



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2024 – 08:41 am BST

PDB ID : 8AWR
Title : Structure of recombinant human beta-glucocerebrosidase in complex with L-carboxylosyl chloride
Authors : Rowland, R.J.; Davies, G.J.
Deposited on : 2022-08-30
Resolution : 1.49 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

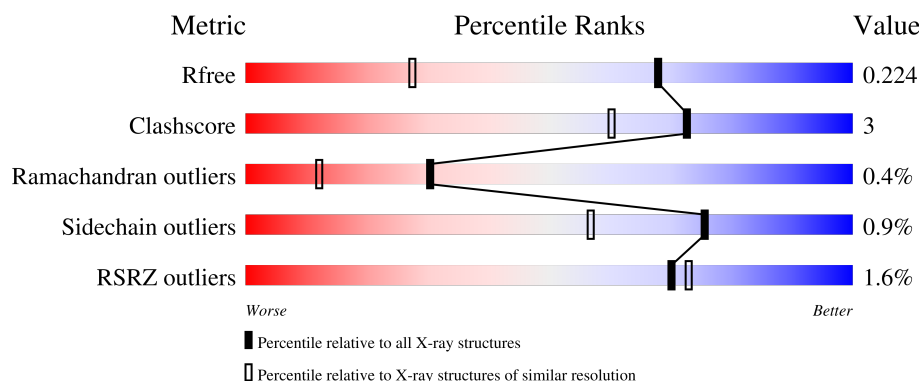
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.49 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}	164625	3717 (1.50-1.50)
Clashscore	180529	4048 (1.50-1.50)
Ramachandran outliers	177936	3970 (1.50-1.50)
Sidechain outliers	177891	3967 (1.50-1.50)
RSRZ outliers	164620	3718 (1.50-1.50)

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	AAA	497	<div> <div>2%</div> <div>93%</div> <div>7%</div> </div>
2	AcA	4	<div> <div>25%</div> <div>75%</div> </div>

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
4	EDO	AAA	527	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 4670 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 Lysosomal acid glucosylceramidase.

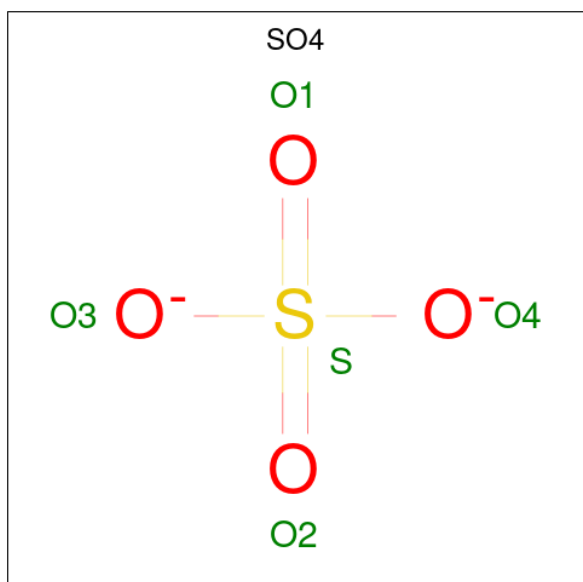
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	497	Total	C	N	O	S	0	9	0
			3995	2570	686	723	16			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



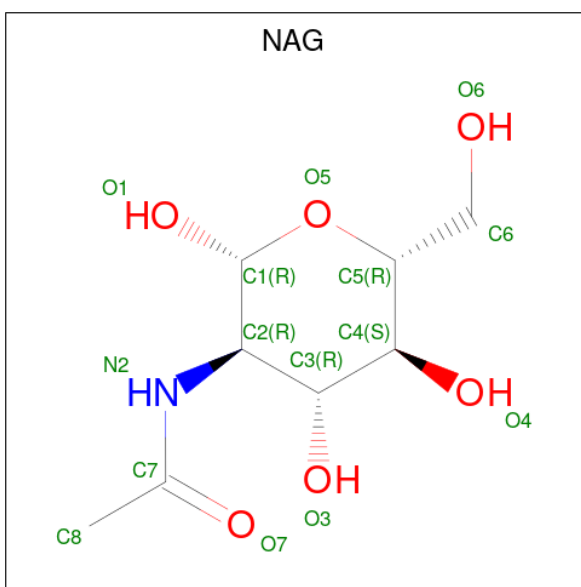
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0

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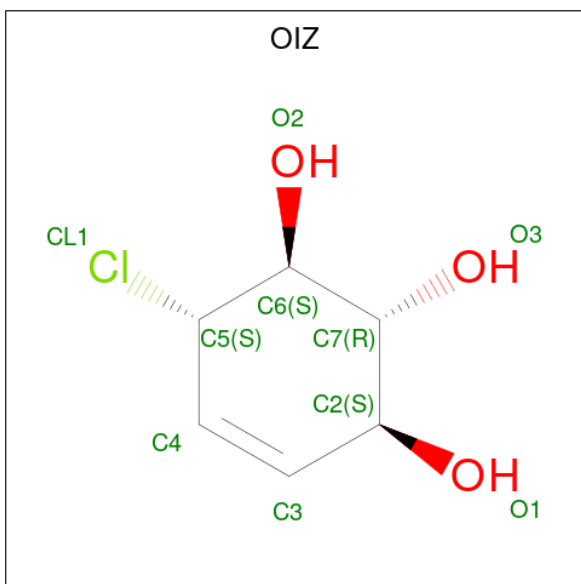
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



