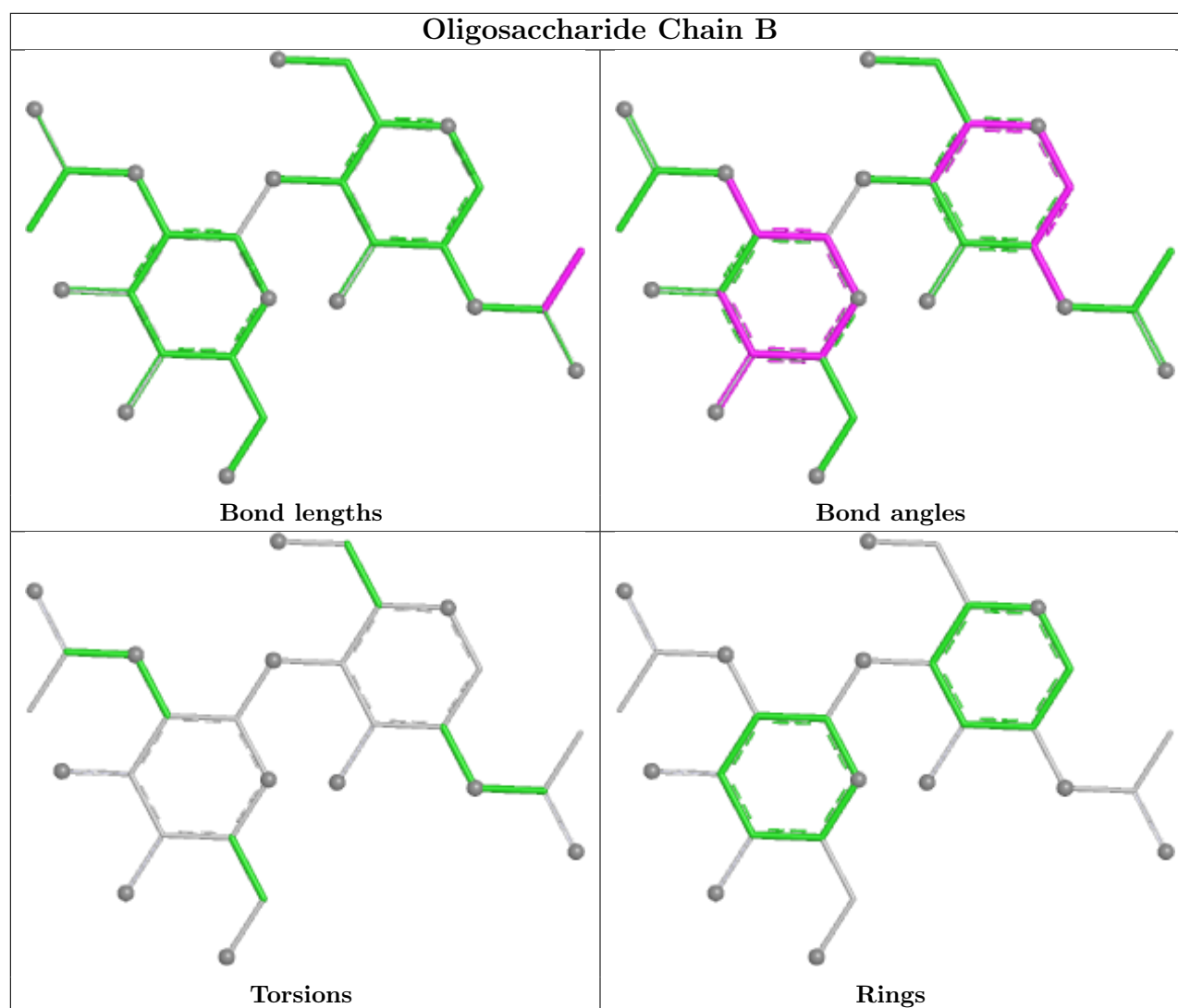
There are no chirality outliers.

There are no torsion outliers.

