



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:11 PM UTC

PDB ID : 5J3J / pdb_00005j3j
Title : Crystal Structure of human DPP-IV in complex with HL1
Authors : Wu, F.; Li, H.; Zhao, Z.; Zhu, L.; Xu, H.; Li, S.
Deposited on : 2016-03-31
Resolution : 2.75 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

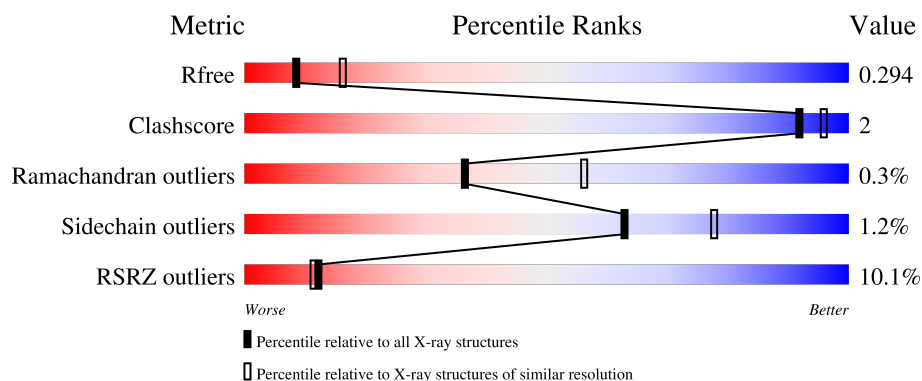
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	734	10% 95% . .
1	B	734	10% 92% 7% .
2	C	4	100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12141 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.

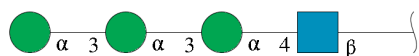
- Molecule 1 is a protein called Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			
1	B	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 14 discrepancies between the modelled and reference sequences:

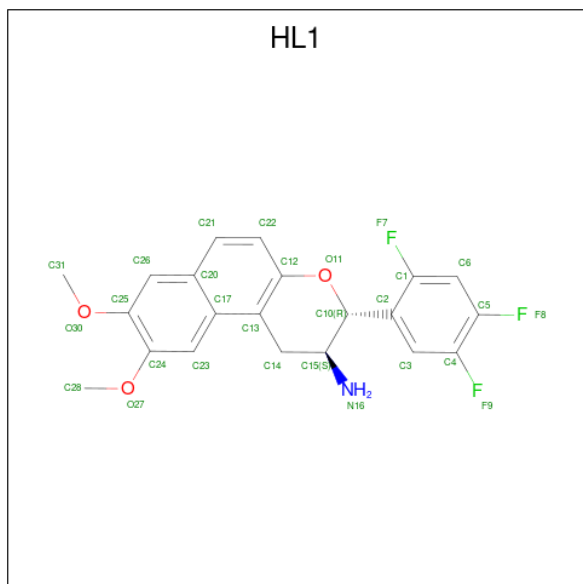
Chain	Residue	Modelled	Actual	Comment	Reference
A	767	GLY	-	expression tag	UNP P27487
A	768	HIS	-	expression tag	UNP P27487
A	769	HIS	-	expression tag	UNP P27487
A	770	HIS	-	expression tag	UNP P27487
A	771	HIS	-	expression tag	UNP P27487
A	772	HIS	-	expression tag	UNP P27487
A	773	HIS	-	expression tag	UNP P27487
B	767	GLY	-	expression tag	UNP P27487
B	768	HIS	-	expression tag	UNP P27487
B	769	HIS	-	expression tag	UNP P27487
B	770	HIS	-	expression tag	UNP P27487
B	771	HIS	-	expression tag	UNP P27487
B	772	HIS	-	expression tag	UNP P27487
B	773	HIS	-	expression tag	UNP P27487

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			47	26	1	20			

- Molecule 3 is (2 {S},3 {R})-8,9-dimethoxy-3-[2,4,5-tris(fluoranyl)phenyl]-2,3-dihydro-1 {H} -benzo[f]chromen-2-amine (CCD ID: HL1) (formula: C₂₁H₁₈F₃NO₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 21	F 3	N 1	O 3	0	0
3	B	1	Total 28	C 21	F 3	N 1	O 3	0	0