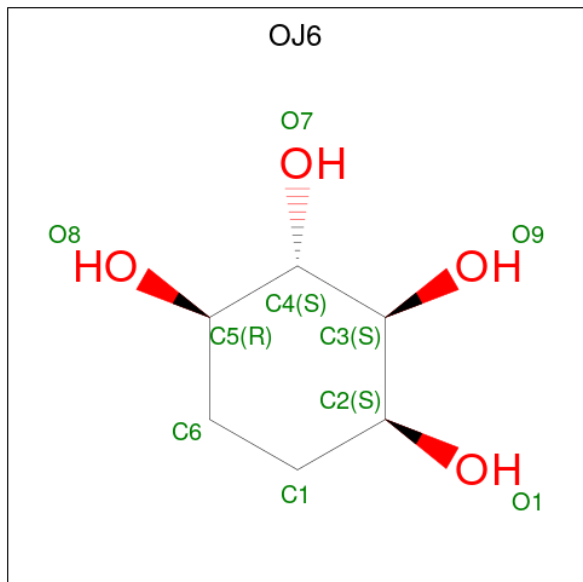
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
5	AAA	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is (1 {S},2 {R},3 {S},6 {S})-6-chloranycyclohex-4-ene-1,2,3-triol (three-letter code: OIZ) (formula: C₆H₉ClO₃) (labeled as "Ligand of Interest" by depositor).



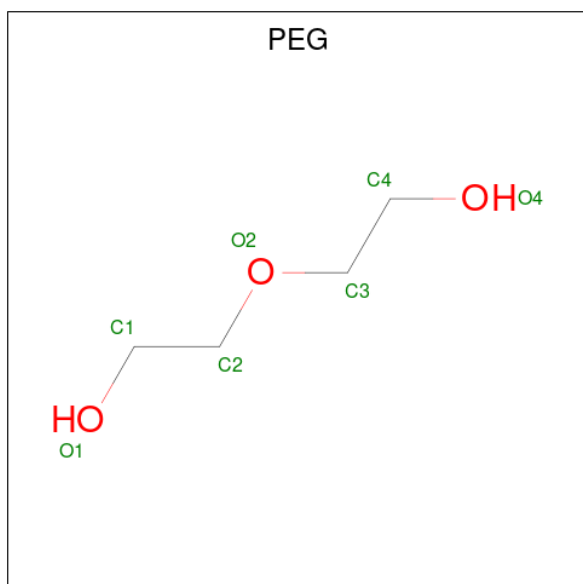
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	Cl	O	0	0
			10	6	1	3		

- Molecule 7 is (1 {S},2 {S},3 {S},4 {R})-cyclohexane-1,2,3,4-tetrol (three-letter code: OJ6) (formula: $C_6H_{12}O_4$) (labeled as "Ligand of Interest" by depositor).



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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	AAA	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	2	Total 2	Na 2	0	0

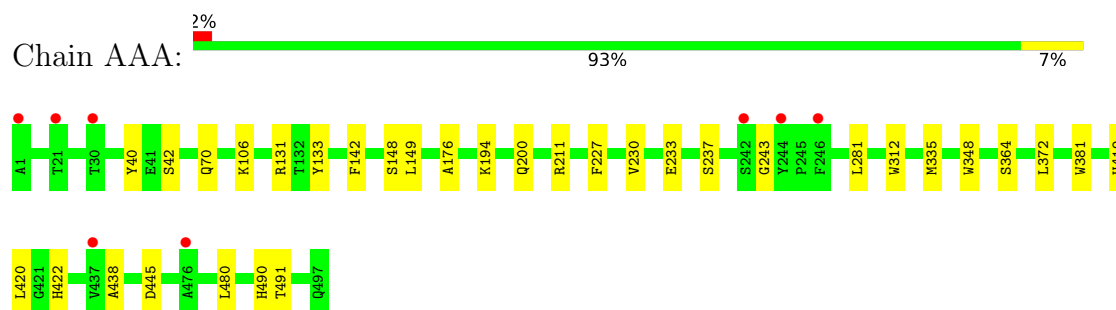
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	AAA	465	Total 467	O 467	0	2

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: Lysosomal acid glucosylceramidase



- Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-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	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.11Å 76.48Å 68.15Å 90.00° 101.96° 90.00°	Depositor
Resolution (Å)	51.96 – 1.49 51.96 – 1.49	Depositor EDS
% Data completeness (in resolution range)	98.6 (51.96-1.49) 98.6 (51.96-1.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.49Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.183 , 0.222 0.185 , 0.224	Depositor DCC
R_{free} test set	4275 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4670	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 5.68% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO, PEG, OIZ, NA, OJ6, BMA, MAN, NAG