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](#)

34 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	EDO	A	532	-	3,3,3	0.21	0	2,2,2	0.53	0
6	KHP	A	513	-	20,20,20	1.34	3 (15%)	26,28,28	2.29	8 (30%)
8	PEG	A	514	-	4,4,6	0.24	0	3,3,5	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	KHP	A	507	-	20,20,20	0.84	1 (5%)	26,28,28	1.58	2 (7%)
8	PEG	A	516	-	4,4,6	0.30	0	3,3,5	0.18	0
10	1PE	A	533	-	12,12,15	0.84	0	11,11,14	1.24	3 (27%)
7	EDO	A	522	-	3,3,3	0.11	0	2,2,2	0.19	0
7	EDO	A	528	-	3,3,3	0.22	0	2,2,2	0.19	0
8	PEG	A	530	-	6,6,6	0.55	0	5,5,5	0.52	0
5	ACT	A	505	-	3,3,3	1.89	2 (66%)	3,3,3	1.01	0
7	EDO	A	523	-	3,3,3	0.10	0	2,2,2	0.23	0
7	EDO	A	527	-	3,3,3	0.17	0	2,2,2	0.41	0
7	EDO	A	511	-	3,3,3	0.34	0	2,2,2	0.41	0
7	EDO	A	531	-	3,3,3	0.14	0	2,2,2	0.16	0
9	PGE	A	521	-	9,9,9	0.20	0	8,8,8	0.14	0
4	SO4	A	504	-	4,4,4	0.39	0	6,6,6	0.32	0
5	ACT	A	510	-	3,3,3	0.88	0	3,3,3	1.30	0
7	EDO	A	519	-	3,3,3	0.19	0	2,2,2	0.15	0
8	PEG	A	518	-	4,4,6	0.29	0	3,3,5	0.18	0
8	PEG	A	517	-	6,6,6	0.31	0	5,5,5	0.19	0
3	NAG	A	503	1	14,14,15	0.76	0	17,19,21	1.09	2 (11%)
7	EDO	A	534	-	3,3,3	0.15	0	2,2,2	0.45	0
7	EDO	A	508	-	3,3,3	0.20	0	2,2,2	0.46	0
7	EDO	A	512	-	3,3,3	0.35	0	2,2,2	0.55	0
7	EDO	A	529	-	3,3,3	0.41	0	2,2,2	0.57	0
8	PEG	A	515	-	6,6,6	0.26	0	5,5,5	0.37	0
4	SO4	A	509	-	4,4,4	0.38	0	6,6,6	0.10	0
10	1PE	A	525	-	14,14,15	0.82	0	13,13,14	0.58	0
6	KHP	A	506	-	20,20,20	1.03	2 (10%)	26,28,28	1.29	3 (11%)
7	EDO	A	526	-	3,3,3	0.16	0	2,2,2	0.08	0
8	PEG	A	524	-	6,6,6	0.32	0	5,5,5	0.21	0
4	SO4	A	535	-	4,4,4	0.26	0	6,6,6	0.15	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	EDO	A	532	-	-	1/1/1/1	-
6	KHP	A	513	-	-	2/7/26/26	0/2/2/2
8	PEG	A	514	-	-	1/2/2/4	-
6	KHP	A	507	-	-	2/7/26/26	0/2/2/2
8	PEG	A	516	-	-	0/2/2/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	1PE	A	533	-	-	4/10/10/13	-
7	EDO	A	522	-	-	1/1/1/1	-
7	EDO	A	528	-	-	1/1/1/1	-
8	PEG	A	530	-	-	3/4/4/4	-
7	EDO	A	523	-	-	1/1/1/1	-
7	EDO	A	527	-	-	1/1/1/1	-
7	EDO	A	511	-	-	1/1/1/1	-
7	EDO	A	531	-	-	1/1/1/1	-
9	PGE	A	521	-	-	3/7/7/7	-
7	EDO	A	519	-	-	1/1/1/1	-
8	PEG	A	518	-	-	1/2/2/4	-
8	PEG	A	517	-	-	0/4/4/4	-
7	EDO	A	534	-	-	1/1/1/1	-
3	NAG	A	503	1	-	0/6/23/26	0/1/1/1
7	EDO	A	508	-	-	1/1/1/1	-
7	EDO	A	512	-	-	1/1/1/1	-
7	EDO	A	529	-	-	0/1/1/1	-
8	PEG	A	515	-	-	2/4/4/4	-
10	1PE	A	525	-	-	7/12/12/13	-
6	KHP	A	506	-	-	4/7/26/26	0/2/2/2
7	EDO	A	526	-	-	1/1/1/1	-
8	PEG	A	524	-	-	1/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	513	KHP	O4-C1	3.99	1.48	1.41
6	A	513	KHP	C4'-N1'	-2.45	1.39	1.45
6	A	513	KHP	C3-C4	2.41	1.59	1.53
6	A	506	KHP	C4'-N1'	-2.39	1.39	1.45
5	A	505	ACT	O-C	2.31	1.32	1.22
5	A	505	ACT	OXT-C	-2.11	1.21	1.30
6	A	506	KHP	O4-C4	-2.08	1.40	1.45
6	A	507	KHP	C4'-N1'	-2.04	1.40	1.45

