Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 07:44 PM JST

PDB ID	:	6M47
Title	:	X-ray structure of a Drosophila dopamine transporter with NET-like mutations (D121G/S426M/F471L) in tramadol bound form
Authors	:	Shabareesh, P.; Mallela, A.K.; Joseph, D.; Penmatsa, A.
Deposited on	:	2020-03-05
Resolution	:	3.25 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:

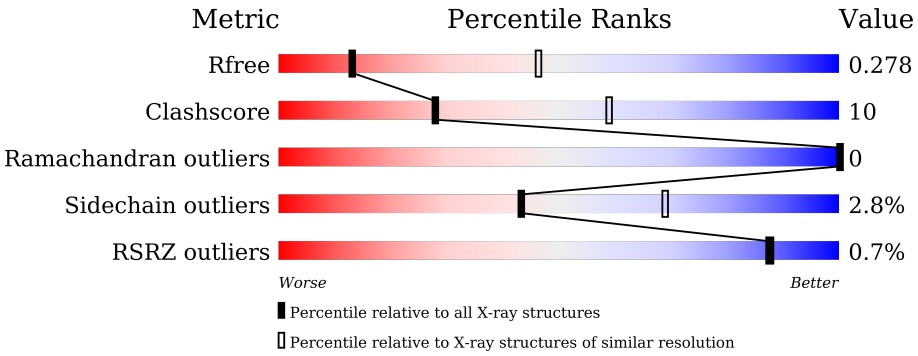
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	534	74% 25%
2	L	214	2% 76% 23%
3	H	219	% 78% 21%
4	B	2	50% 50%
4	C	2	100%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7615 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 Sodium-dependent dopamine transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	534	4212	2828	650	715	19	0	2	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	VAL	engineered mutation	UNP Q7K4Y6
A	121	GLY	ASP	engineered mutation	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	GLN	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	ALA	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	ARG	deletion	UNP Q7K4Y6
A	?	-	VAL	deletion	UNP Q7K4Y6
A	?	-	PRO	deletion	UNP Q7K4Y6
A	?	-	VAL	deletion	UNP Q7K4Y6
A	?	-	ILE	deletion	UNP Q7K4Y6
A	?	-	GLY	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	ASP	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	ALA	deletion	UNP Q7K4Y6
A	?	-	MET	deletion	UNP Q7K4Y6
A	?	-	GLY	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	GLN	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	GLU	deletion	UNP Q7K4Y6
A	?	-	THR	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	MET	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	GLY	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	ASP	deletion	UNP Q7K4Y6
A	?	-	THR	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	ALA	deletion	UNP Q7K4Y6
A	?	-	VAL	deletion	UNP Q7K4Y6
A	415	ALA	LEU	engineered mutation	UNP Q7K4Y6
A	426	MET	SER	engineered mutation	UNP Q7K4Y6
A	471	LEU	PHE	engineered mutation	UNP Q7K4Y6

- Molecule 2 is a protein called Antibody fragment 9D5 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1619	1007	268	336	8			

- Molecule 3 is a protein called Antibody fragment Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1624	1022	276	318	8			

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	B	2	Total	C	O	0	0	0
			23	12	11			

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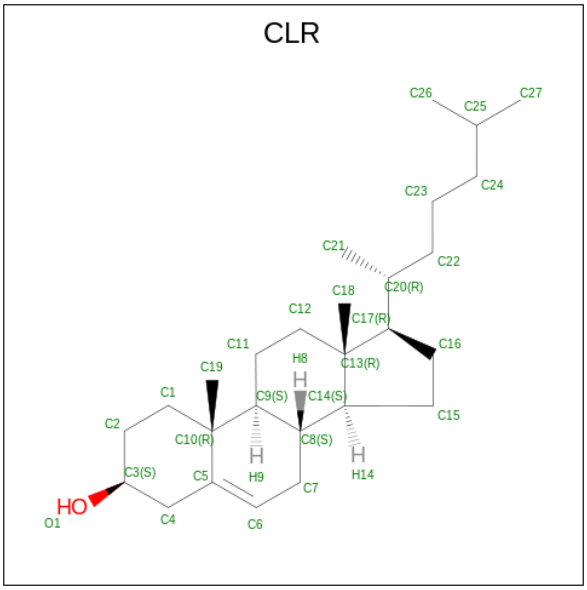
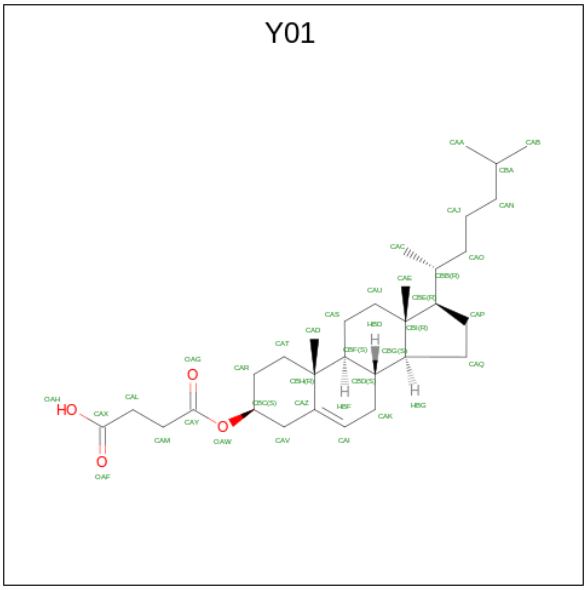
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	C	2	Total C O 23 12 11	0	0	0