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	0.30	0/4114	0.62	0/5607

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	3995	0	3899	24	0
2	AcA	50	0	43	0	0
3	AAA	10	0	0	0	0
4	AAA	92	0	138	16	0
5	AAA	28	0	26	0	0
6	AAA	10	0	0	0	0
7	AAA	9	0	0	0	0
8	AAA	7	0	10	0	0
9	AAA	2	0	0	0	0
10	AAA	467	0	0	4	0
All	All	4670	0	4116	26	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 (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:AAA:131:ARG:HH22	4:AAA:527:EDO:H11	1.46	0.80
1:AAA:243:GLY:H	4:AAA:513:EDO:H12	1.50	0.75
1:AAA:133:TYR:HB2	4:AAA:527:EDO:H12	1.76	0.67
1:AAA:148:SER:HB2	4:AAA:528:EDO:H22	1.75	0.66
1:AAA:42:SER:OG	1:AAA:422:HIS:HE1	1.80	0.62
1:AAA:131:ARG:HH22	4:AAA:527:EDO:C1	2.12	0.61
4:AAA:527:EDO:H21	10:AAA:611:HOH:O	2.00	0.61
1:AAA:364:SER:OG	1:AAA:419:HIS:HD2	1.86	0.59
1:AAA:149:LEU:HB2	4:AAA:528:EDO:H11	1.85	0.59
1:AAA:142:PHE:O	1:AAA:211:ARG:NH2	2.36	0.58
1:AAA:372:LEU:HD12	4:AAA:511:EDO:H11	1.90	0.54
4:AAA:527:EDO:C2	10:AAA:611:HOH:O	2.55	0.53
1:AAA:348:TRP:O	4:AAA:529:EDO:H11	2.10	0.52
1:AAA:237:SER:OG	4:AAA:505:EDO:H22	2.10	0.51
1:AAA:176:ALA:HB3	1:AAA:230:VAL:HG12	1.93	0.50
1:AAA:480:LEU:HD12	1:AAA:480:LEU:N	2.27	0.50
1:AAA:438:ALA:HB2	4:AAA:519:EDO:H22	1.98	0.46
1:AAA:176:ALA:HB2	1:AAA:227:PHE:CE2	2.53	0.43
1:AAA:445:ASP:OD1	4:AAA:511:EDO:H21	2.19	0.43
1:AAA:194:LYS:H	4:AAA:513:EDO:H11	1.84	0.42
1:AAA:70[B]:GLN:NE2	10:AAA:614:HOH:O	2.48	0.41
1:AAA:200:GLN:NE2	10:AAA:622:HOH:O	2.53	0.41
1:AAA:372:LEU:HD12	4:AAA:511:EDO:C1	2.50	0.41
1:AAA:422:HIS:HD2	1:AAA:491:THR:OG1	2.03	0.41
1:AAA:106:LYS:HE2	4:AAA:520:EDO:H11	2.02	0.41
1:AAA:40:TYR:O	1:AAA:490:HIS:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	503/497 (101%)	487 (97%)	14 (3%)	2 (0%)	30 12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	233	GLU
1	AAA	281	LEU

5.3.2 Protein sidechains ⓘ

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	431/424 (102%)	427 (99%)	4 (1%)	75 57

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

Mol	Chain	Res	Type
1	AAA	312	TRP
1	AAA	335	MET
1	AAA	381	TRP
1	AAA	420	LEU

Sometimes 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

4 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	AcA	1	1,2	14,14,15	0.49	0	17,19,21	0.90	0
2	NAG	AcA	2	2	14,14,15	0.43	0	17,19,21	1.28	3 (17%)
2	BMA	AcA	3	2	11,11,12	0.34	0	15,15,17	0.81	1 (6%)
2	MAN	AcA	4	2	11,11,12	0.44	0	15,15,17	1.10	2 (13%)

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AcA	2	NAG	C4-C3-C2	2.78	115.09	111.02
2	AcA	3	BMA	C1-O5-C5	2.59	115.70	112.19
2	AcA	2	NAG	C1-O5-C5	2.41	115.45	112.19
2	AcA	2	NAG	C3-C4-C5	2.32	114.39	110.24
2	AcA	4	MAN	C2-C3-C4	2.31	114.89	110.89
2	AcA	4	MAN	C1-C2-C3	2.25	112.43	109.67

There are no chirality outliers.