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	513	KHP	O4-C1-C2	7.66	114.72	104.98
6	A	507	KHP	O4-C1-C2	5.76	112.30	104.98
6	A	513	KHP	O3-C3-C4	3.79	121.97	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	513	KHP	O1-C1-C2	-3.52	100.99	106.69
6	A	506	KHP	O4-C1-C2	3.21	109.07	104.98
6	A	507	KHP	C1'-O1-C1	3.17	122.28	117.82
3	A	503	NAG	C8-C7-N2	2.83	120.81	116.12
6	A	513	KHP	O2-C2-C1	2.81	119.73	111.82
3	A	503	NAG	O7-C7-C8	-2.66	117.31	122.05
6	A	513	KHP	O4-C4-C5	-2.55	103.82	109.22
6	A	513	KHP	C5-C4-C3	2.49	120.96	115.10
6	A	506	KHP	O2-C2-C1	-2.41	105.02	111.82
10	A	533	1PE	C25-OH5-C14	2.29	123.29	113.26
10	A	533	1PE	C22-OH3-C23	2.27	121.01	113.06
10	A	533	1PE	C24-OH4-C13	2.13	122.59	113.26
6	A	513	KHP	O5-C5-C4	-2.11	104.15	111.33
6	A	506	KHP	C2'-C3'-C4'	-2.08	117.32	120.08
6	A	513	KHP	O3-C3-C2	-2.05	105.24	111.82

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	513	KHP	C3'-C4'-N1'-O2'
6	A	513	KHP	C5'-C4'-N1'-O2'
8	A	518	PEG	O2-C3-C4-O4
8	A	530	PEG	O2-C3-C4-O4
10	A	525	1PE	OH4-C13-C23-OH3
10	A	533	1PE	OH4-C13-C23-OH3
10	A	525	1PE	OH6-C15-C25-OH5
8	A	524	PEG	O1-C1-C2-O2
8	A	530	PEG	O1-C1-C2-O2
6	A	506	KHP	C3'-C4'-N1'-O2'
6	A	506	KHP	C5'-C4'-N1'-O2'
6	A	507	KHP	C3'-C4'-N1'-O2'
9	A	521	PGE	O1-C1-C2-O2
7	A	511	EDO	O1-C1-C2-O2
7	A	532	EDO	O1-C1-C2-O2
9	A	521	PGE	O2-C3-C4-O3
10	A	525	1PE	OH5-C14-C24-OH4
7	A	519	EDO	O1-C1-C2-O2
7	A	527	EDO	O1-C1-C2-O2
7	A	528	EDO	O1-C1-C2-O2
7	A	531	EDO	O1-C1-C2-O2
7	A	534	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	506	KHP	C2'-C1'-O1-C1
6	A	507	KHP	C5'-C4'-N1'-O2'
10	A	525	1PE	C25-C15-OH6-C26
6	A	506	KHP	C6'-C1'-O1-C1
8	A	515	PEG	C4-C3-O2-C2
8	A	530	PEG	C4-C3-O2-C2
9	A	521	PGE	C6-C5-O3-C4
10	A	533	1PE	C13-C23-OH3-C22
7	A	522	EDO	O1-C1-C2-O2
10	A	525	1PE	C23-C13-OH4-C24
8	A	515	PEG	C1-C2-O2-C3
10	A	525	1PE	C24-C14-OH5-C25
7	A	512	EDO	O1-C1-C2-O2
8	A	514	PEG	O2-C3-C4-O4
10	A	525	1PE	C15-C25-OH5-C14
7	A	508	EDO	O1-C1-C2-O2
7	A	523	EDO	O1-C1-C2-O2
7	A	526	EDO	O1-C1-C2-O2
10	A	533	1PE	C23-C13-OH4-C24
10	A	533	1PE	C24-C14-OH5-C25