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 28 27 1	0	0

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 35 31 4	0	0

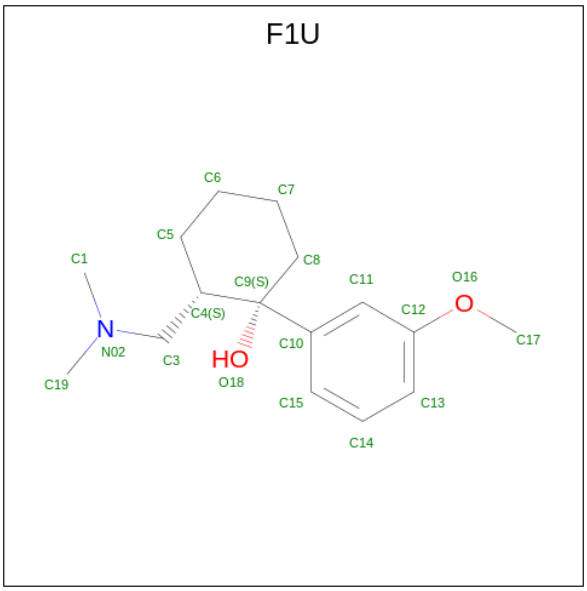
- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Na 2 2	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

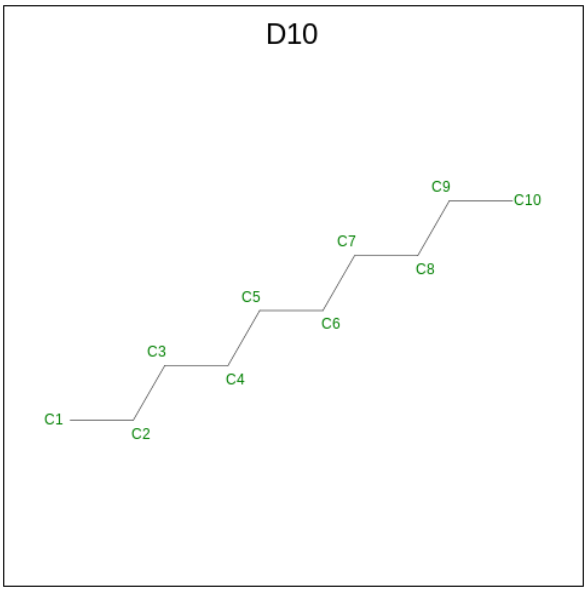
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is (1S,2S)-2-[(dimethylamino)methyl]-1-(3-methoxyphenyl)cyclohexan -1-ol (three-letter code: F1U) (formula: $C_{16}H_{25}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O 19 16 1 2	0	0

- Molecule 10 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C 10 10	0	0

- Molecule 11 is water.