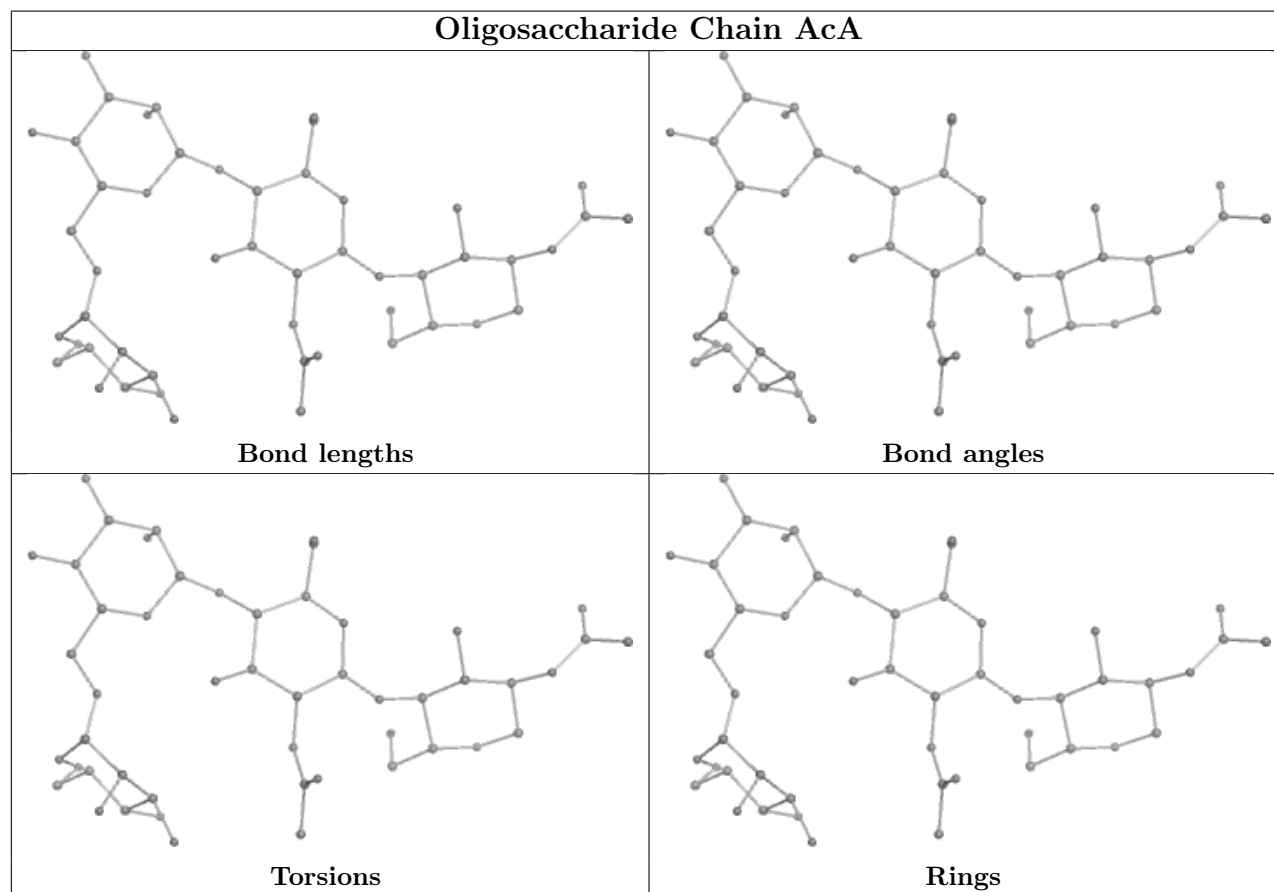
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AcA	4	MAN	O5-C5-C6-O6
2	AcA	4	MAN	C4-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 ⓘ