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



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

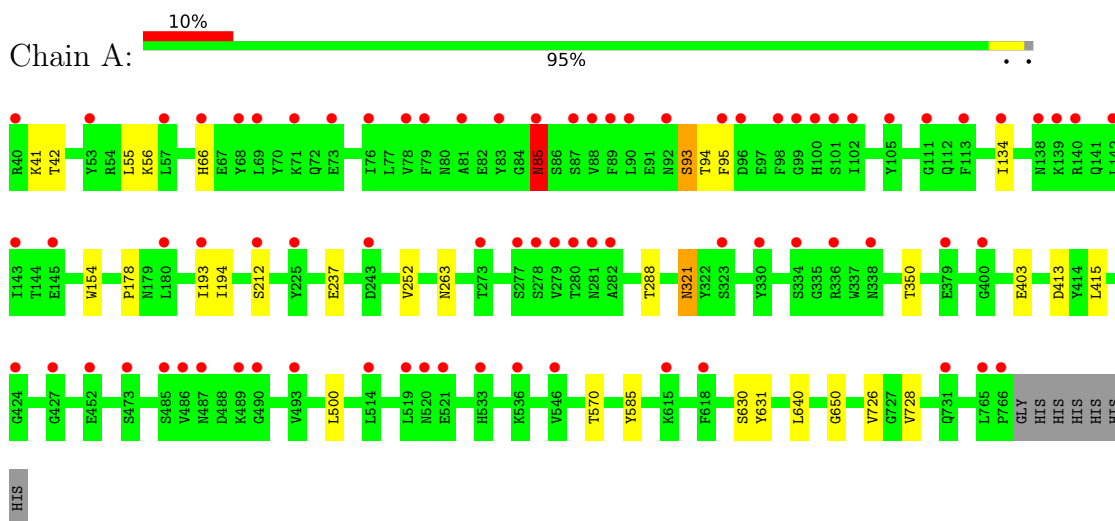
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	59	Total	O	0	0
			59	59		
5	B	37	Total	O	0	0
			37	37		

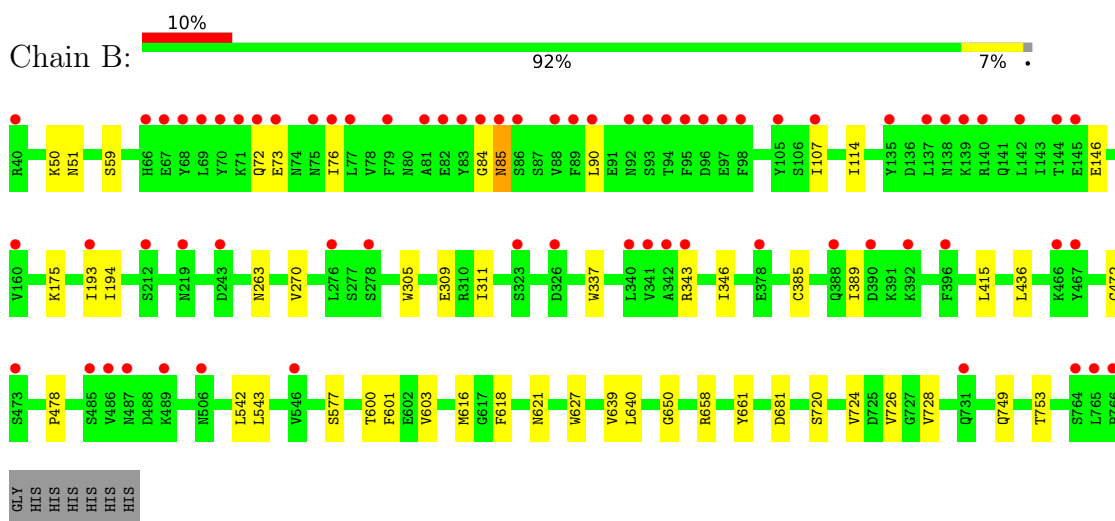
3 Residue-property plots [i](#)

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: Dipeptidyl peptidase 4



- Molecule 1: Dipeptidyl peptidase 4



- Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MA1
MA2
MA3
MA4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.36Å 126.82Å 112.62Å 90.00° 99.95° 90.00°	Depositor
Resolution (Å)	55.11 – 2.75 55.11 – 2.75	Depositor EDS
% Data completeness (in resolution range)	94.7 (55.11-2.75) 94.7 (55.11-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.235 , 0.298 0.236 , 0.294	Depositor DCC
R_{free} test set	2248 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12141	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: NAG, HL1, MAN

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	0.44	1/6129 (0.0%)	0.65	0/8336
1	B	0.41	0/6129	0.65	0/8336
All	All	0.42	1/12258 (0.0%)	0.65	0/16672

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	631	TYR	C-O	-6.06	1.17	1.24

There are no bond angle outliers.

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	5957	0	5679	15	0
1	B	5957	0	5678	22	0
2	C	47	0	40	0	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	59	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	37	0	0	0	0
All	All	12141	0	11423	37	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 2.