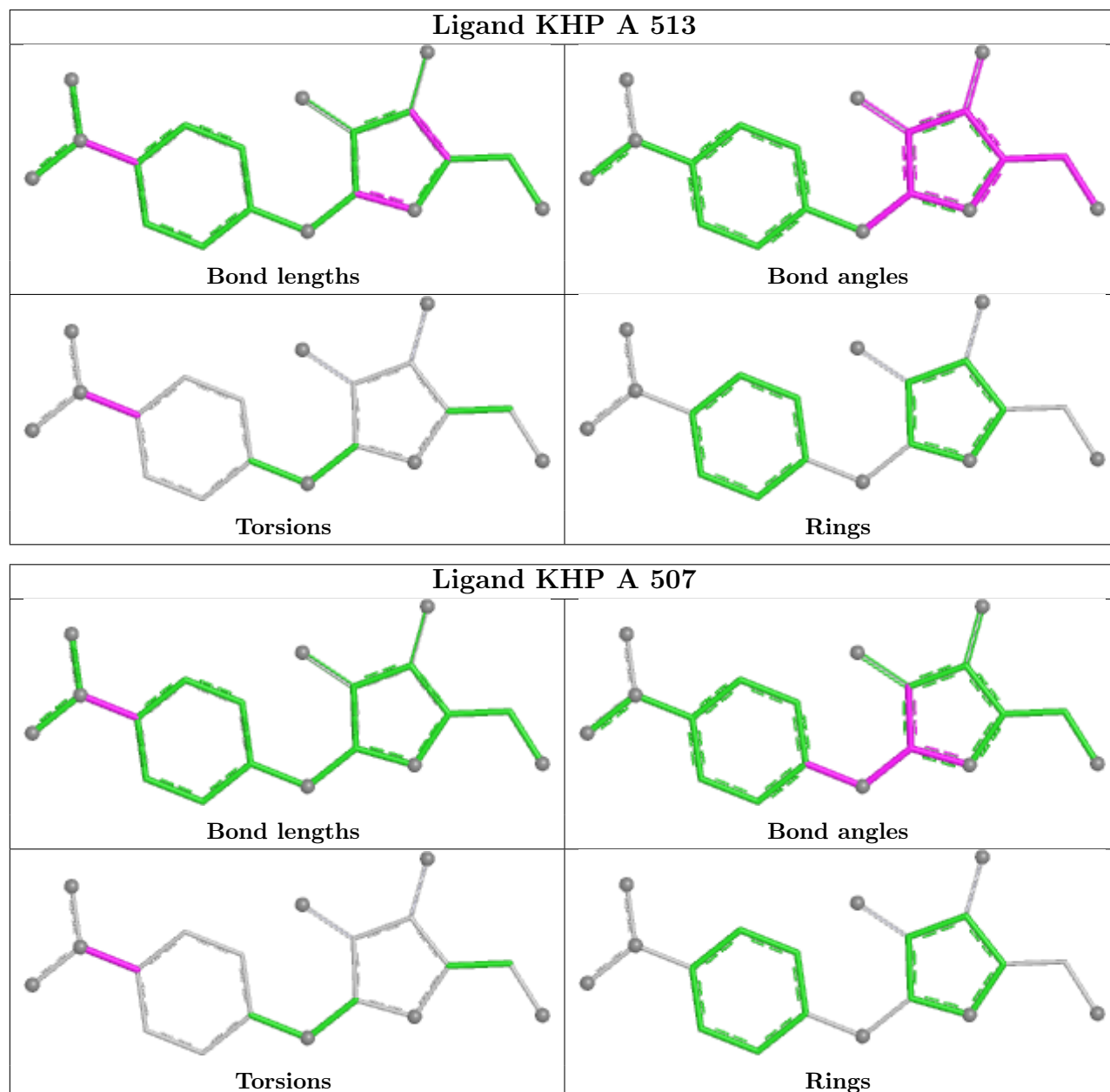
There are no ring outliers.