Of 32 ligands modelled in this entry, 2 are monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PEG	AAA	530	-	6,6,6	0.16	0	5,5,5	0.08	0
4	EDO	AAA	515	-	3,3,3	0.18	0	2,2,2	0.11	0
4	EDO	AAA	503	-	3,3,3	0.16	0	2,2,2	0.15	0
4	EDO	AAA	509	-	3,3,3	0.14	0	2,2,2	0.18	0
4	EDO	AAA	518	-	3,3,3	0.07	0	2,2,2	0.09	0
4	EDO	AAA	513	-	3,3,3	0.09	0	2,2,2	0.02	0
4	EDO	AAA	516	-	3,3,3	0.05	0	2,2,2	0.12	0
3	SO4	AAA	501	-	4,4,4	0.42	0	6,6,6	0.18	0
4	EDO	AAA	529	-	3,3,3	0.14	0	2,2,2	0.51	0
4	EDO	AAA	522	-	3,3,3	0.07	0	2,2,2	0.16	0
4	EDO	AAA	508	-	3,3,3	0.04	0	2,2,2	0.10	0
7	OJ6	AAA	524	1	9,9,10	2.41	1 (11%)	12,12,14	2.52	4 (33%)
4	EDO	AAA	526	-	3,3,3	0.08	0	2,2,2	0.32	0
5	NAG	AAA	510	1	14,14,15	0.47	0	17,19,21	1.49	3 (17%)
4	EDO	AAA	528	-	3,3,3	0.09	0	2,2,2	0.12	0
4	EDO	AAA	505	-	3,3,3	0.08	0	2,2,2	0.18	0
4	EDO	AAA	527	-	3,3,3	0.08	0	2,2,2	0.32	0
3	SO4	AAA	502	-	4,4,4	0.39	0	6,6,6	0.12	0
4	EDO	AAA	512	-	3,3,3	0.26	0	2,2,2	0.39	0
5	NAG	AAA	525	1	14,14,15	0.34	0	17,19,21	0.72	0
4	EDO	AAA	507	-	3,3,3	0.12	0	2,2,2	0.41	0
4	EDO	AAA	514	-	3,3,3	0.08	0	2,2,2	0.12	0
6	OIZ	AAA	523	-	9,10,10	0.39	0	7,14,14	0.69	0
4	EDO	AAA	506	-	3,3,3	0.05	0	2,2,2	0.11	0
4	EDO	AAA	517	-	3,3,3	0.15	0	2,2,2	0.08	0
4	EDO	AAA	520	-	3,3,3	0.04	0	2,2,2	0.36	0
4	EDO	AAA	519	-	3,3,3	0.07	0	2,2,2	0.30	0
4	EDO	AAA	511	-	3,3,3	0.18	0	2,2,2	0.13	0
4	EDO	AAA	521	-	3,3,3	0.05	0	2,2,2	0.14	0
4	EDO	AAA	504	-	3,3,3	0.11	0	2,2,2	0.28	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
8	PEG	AAA	530	-	-	2/4/4/4	-
4	EDO	AAA	515	-	-	0/1/1/1	-
4	EDO	AAA	503	-	-	0/1/1/1	-
4	EDO	AAA	509	-	-	0/1/1/1	-
4	EDO	AAA	518	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	AAA	513	-	-	0/1/1/1	-
4	EDO	AAA	516	-	-	0/1/1/1	-
4	EDO	AAA	529	-	-	0/1/1/1	-
4	EDO	AAA	522	-	-	1/1/1/1	-
4	EDO	AAA	508	-	-	0/1/1/1	-
7	OJ6	AAA	524	1	-	-	0/1/1/1
4	EDO	AAA	526	-	-	0/1/1/1	-
5	NAG	AAA	510	1	-	2/6/23/26	0/1/1/1
4	EDO	AAA	528	-	-	1/1/1/1	-
4	EDO	AAA	505	-	-	1/1/1/1	-
4	EDO	AAA	527	-	-	1/1/1/1	-
4	EDO	AAA	512	-	-	1/1/1/1	-
5	NAG	AAA	525	1	-	0/6/23/26	0/1/1/1
4	EDO	AAA	507	-	-	1/1/1/1	-
4	EDO	AAA	514	-	-	1/1/1/1	-
6	OIZ	AAA	523	-	-	-	0/1/1/1
4	EDO	AAA	506	-	-	1/1/1/1	-
4	EDO	AAA	517	-	-	1/1/1/1	-
4	EDO	AAA	520	-	-	1/1/1/1	-
4	EDO	AAA	519	-	-	1/1/1/1	-
4	EDO	AAA	511	-	-	1/1/1/1	-
4	EDO	AAA	521	-	-	1/1/1/1	-
4	EDO	AAA	504	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	AAA	524	OJ6	C1-C6	-7.03	1.34	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AAA	524	OJ6	C1-C6-C5	5.88	122.21	111.47
7	AAA	524	OJ6	C1-C2-C3	-3.94	104.27	111.47
7	AAA	524	OJ6	C2-C3-C4	-3.43	107.21	111.16
5	AAA	510	NAG	C2-N2-C7	3.13	127.36	122.90
7	AAA	524	OJ6	C6-C1-C2	3.01	121.65	112.87
5	AAA	510	NAG	C1-O5-C5	2.99	116.24	112.19
5	AAA	510	NAG	C1-C2-N2	2.27	114.37	110.49

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	AAA	530	PEG	O2-C3-C4-O4
4	AAA	511	EDO	O1-C1-C2-O2
4	AAA	528	EDO	O1-C1-C2-O2
8	AAA	530	PEG	O1-C1-C2-O2
4	AAA	506	EDO	O1-C1-C2-O2
4	AAA	512	EDO	O1-C1-C2-O2
4	AAA	517	EDO	O1-C1-C2-O2
4	AAA	519	EDO	O1-C1-C2-O2
4	AAA	520	EDO	O1-C1-C2-O2
4	AAA	527	EDO	O1-C1-C2-O2
4	AAA	507	EDO	O1-C1-C2-O2
4	AAA	521	EDO	O1-C1-C2-O2
4	AAA	522	EDO	O1-C1-C2-O2
4	AAA	514	EDO	O1-C1-C2-O2
5	AAA	510	NAG	C1-C2-N2-C7
5	AAA	510	NAG	C3-C2-N2-C7
4	AAA	505	EDO	O1-C1-C2-O2