All (37) 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:B:658:ARG:HD3	1:B:661:TYR:CZ	2.31	0.65
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.83	0.60
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.84	0.59
1:B:76:ILE:HD12	1:B:90:LEU:HD23	1.86	0.57
1:B:472:CYS:O	1:B:478:PRO:HA	2.07	0.54
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.92	0.51
1:B:415:LEU:HB2	1:B:436:LEU:HD21	1.93	0.49
1:B:346:ILE:HD12	1:B:346:ILE:N	2.28	0.49
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.94	0.48
1:B:749:GLN:O	1:B:753:THR:OG1	2.26	0.46
1:B:305:TRP:CE2	1:B:311:ILE:HD12	2.51	0.46
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.45	0.46
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.97	0.45
1:B:270:VAL:HG11	1:B:337:TRP:CZ2	2.51	0.45
1:A:85:ASN:ND2	1:A:85:ASN:C	2.74	0.45
1:A:42:THR:HG21	1:A:570:THR:HG23	1.99	0.44
1:B:107:ILE:HD11	1:B:114:ILE:HD12	1.99	0.44
1:B:603:VAL:HG13	1:B:639:VAL:HG23	1.98	0.44
1:B:616:MET:HB3	1:B:618:PHE:CE2	2.53	0.44
1:A:85:ASN:C	1:A:85:ASN:HD22	2.25	0.44
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.99	0.44
1:B:343:ARG:NE	1:B:389:ILE:HD12	2.33	0.43
1:B:50:LYS:O	1:B:51:ASN:C	2.61	0.43
1:B:146:GLU:O	1:B:175:LYS:NZ	2.49	0.43
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.54	0.42
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.19	0.42
1:B:84:GLY:O	1:B:85:ASN:C	2.62	0.42
1:A:415:LEU:HD23	1:A:415:LEU:C	2.44	0.42
1:A:134:ILE:HG21	1:A:178:PRO:HB3	2.02	0.41
1:B:542:LEU:HD23	1:B:543:LEU:N	2.35	0.41
1:B:72:GLN:HG2	1:B:73:GLU:HG2	2.03	0.41
1:A:321:ASN:C	1:A:321:ASN:HD22	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:SER:O	1:A:95:PHE:N	2.50	0.41
1:A:237:GLU:HA	1:A:252:VAL:O	2.20	0.41
1:B:600:THR:OG1	1:B:601:PHE:N	2.54	0.41
1:A:413:ASP:OD1	1:A:413:ASP:N	2.55	0.40
1:B:720:SER:O	1:B:724:VAL:HG23	2.21	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	A	725/734 (99%)	677 (93%)	44 (6%)	4 (1%)	21	38
1	B	725/734 (99%)	682 (94%)	42 (6%)	1 (0%)	48	71
All	All	1450/1468 (99%)	1359 (94%)	86 (6%)	5 (0%)	36	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	ASN
1	A	85	ASN
1	A	93	SER
1	A	630	SER
1	A	94	THR

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	652/658 (99%)	644 (99%)	8 (1%)	63	78
1	B	652/658 (99%)	644 (99%)	8 (1%)	63	78
All	All	1304/1316 (99%)	1288 (99%)	16 (1%)	63	78

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	56	LYS
1	A	66	HIS
1	A	85	ASN
1	A	263	ASN
1	A	288	THR
1	A	321	ASN
1	A	350	THR
1	B	59	SER
1	B	263	ASN
1	B	309	GLU
1	B	385	CYS
1	B	577	SER
1	B	621	ASN
1	B	627	TRP
1	B	681	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	281	ASN
1	A	314	GLN
1	A	321	ASN
1	A	344	GLN
1	A	748	HIS
1	B	138	ASN
1	B	141	GLN
1	B	227	GLN
1	B	263	ASN
1	B	363	HIS
1	B	435	GLN

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Mol	Chain	Res	Type
1	B	606	GLN
1	B	731	GLN

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	C	1	2,1	14,14,15	0.55	0	17,19,21	1.36	3 (17%)
2	MAN	C	2	2	11,11,12	0.94	0	15,15,17	1.50	2 (13%)
2	MAN	C	3	2	11,11,12	0.52	0	15,15,17	1.03	1 (6%)
2	MAN	C	4	2	11,11,12	0.59	0	15,15,17	1.11	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	C	1	2,1	-	3/6/23/26	0/1/1/1
2	MAN	C	2	2	-	2/2/19/22	0/1/1/1
2	MAN	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	MAN	C1-C2-C3	4.80	116.63	109.64
2	C	3	MAN	C1-O5-C5	2.62	115.69	112.19
2	C	1	NAG	C8-C7-N2	2.62	120.46	116.12
2	C	4	MAN	C1-O5-C5	2.49	115.52	112.19
2	C	2	MAN	O5-C5-C4	-2.45	104.88	110.83
2	C	1	NAG	C1-O5-C5	2.36	115.35	112.19
2	C	1	NAG	O5-C1-C2	-2.30	107.73	111.29
2	C	4	MAN	C3-C4-C5	2.28	114.38	110.23

There are no chirality outliers.