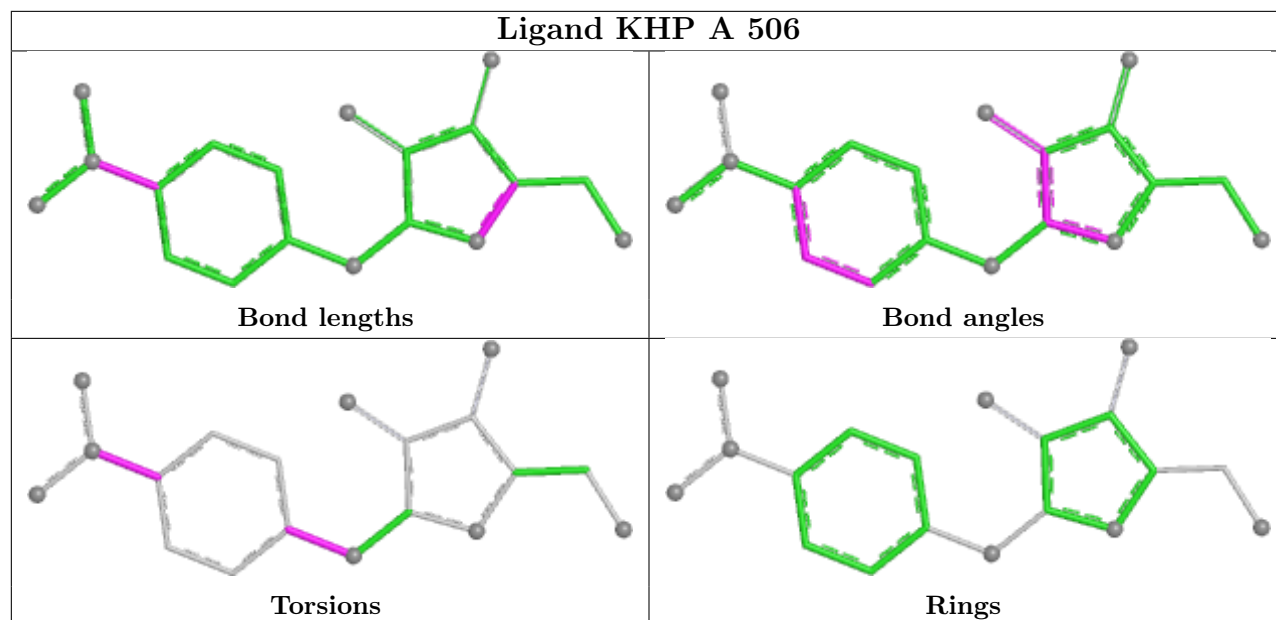
7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	532	EDO	1	0
6	A	513	KHP	1	0
10	A	533	1PE	2	0
8	A	530	PEG	5	0
5	A	505	ACT	4	0
7	A	529	EDO	2	0
8	A	515	PEG	2	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, 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	481/482 (99%)	-0.37	1 (0%) 91 92	17, 25, 35, 53	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	498	ALA	4.0