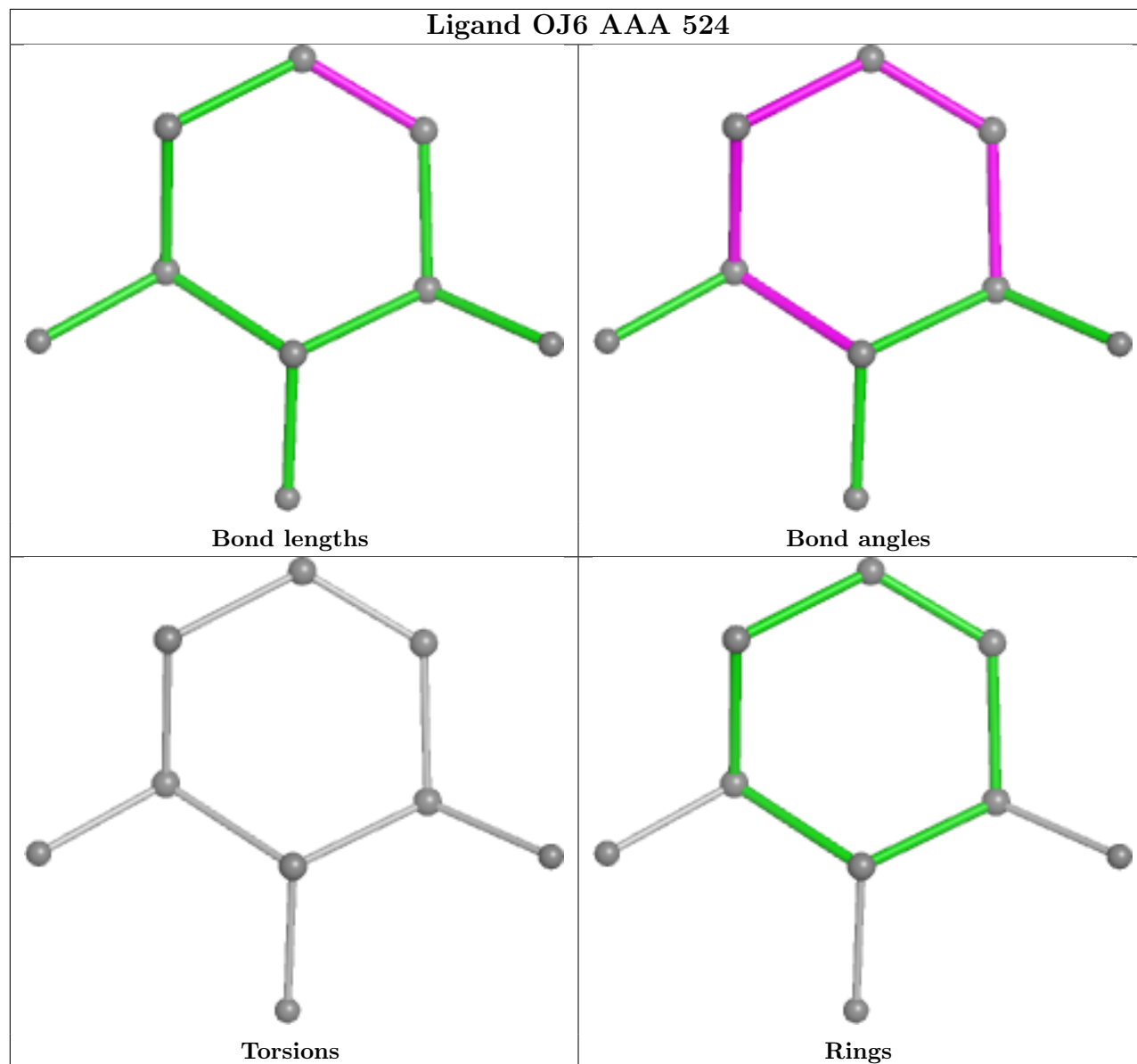
There are no ring outliers.