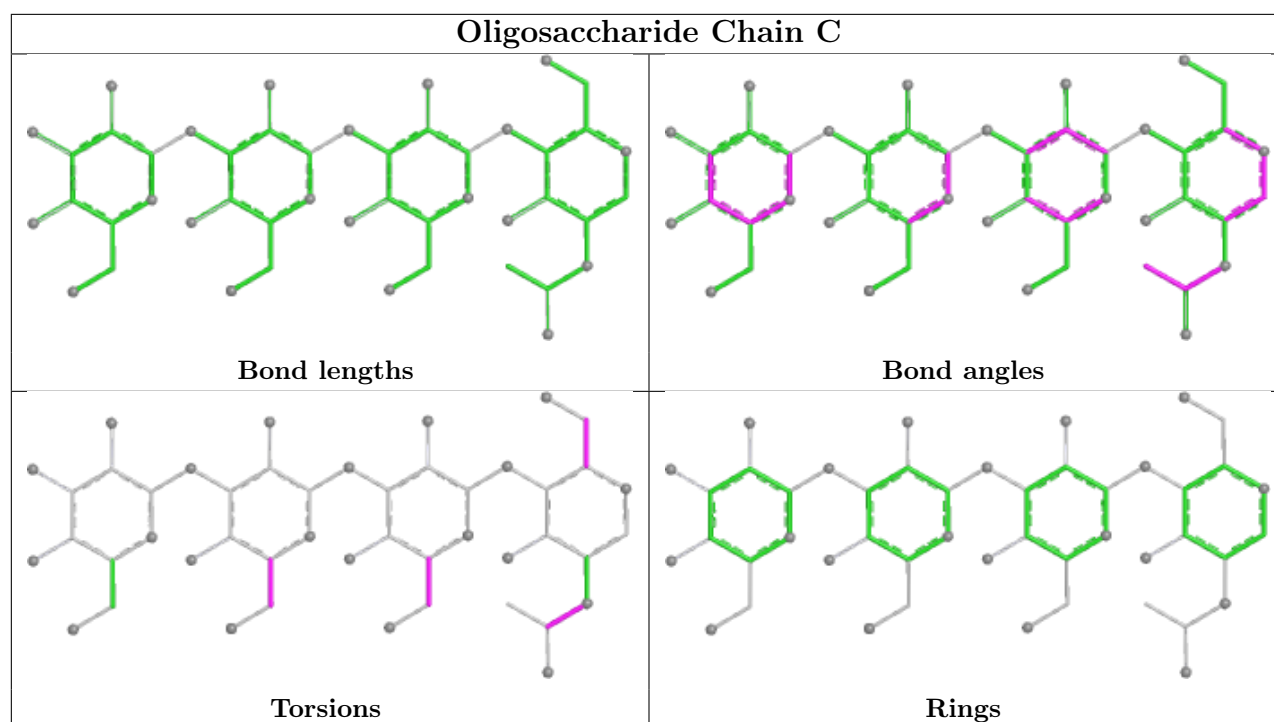
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	MAN	C4-C5-C6-O6
2	C	2	MAN	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	3	MAN	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	3	MAN	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](#)

4 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	$\# Z > 2$
4	NAG	B	802	1	14,14,15	0.49	0	17,19,21	1.30	1 (5%)
3	HL1	B	801	-	31,31,31	1.83	6 (19%)	42,46,46	1.65	8 (19%)
4	NAG	A	802	1	14,14,15	0.46	0	17,19,21	1.44	1 (5%)
3	HL1	A	801	-	31,31,31	1.80	4 (12%)	42,46,46	1.71	7 (16%)

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
4	NAG	B	802	1	-	2/6/23/26	0/1/1/1
3	HL1	B	801	-	-	0/8/20/20	0/4/4/4
4	NAG	A	802	1	-	1/6/23/26	0/1/1/1
3	HL1	A	801	-	-	2/8/20/20	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	HL1	C12-C13	6.40	1.49	1.38
3	B	801	HL1	C12-C13	6.12	1.48	1.38
3	B	801	HL1	C25-C24	4.12	1.49	1.40
3	A	801	HL1	C25-C24	3.81	1.48	1.40
3	B	801	HL1	C17-C20	3.47	1.49	1.43
3	A	801	HL1	C17-C20	3.37	1.49	1.43
3	A	801	HL1	C13-C17	3.03	1.49	1.43
3	B	801	HL1	C13-C17	2.93	1.48	1.43
3	B	801	HL1	C26-C25	2.19	1.40	1.36
3	B	801	HL1	C23-C24	2.04	1.40	1.36