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

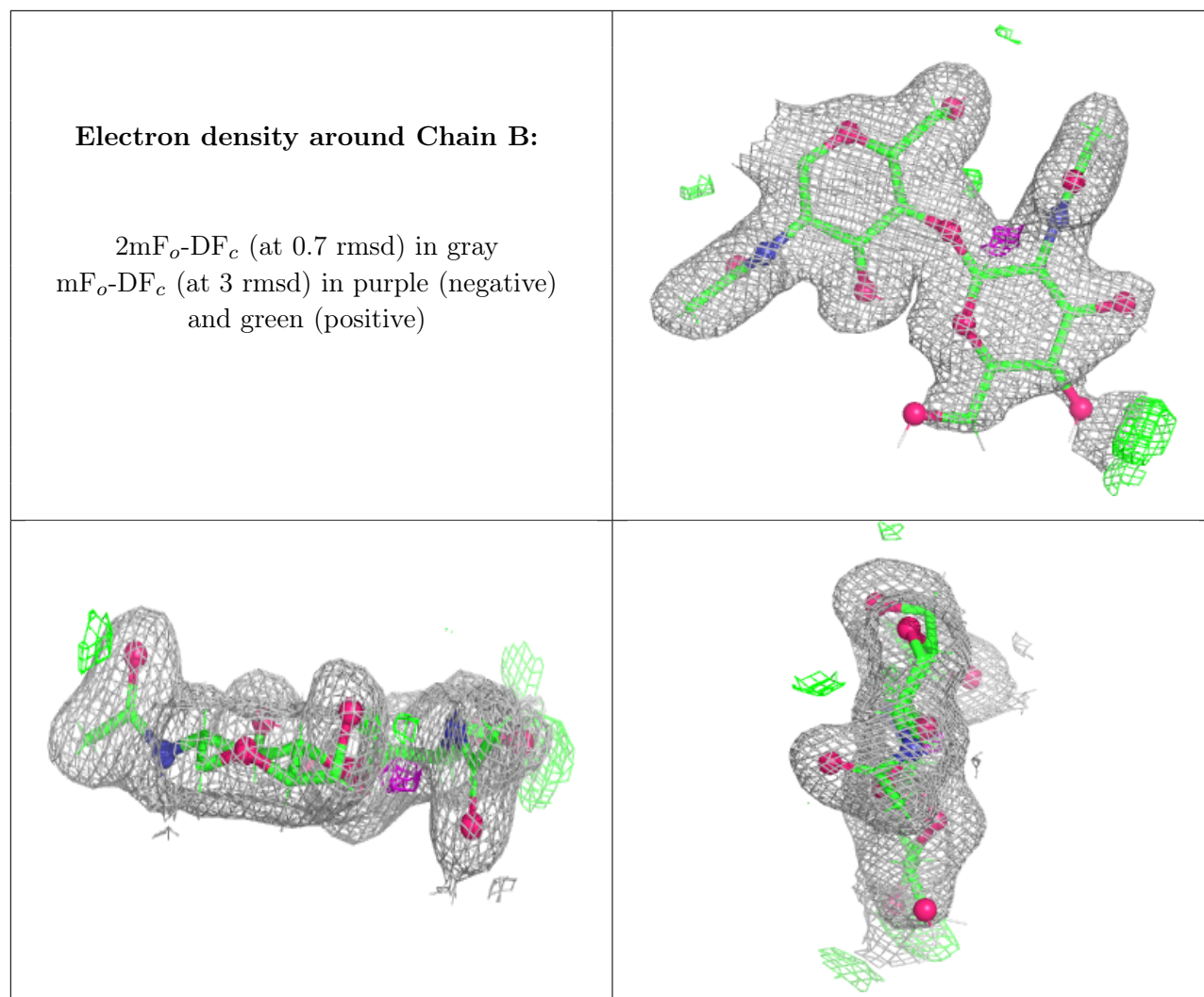
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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
2	NAG	B	2	14/15	0.87	0.14	36,50,73,75	3
2	NAG	B	1	14/15	0.96	0.06	26,31,39,42	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.