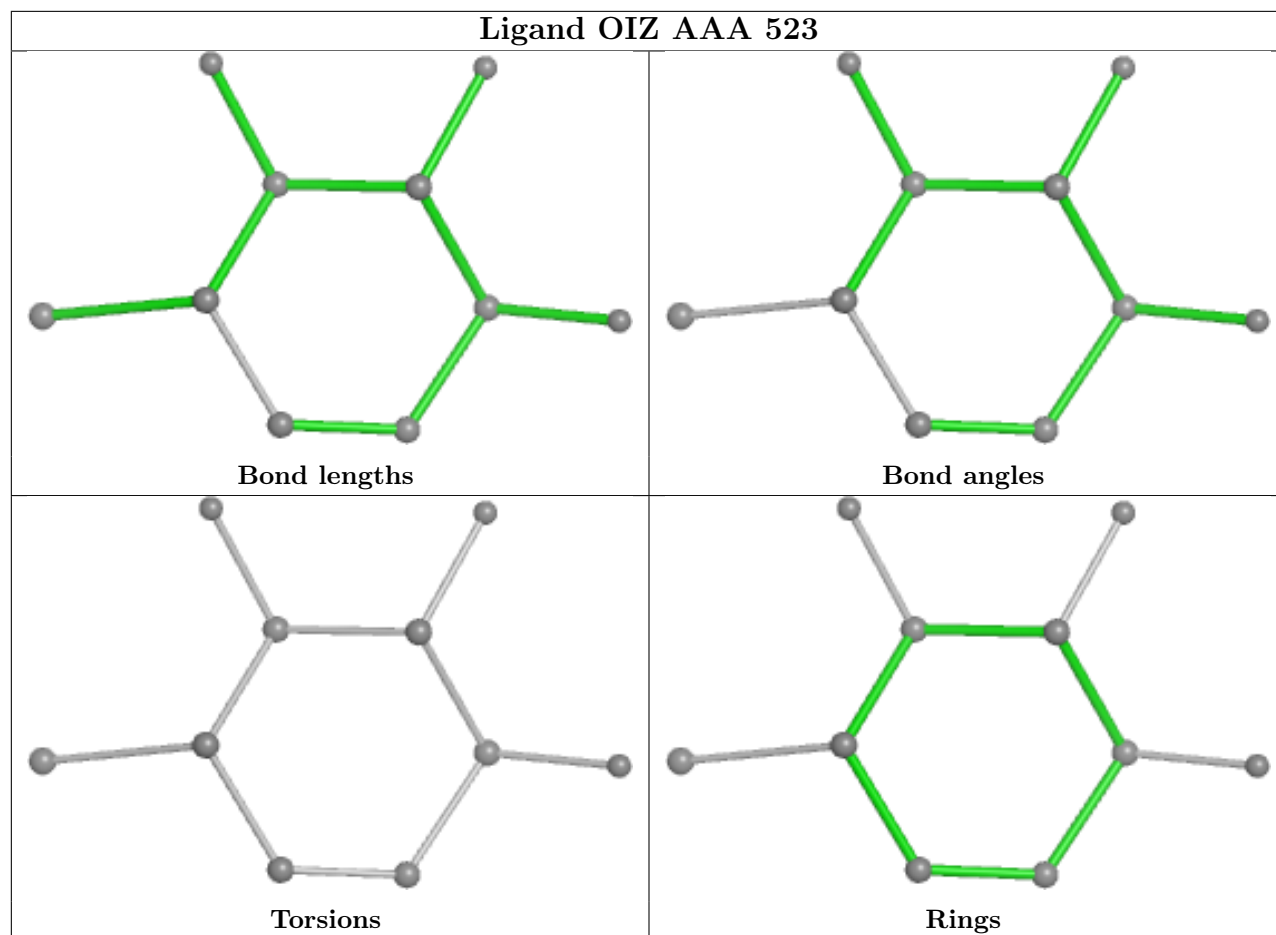
8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	513	EDO	2	0
4	AAA	529	EDO	1	0
4	AAA	528	EDO	2	0
4	AAA	505	EDO	1	0
4	AAA	527	EDO	5	0
4	AAA	520	EDO	1	0
4	AAA	519	EDO	1	0
4	AAA	511	EDO	3	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	AAA	497/497 (100%)	-0.02	8 (1%) 70 73	8, 19, 28, 37	9 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	437[A]	VAL	2.9
1	AAA	246	PHE	2.7
1	AAA	1	ALA	2.6
1	AAA	476	ALA	2.3
1	AAA	30	THR	2.1
1	AAA	21	THR	2.1
1	AAA	244	TYR	2.1
1	AAA	242	SER	2.0

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](#)