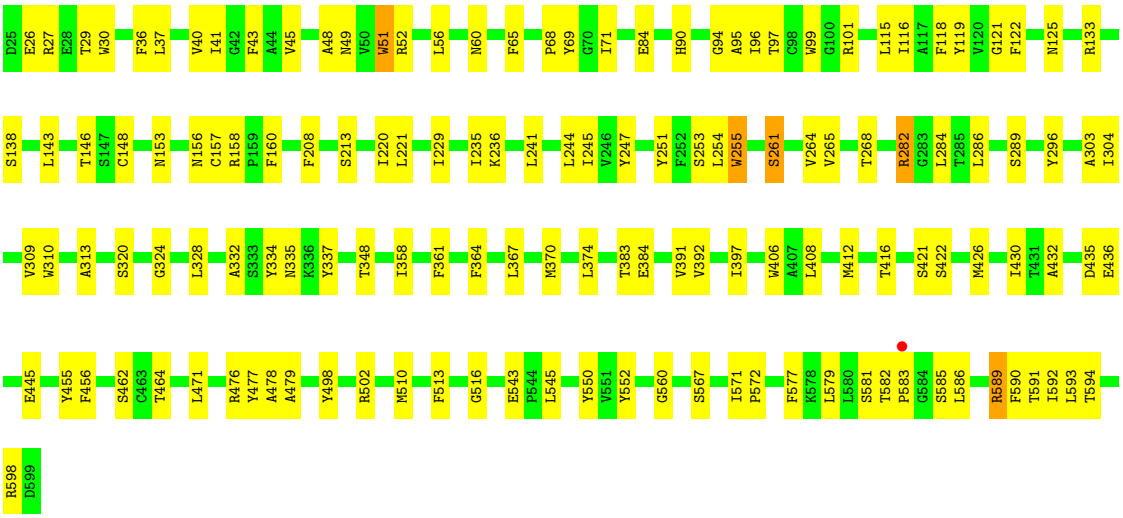
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	14	Total O 14 14	0	0
11	L	3	Total O 3 3	0	0
11	H	2	Total O 2 2	0	0

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.

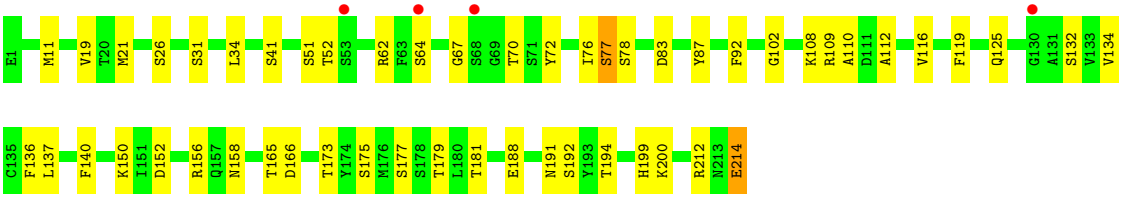
• Molecule 1: Sodium-dependent dopamine transporter

Chain A:



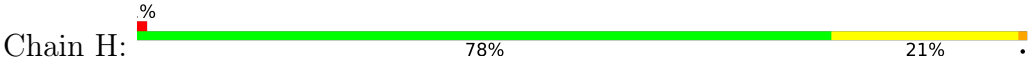
• Molecule 2: Antibody fragment 9D5 light chain

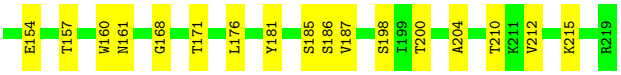
Chain L:



• Molecule 3: Antibody fragment Heavy chain

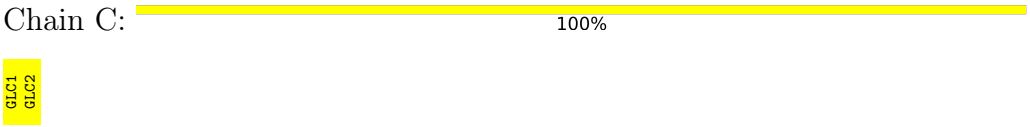
Chain H:





• Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

• Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.00Å 140.96Å 167.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.50 – 3.25 48.50 – 3.25	Depositor EDS
% Data completeness (in resolution range)	95.4 (48.50-3.25) 95.6 (48.50-3.25)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.241 , 0.275 0.242 , 0.278	Depositor DCC
R_{free} test set	1805 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	95.2	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	7615	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: F1U, Y01, GLC, CL, CLR, NA, D10

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	0.30	0/4361	0.49	0/5965
2	L	0.28	0/1657	0.52	0/2254
3	H	0.30	0/1663	0.59	2/2270 (0.1%)
All	All	0.30	0/7681	0.52	2/10489 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	33	ALA	CB-CA-C	9.41	124.21	110.10
3	H	33	ALA	N-CA-C	-5.21	96.95	111.00

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	4212	0	4116	90	0
2	L	1619	0	1523	28	0
3	H	1624	0	1550	32	0
4	B	23	0	21	1	0
4	C	23	0	21	0	0
5	A	28	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	35	0	49	2	0
7	A	2	0	0	0	0
8	A	1	0	0	1	0
9	A	19	0	0	1	0
10	A	10	0	22	0	0
11	A	14	0	0	1	0
11	H	2	0	0	0	0
11	L	3	0	0	1	0
All	All	7615	0	7348	148	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 10.