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	HL1	C3-C2-C1	4.71	120.36	116.42
3	A	801	HL1	C31-O30-C25	4.70	124.41	117.51
3	B	801	HL1	C31-O30-C25	4.57	124.22	117.51
4	B	802	NAG	C1-O5-C5	4.48	118.19	112.19
3	B	801	HL1	C6-C1-C2	-4.18	119.29	123.93
3	B	801	HL1	C3-C2-C1	4.10	119.85	116.42
4	A	802	NAG	C1-O5-C5	4.10	117.68	112.19
3	A	801	HL1	C6-C1-C2	-3.98	119.51	123.93
3	A	801	HL1	C28-O27-C24	3.33	122.40	117.51
3	B	801	HL1	C28-O27-C24	3.05	121.98	117.51
3	A	801	HL1	O30-C25-C26	-2.64	121.81	125.16
3	A	801	HL1	O27-C24-C23	-2.47	122.03	125.16
3	B	801	HL1	O11-C12-C22	2.46	120.69	116.20
3	B	801	HL1	O27-C24-C23	-2.21	122.36	125.16
3	B	801	HL1	O11-C12-C13	-2.19	118.64	122.28
3	B	801	HL1	C5-C6-C1	2.07	120.71	117.22
3	A	801	HL1	O30-C25-C24	2.01	118.13	115.40

There are no chirality outliers.

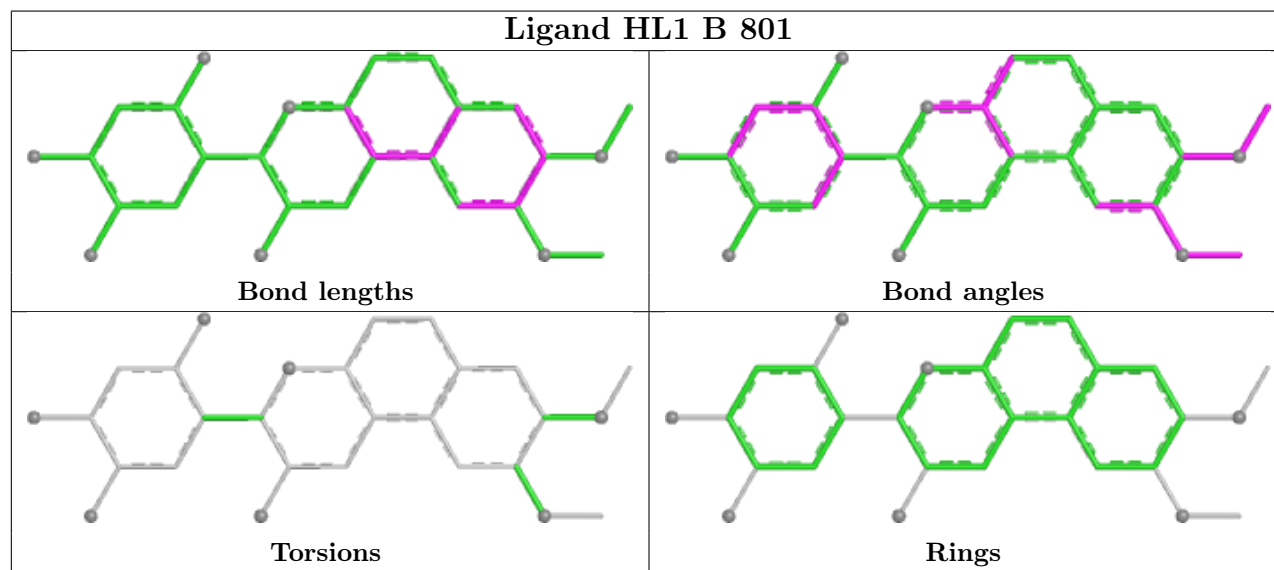
All (5) torsion outliers are listed below:

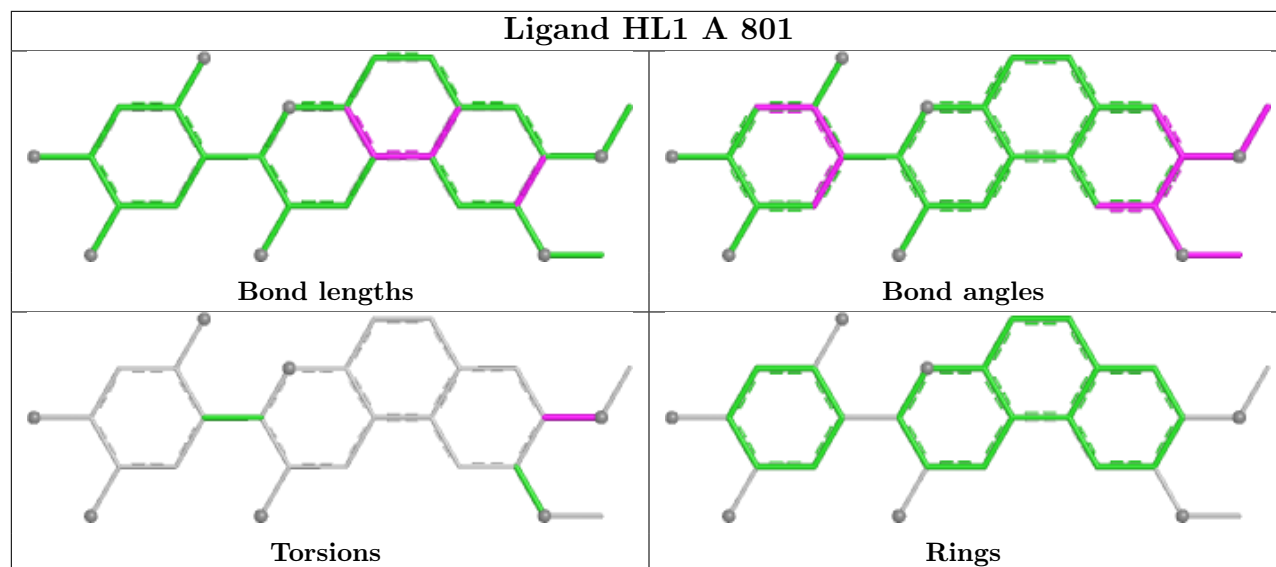
Mol	Chain	Res	Type	Atoms
4	B	802	NAG	O5-C5-C6-O6
3	A	801	HL1	C24-C25-O30-C31
4	B	802	NAG	C4-C5-C6-O6
3	A	801	HL1	C26-C25-O30-C31
4	A	802	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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

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, 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	727/734 (99%)	0.89	77 (10%)	11 10	8, 32, 59, 73	8 (1%)
1	B	727/734 (99%)	0.83	70 (9%)	13 13	8, 30, 64, 82	8 (1%)
All	All	1454/1468 (99%)	0.86	147 (10%)	12 11	8, 31, 61, 82	16 (1%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	731	GLN	8.2
1	B	473	SER	7.9
1	B	546	VAL	7.8
1	B	243	ASP	7.6
1	B	193	ILE	7.6
1	A	546	VAL	7.2
1	A	193	ILE	7.2
1	A	473	SER	7.1
1	B	731	GLN	6.5
1	A	243	ASP	6.4
1	B	485	SER	6.3
1	A	485	SER	6.2
1	B	766	PRO	5.8
1	A	212	SER	5.5
1	A	279	VAL	5.3
1	B	212	SER	4.8
1	B	84	GLY	4.6
1	A	766	PRO	4.5
1	B	71	LYS	4.3
1	B	88	VAL	4.2
1	B	95	PHE	4.1
1	B	765	LEU	4.1
1	B	85	ASN	4.1
1	A	323	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	323	SER	3.9
1	B	392	LYS	3.9
1	A	278	SER	3.9
1	B	83	TYR	3.6
1	B	93	SER	3.4
1	A	615	LYS	3.4
1	A	87	SER	3.3
1	B	98	PHE	3.3
1	A	379	GLU	3.3
1	B	76	ILE	3.3
1	B	90	LEU	3.2
1	A	96	ASP	3.2
1	A	83	TYR	3.2
1	A	490	GLY	3.2
1	B	139	LYS	3.2
1	B	489	LYS	3.2
1	B	97	GLU	3.1
1	A	102	ILE	3.1
1	A	85	ASN	3.1
1	A	282	ALA	3.1
1	A	138	ASN	3.0
1	A	338	ASN	3.0
1	B	487	ASN	3.0
1	A	98	PHE	3.0
1	A	487	ASN	3.0
1	B	72	GLN	2.9
1	B	86	SER	2.9
1	A	486	VAL	2.9
1	B	70	TYR	2.8
1	B	105	TYR	2.8
1	B	79	PHE	2.8
1	B	278	SER	2.8
1	A	143	ILE	2.8
1	A	280	THR	2.8
1	B	341	VAL	2.8
1	B	40	ARG	2.7
1	B	77	LEU	2.7
1	B	137	LEU	2.7
1	A	424	GLY	2.7
1	A	140	ARG	2.7
1	B	96	ASP	2.7
1	B	388	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	92	ASN	2.7
1	A	90	LEU	2.7
1	B	340	LEU	2.6
1	A	78	VAL	2.6
1	B	94	THR	2.6
1	A	180	LEU	2.6
1	A	92	ASN	2.6
1	A	334	SER	2.6
1	B	378	GLU	2.6
1	A	73	GLU	2.6
1	A	79	PHE	2.5
1	A	95	PHE	2.5
1	A	618	PHE	2.5
1	B	506	ASN	2.5
1	A	765	LEU	2.5
1	A	66	HIS	2.5
1	B	66	HIS	2.5
1	B	68	TYR	2.5
1	B	160	VAL	2.5
1	A	514	LEU	2.5
1	B	276	LEU	2.5
1	A	277	SER	2.5
1	B	396	PHE	2.5
1	A	489	LYS	2.4
1	B	75	ASN	2.4
1	A	100	HIS	2.4
1	A	536	LYS	2.4
1	A	68	TYR	2.4
1	A	452	GLU	2.4
1	B	73	GLU	2.4
1	B	486	VAL	2.4
1	B	135	TYR	2.4
1	B	69	LEU	2.4
1	A	521	GLU	2.4
1	B	145	GLU	2.4
1	A	71	LYS	2.4
1	B	140	ARG	2.4
1	A	330	TYR	2.3
1	B	81	ALA	2.3
1	B	142	LEU	2.3
1	A	533	HIS	2.3
1	B	390	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	69	LEU	2.3
1	A	89	PHE	2.3
1	B	342	ALA	2.3
1	A	105	TYR	2.3
1	A	145	GLU	2.3
1	B	326	ASP	2.3
1	A	99	GLY	2.3
1	B	89	PHE	2.3
1	A	53	TYR	2.2
1	A	76	ILE	2.2
1	B	67	GLU	2.2
1	A	520	ASN	2.2
1	A	400	GLY	2.2
1	A	427	GLY	2.2
1	B	219	ASN	2.2
1	B	467	TYR	2.2
1	A	57	LEU	2.2
1	A	142	LEU	2.2
1	B	764	SER	2.2
1	A	281	ASN	2.2
1	B	138	ASN	2.2
1	A	134	ILE	2.2
1	B	466	LYS	2.1
1	A	273	THR	2.1
1	A	111	GLY	2.1
1	B	107	ILE	2.1
1	A	40	ARG	2.1
1	B	144	THR	2.1
1	A	139	LYS	2.1
1	A	88	VAL	2.1
1	B	82	GLU	2.1
1	A	493	VAL	2.1
1	A	113	PHE	2.1
1	A	81	ALA	2.0
1	A	101	SER	2.0
1	A	519	LEU	2.0
1	A	336	ARG	2.0
1	B	343	ARG	2.0
1	A	225	TYR	2.0