SUGAR-RSR INFOmissingINFO

6.4 Ligands [i](#)

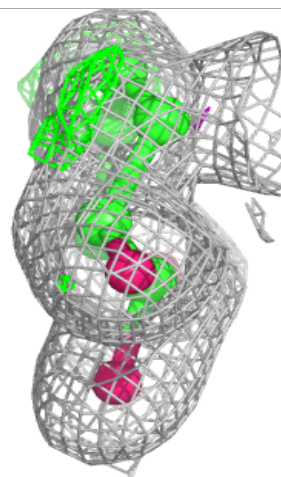
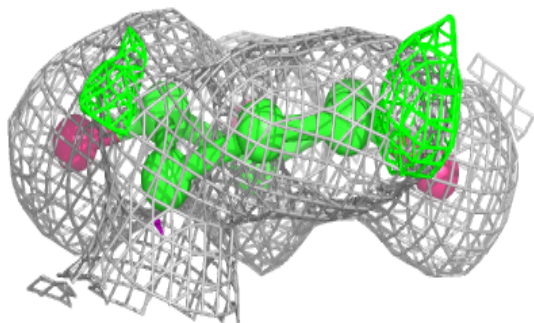
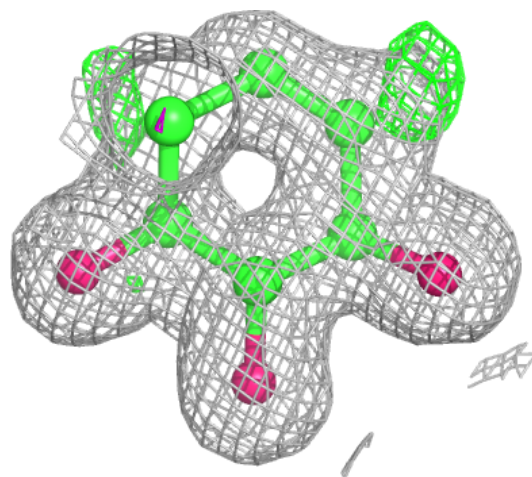
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	AAA	510	14/15	0.59	0.16	57,64,69,75	0
4	EDO	AAA	513	4/4	0.72	0.19	47,49,50,53	0
5	NAG	AAA	525	14/15	0.73	0.19	29,32,34,34	14
4	EDO	AAA	507	4/4	0.76	0.19	46,51,51,52	0
4	EDO	AAA	527	4/4	0.76	0.15	48,49,51,56	0
4	EDO	AAA	522	4/4	0.77	0.17	45,47,49,50	0
8	PEG	AAA	530	7/7	0.77	0.18	48,53,58,58	0
4	EDO	AAA	518	4/4	0.79	0.17	37,42,43,45	0
4	EDO	AAA	526	4/4	0.79	0.18	53,54,56,56	0
4	EDO	AAA	521	4/4	0.81	0.14	53,53,56,57	0
4	EDO	AAA	529	4/4	0.82	0.15	37,39,40,43	0
4	EDO	AAA	519	4/4	0.82	0.18	45,50,51,52	0
4	EDO	AAA	520	4/4	0.83	0.16	49,50,50,54	0
4	EDO	AAA	528	4/4	0.83	0.13	37,39,40,41	0
4	EDO	AAA	512	4/4	0.84	0.14	27,30,32,39	0
4	EDO	AAA	508	4/4	0.85	0.14	39,40,40,46	0
4	EDO	AAA	517	4/4	0.85	0.15	43,45,45,45	0
4	EDO	AAA	516	4/4	0.86	0.12	37,38,38,38	0
4	EDO	AAA	514	4/4	0.86	0.12	45,47,48,50	0
4	EDO	AAA	506	4/4	0.87	0.11	42,42,43,44	0
4	EDO	AAA	511	4/4	0.90	0.11	39,39,40,40	0
4	EDO	AAA	505	4/4	0.93	0.10	31,37,38,40	0
7	OJ6	AAA	524	9/10	0.94	0.07	14,15,15,16	9
6	OIZ	AAA	523	10/10	0.94	0.08	27,29,31,32	0
4	EDO	AAA	503	4/4	0.95	0.07	23,24,25,25	0
3	SO4	AAA	502	5/5	0.96	0.07	32,32,33,34	0
4	EDO	AAA	509	4/4	0.97	0.06	24,25,25,26	0
3	SO4	AAA	501	5/5	0.97	0.07	25,27,28,31	0
4	EDO	AAA	504	4/4	0.97	0.07	24,24,25,26	0
4	EDO	AAA	515	4/4	0.98	0.04	20,20,20,21	0
9	NA	AAA	532	1/1	0.98	0.07	25,25,25,25	0
9	NA	AAA	531	1/1	0.99	0.04	20,20,20,20	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.

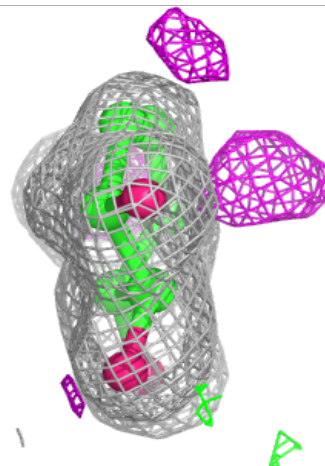
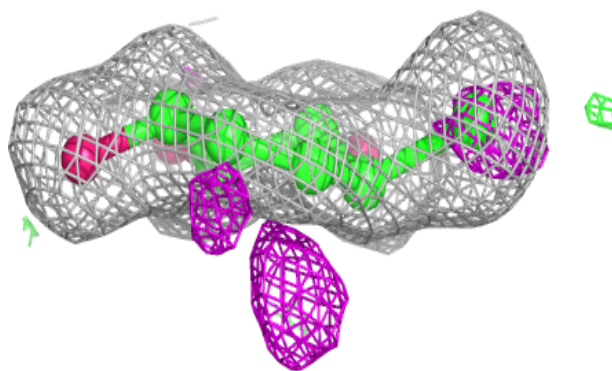
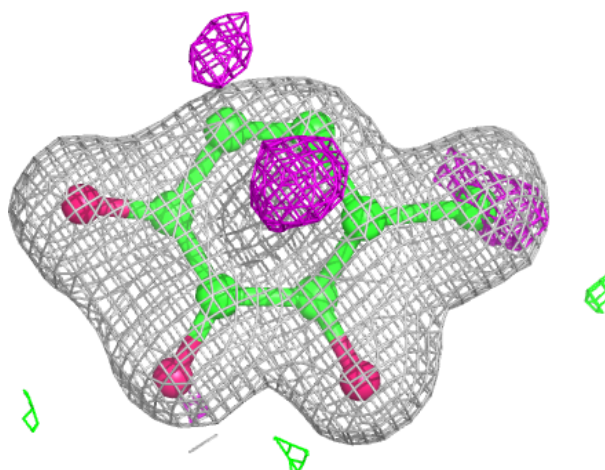
Electron density around OJ6 AAA 524:

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



Electron density around OIZ AAA 523:

$2mF_o-DF_c$ (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.