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, 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($\text{\AA}^2$)	Q<0.9
8	PEG	A	530	7/7	0.74	0.23	43,51,62,70	1
7	EDO	A	523	4/4	0.80	0.29	81,91,99,99	1
7	EDO	A	534	4/4	0.82	0.24	61,63,63,63	1
6	KHP	A	513	19/19	0.83	0.26	19,31,66,73	32
8	PEG	A	520[A]	5/7	0.83	0.20	52,61,65,65	1
8	PEG	A	520[B]	5/7	0.83	0.20	52,61,65,65	0
8	PEG	A	524	7/7	0.83	0.23	58,60,65,65	1
7	EDO	A	529	4/4	0.83	0.23	55,57,62,62	1
10	1PE	A	533	13/16	0.83	0.21	0,55,62,69	2

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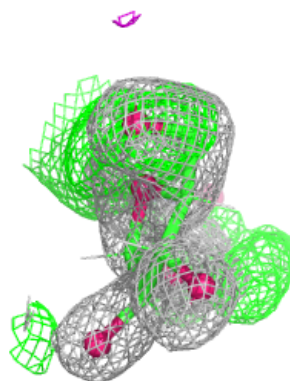
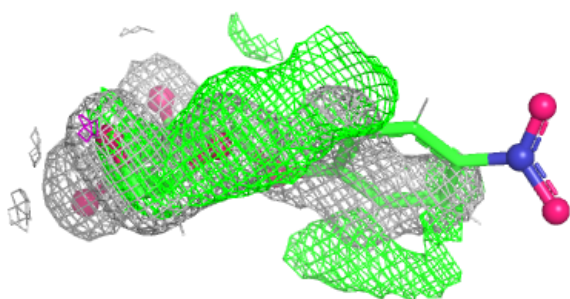
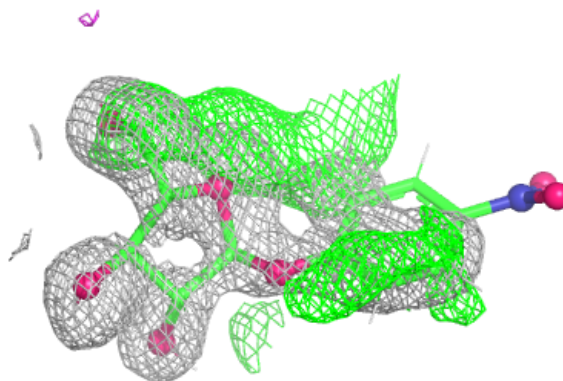
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	PEG	A	518	5/7	0.84	0.22	0,51,58,58	2
5	ACT	A	510	4/4	0.84	0.22	43,59,59,61	0
10	1PE	A	525	15/16	0.85	0.24	48,59,73,73	36
8	PEG	A	515	7/7	0.85	0.17	51,52,55,63	1
4	SO4	A	535	5/5	0.86	0.11	60,65,79,88	0
8	PEG	A	514	5/7	0.87	0.20	0,68,74,74	2
5	ACT	A	505	4/4	0.89	0.17	28,32,32,38	0
9	PGE	A	521	10/10	0.89	0.16	46,58,67,69	1
8	PEG	A	516	5/7	0.89	0.15	0,45,51,51	2
7	EDO	A	532	4/4	0.89	0.16	50,57,62,62	1
7	EDO	A	531	4/4	0.90	0.15	52,52,60,60	1
7	EDO	A	519	4/4	0.91	0.14	55,57,62,62	1
7	EDO	A	522	4/4	0.91	0.13	51,55,60,60	1
7	EDO	A	512	4/4	0.92	0.15	40,41,49,49	1
8	PEG	A	517	7/7	0.92	0.15	52,54,58,58	17
7	EDO	A	508	4/4	0.93	0.14	52,54,55,55	1
7	EDO	A	526	4/4	0.93	0.13	48,50,60,60	1
7	EDO	A	527	4/4	0.93	0.15	60,66,71,71	1
7	EDO	A	528	4/4	0.93	0.14	54,57,63,63	1
7	EDO	A	511	4/4	0.94	0.13	44,47,49,49	1
4	SO4	A	504	5/5	0.96	0.08	35,36,38,44	0
6	KHP	A	506	19/19	0.96	0.09	26,32,80,87	3
3	NAG	A	503	14/15	0.97	0.07	28,31,34,35	3
6	KHP	A	507	19/19	0.97	0.08	23,27,65,72	3
4	SO4	A	509	5/5	0.99	0.06	28,29,32,32	5