All (148) 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:476:ARG:HD3	1:A:545:LEU:HD13	1.67	0.76
1:A:27:ARG:NH2	1:A:435:ASP:OD2	2.18	0.75
3:H:29:PHE:O	3:H:72:ARG:NH2	2.22	0.72
3:H:9:GLY:HA2	3:H:18:LEU:HD21	1.74	0.70
2:L:214:GLU:O	3:H:134:CYS:SG	2.49	0.70
1:A:364:PHE:HA	1:A:367:LEU:HB2	1.75	0.68
1:A:513:PHE:HB3	3:H:101:VAL:HG13	1.75	0.68
1:A:96:ILE:HG13	1:A:432:ALA:HB1	1.75	0.67
1:A:52:ARG:NH1	1:A:384:GLU:OE1	2.25	0.65
3:H:157:THR:HB	3:H:204:ALA:HB3	1.80	0.62
2:L:152:ASP:HA	2:L:192:SER:HB3	1.82	0.61
1:A:220:ILE:O	1:A:236:LYS:NZ	2.32	0.61
1:A:97:THR:HG22	1:A:101:ARG:HD2	1.83	0.60
2:L:19:VAL:HG22	2:L:76:ILE:HB	1.84	0.60
3:H:60:TYR:HE1	3:H:70:ILE:HG22	1.66	0.60
1:A:579:LEU:HD23	1:A:593:LEU:HD12	1.84	0.60
1:A:68:PRO:HD3	1:A:304:ILE:HD11	1.84	0.59
3:H:12:VAL:HG11	3:H:86:LEU:HD13	1.82	0.59
2:L:116:VAL:HG22	2:L:137:LEU:HD22	1.83	0.59
1:A:585:SER:O	1:A:589:ARG:N	2.36	0.59
1:A:476:ARG:NH2	1:A:543:GLU:O	2.35	0.59
1:A:282:ARG:HG3	1:A:406:TRP:CZ2	2.39	0.58
2:L:134:VAL:HG22	2:L:179:THR:HG23	1.86	0.57
1:A:477:TYR:CD2	1:A:560:GLY:HA3	2.40	0.57
1:A:516:GLY:HA3	6:A:602:Y01:CAX	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:MET:HE3	1:A:392:VAL:HG12	1.87	0.56
9:A:608:F1U:C5	9:A:608:F1U:C19	2.84	0.55
1:A:52:ARG:O	1:A:56:LEU:HG	2.07	0.55
1:A:71:ILE:HD12	1:A:310:TRP:HH2	1.72	0.55
2:L:77:SER:OG	2:L:78:SER:N	2.39	0.55
1:A:251:TYR:OH	1:A:445:GLU:O	2.20	0.55
2:L:11:MET:HE1	2:L:21:MET:HG2	1.89	0.55
1:A:422:SER:O	1:A:426:MET:HG2	2.06	0.55
3:H:34:MET:HG2	3:H:72:ARG:HH12	1.72	0.55
1:A:462:SER:HB2	1:A:471:LEU:HD11	1.89	0.54
1:A:119:TYR:HB3	1:A:478:ALA:HB1	1.89	0.54
1:A:220:ILE:HG22	1:A:221:LEU:HD12	1.89	0.54
3:H:60:TYR:CE1	3:H:70:ILE:HG22	2.41	0.54
1:A:582:THR:O	1:A:589:ARG:NH1	2.42	0.53
3:H:36:TRP:HD1	3:H:70:ILE:HD12	1.73	0.53
1:A:332:ALA:O	1:A:335:ASN:HB2	2.08	0.53
1:A:268:THR:HG22	1:A:416:THR:HG22	1.90	0.53
2:L:119:PHE:HZ	3:H:143:THR:HG22	1.74	0.53
1:A:571:ILE:HB	1:A:572:PRO:HD3	1.91	0.53
1:A:69:TYR:HA	1:A:313:ALA:HB1	1.91	0.53
1:A:30:TRP:CD1	1:A:36:PHE:HB2	2.44	0.52
1:A:303:ALA:HB1	1:A:309:VAL:HG21	1.91	0.52
3:H:144:LEU:HB2	3:H:187:VAL:HG13	1.92	0.52