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

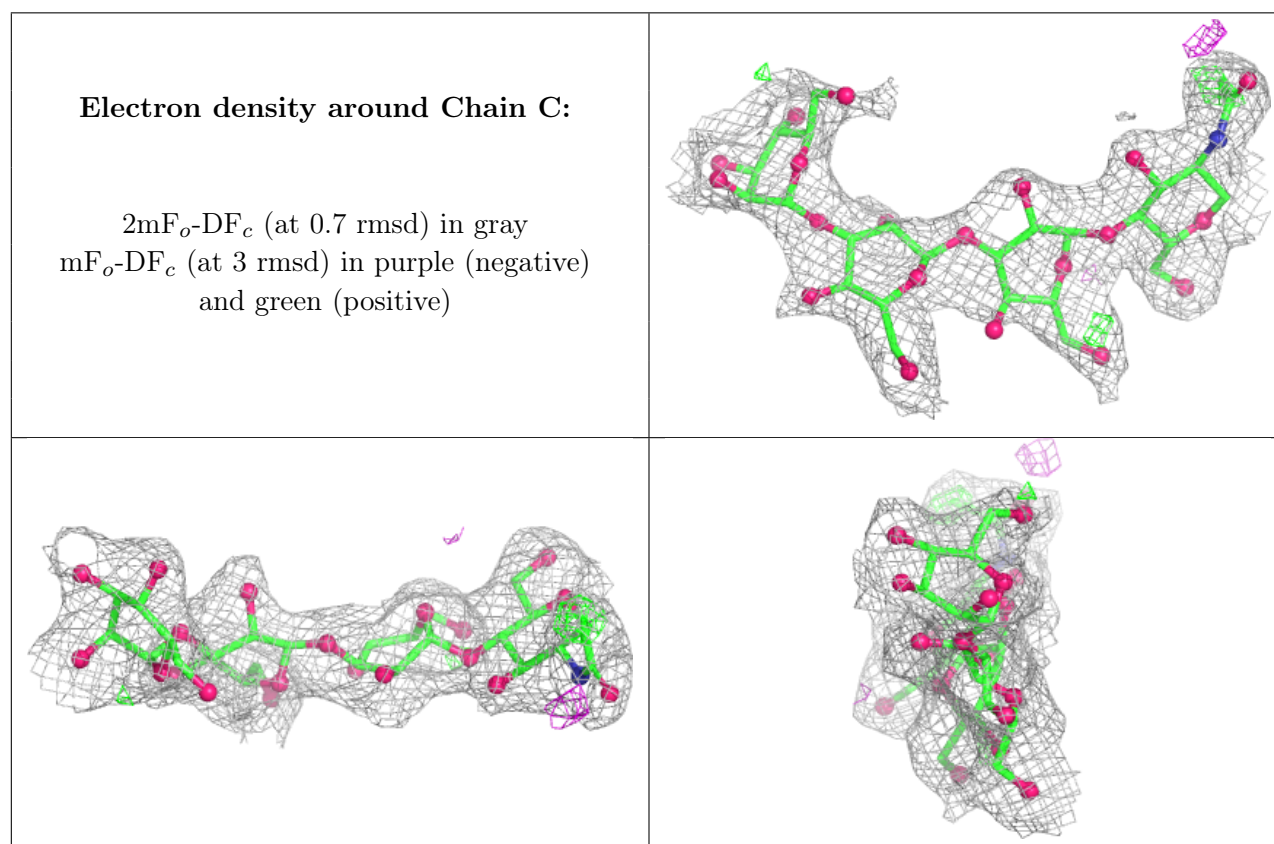
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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
2	MAN	C	3	11/12	0.66	0.14	54,56,57,59	0
2	MAN	C	2	11/12	0.72	0.17	46,48,52,53	0
2	MAN	C	4	11/12	0.72	0.15	58,59,60,60	0
2	NAG	C	1	14/15	0.77	0.14	36,39,42,44	0