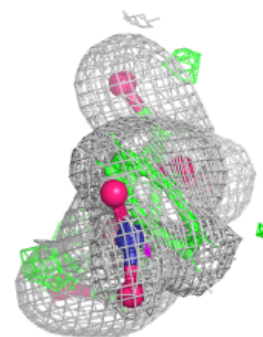
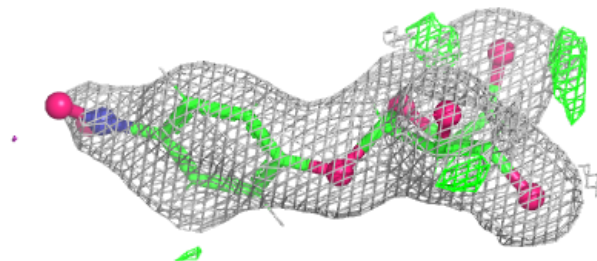
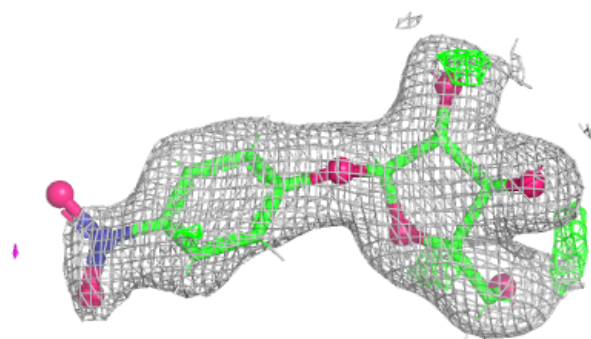
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KHP A 513:

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

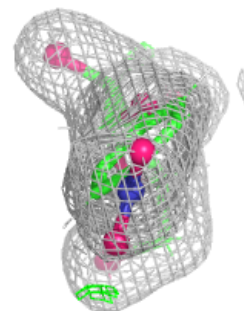
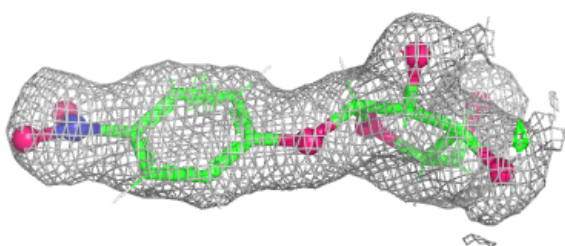
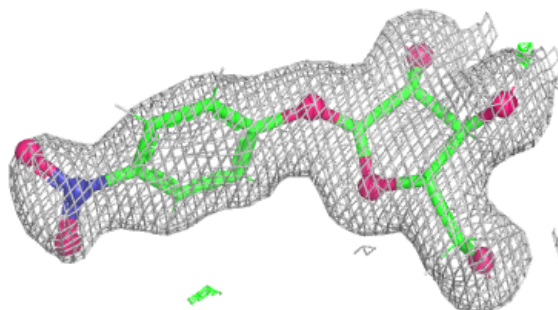
**Electron density around KHP A 506:**

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



Electron density around KHP 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 ⓘ

There are no such residues in this entry.