1:A:121:GLY:O	1:A:125:ASN:ND2	2.44	0.51
1:A:244:LEU:HB2	1:A:456:PHE:CE2	2.45	0.51
1:A:115:LEU:HD11	1:A:567:SER:HA	1.91	0.51
1:A:43:PHE:HA	1:A:421:SER:HA	1.92	0.51
1:A:397:ILE:HG23	1:A:406:TRP:HB2	1.93	0.51
1:A:320:SER:OG	8:A:605:CL:CL	2.66	0.51
1:A:445:GLU:CD	1:A:445:GLU:H	2.14	0.51
1:A:577:PHE:O	1:A:581:SER:OG	2.16	0.51
2:L:132:SER:HA	2:L:181:THR:HA	1.93	0.51
2:L:108:LYS:NZ	11:L:301:HOH:O	2.43	0.50
3:H:2:VAL:HG13	3:H:27:PHE:CD1	2.46	0.50
1:A:160:PHE:CE1	1:A:374:LEU:HD13	2.46	0.50
1:A:358:ILE:HG21	5:A:601:CLR:H263	1.94	0.50
1:A:445:GLU:OE1	1:A:445:GLU:N	2.41	0.50
3:H:35:SER:OG	3:H:50:GLU:HG3	2.11	0.50
3:H:210:THR:HG22	3:H:212:VAL:HG23	1.94	0.50
2:L:67:GLY:HA3	2:L:72:TYR:HA	1.93	0.50
2:L:62:ARG:NH1	2:L:83:ASP:OD2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:171:THR:HG23	3:H:185:SER:HB2	1.92	0.50
1:A:71:ILE:HD12	1:A:310:TRP:CH2	2.48	0.49
1:A:68:PRO:HD3	1:A:304:ILE:CD1	2.43	0.49
1:A:84:GLU:OE1	1:A:324:GLY:N	2.45	0.49
1:A:68:PRO:HB3	1:A:310:TRP:CE2	2.48	0.48
3:H:9:GLY:HA2	3:H:18:LEU:CD2	2.42	0.48
3:H:176:LEU:HD12	3:H:181:TYR:CE2	2.49	0.48
1:A:586:LEU:O	1:A:589:ARG:HB3	2.14	0.48
1:A:60:ASN:O	1:A:65:PHE:HB2	2.14	0.48
1:A:591:THR:HA	1:A:594:THR:HG22	1.95	0.48
1:A:156:ASN:O	1:A:208:PHE:HA	2.13	0.48
1:A:583:PRO:O	1:A:589:ARG:NH2	2.44	0.48
3:H:2:VAL:HG22	3:H:27:PHE:HB3	1.96	0.48
2:L:199:HIS:CD2	2:L:200:LYS:H	2.32	0.48
2:L:109:ARG:NH1	2:L:110:ALA:O	2.47	0.48
1:A:41:ILE:HD13	1:A:348:THR:HG23	1.96	0.47
2:L:41:SER:OG	2:L:166:ASP:OD2	2.24	0.47
2:L:150:LYS:HB2	2:L:194:THR:HB	1.96	0.47
3:H:33:ALA:O	3:H:99:GLY:O	2.32	0.47
1:A:229:ILE:HG22	1:A:550:TYR:OH	2.14	0.47
3:H:151:TYR:OH	3:H:154:GLU:OE2	2.27	0.47
1:A:284:LEU:HA	1:A:289:SER:OG	2.14	0.47
2:L:191:ASN:OD1	2:L:192:SER:N	2.48	0.47
3:H:200:THR:HA	3:H:215:LYS:HA	1.96	0.47
1:A:337:TYR:O	1:A:510:MET:HG2	2.14	0.47
1:A:37:LEU:O	1:A:41:ILE:HG12	2.14	0.46
1:A:247:TYR:CZ	1:A:455:TYR:HB3	2.50	0.46
1:A:328:LEU:N	11:A:703:HOH:O	2.44	0.46
1:A:133:ARG:CZ	4:B:1:GLC:H3	2.46	0.46
1:A:157:CYS:SG	1:A:158:ARG:N	2.88	0.46
6:A:602:Y01:HAA1	6:A:602:Y01:HAJ2	1.65	0.46
1:A:426:MET:O	1:A:430:ILE:HG13	2.16	0.45