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 [i](#)

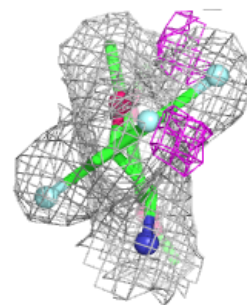
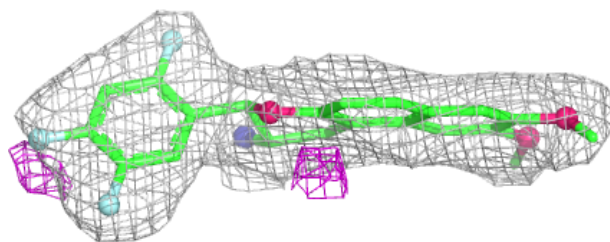
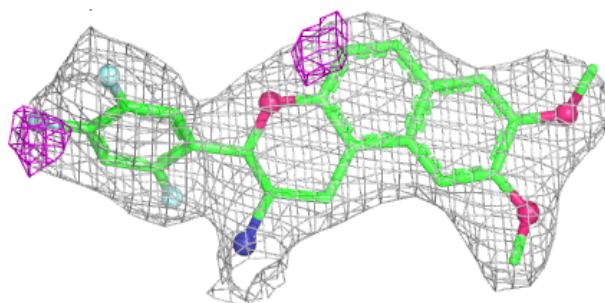
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	802	14/15	0.78	0.14	35,35,37,37	0
4	NAG	B	802	14/15	0.83	0.14	52,53,54,54	0
3	HL1	A	801	28/28	0.90	0.11	23,24,26,26	0
3	HL1	B	801	28/28	0.95	0.09	18,18,18,19	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.

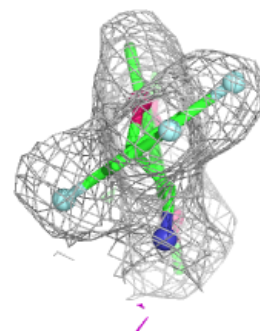
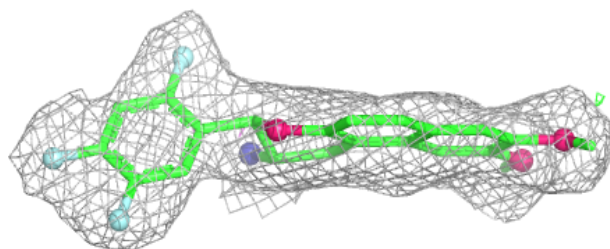
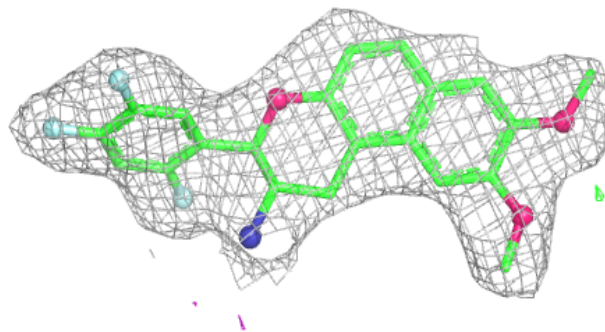
Electron density around HL1 A 801:

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 HL1 B 801:

$2mF_o-DF_c$ (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.