1:A:244:LEU:HB2	1:A:456:PHE:HE2	1.81	0.45
1:A:583:PRO:C	1:A:589:ARG:HH12	2.20	0.45
1:A:115:LEU:HA	1:A:118:PHE:HB3	1.99	0.45
1:A:498:TYR:O	1:A:502:ARG:HD2	2.16	0.45
2:L:109:ARG:HH12	2:L:112:ALA:HB2	1.82	0.45
2:L:156:ARG:NH1	2:L:158:ASN:O	2.50	0.44
2:L:70:THR:O	2:L:70:THR:OG1	2.32	0.44
1:A:95:ALA:O	1:A:99:TRP:HD1	1.99	0.44
3:H:91:THR:HG23	3:H:116:THR:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:SER:HB2	1:A:408:LEU:HD23	2.00	0.44
1:A:235:ILE:HG12	1:A:464:THR:HG22	1.99	0.43
1:A:383:THR:OG1	1:A:384:GLU:N	2.50	0.43
1:A:143:LEU:O	1:A:146:THR:HG22	2.18	0.43
1:A:296:TYR:HE2	1:A:361:PHE:CD1	2.36	0.43
1:A:94:GLY:N	1:A:435:ASP:OD2	2.48	0.43
3:H:125:PRO:HB3	3:H:151:TYR:HB3	2.01	0.43
1:A:286:LEU:HD12	1:A:286:LEU:HA	1.88	0.42
2:L:31:SER:O	2:L:52:THR:OG1	2.36	0.42
2:L:140:PHE:N	2:L:173:THR:OG1	2.52	0.42
1:A:255:TRP:HD1	1:A:255:TRP:H	1.65	0.42
3:H:6:GLU:OE2	3:H:96:CYS:N	2.41	0.42
1:A:213:SER:HB2	1:A:391:VAL:HG11	2.01	0.42
1:A:589:ARG:O	1:A:592:ILE:HG22	2.18	0.42
3:H:67:ARG:NH1	3:H:90:ASP:OD2	2.53	0.42
1:A:590:PHE:O	1:A:594:THR:N	2.53	0.42
2:L:188:GLU:HA	2:L:212:ARG:CZ	2.50	0.42
1:A:304:ILE:HD13	1:A:304:ILE:HA	1.89	0.42
1:A:90:HIS:HB2	1:A:510:MET:CE	2.49	0.41
1:A:29:THR:HA	1:A:334:TYR:O	2.20	0.41
1:A:45:VAL:HG22	1:A:49:ASN:ND2	2.35	0.41
3:H:168:GLY:O	3:H:187:VAL:HA	2.20	0.41
1:A:253:SER:HB2	1:A:264:VAL:HG11	2.01	0.41
2:L:87:TYR:O	2:L:102:GLY:HA2	2.20	0.41
3:H:30:SER:O	3:H:53:SER:HB2	2.20	0.41
3:H:161:ASN:ND2	3:H:198:SER:O	2.41	0.41
1:A:119:TYR:O	1:A:122:PHE:HB2	2.20	0.41
2:L:125:GLN:NE2	2:L:132:SER:OG	2.35	0.41
2:L:136:PHE:CE1	3:H:186:SER:HB3	2.55	0.41
2:L:214:GLU:H	2:L:214:GLU:HG2	1.33	0.41
3:H:146:CYS:HB2	3:H:160:TRP:CH2	2.55	0.41
1:A:40:VAL:HG12	1:A:348:THR:HG21	2.04	0.41
1:A:282:ARG:O	1:A:282:ARG:HD3	2.20	0.41
3:H:171:THR:HA	3:H:185:SER:HB2	2.03	0.41
1:A:48:ALA:HA	1:A:51:TRP:CD1	2.56	0.40
1:A:241:LEU:O	1:A:245:ILE:HG13	2.21	0.40
1:A:116:ILE:HG23	1:A:479:ALA:HB2	2.03	0.40
1:A:221:LEU:C	1:A:236:LYS:HZ1	2.25	0.40
2:L:165:THR:HG23	2:L:175:SER:O	2.21	0.40
1:A:261:SER:O	1:A:265:VAL:HG13	2.22	0.40
1:A:545:LEU:HG	1:A:552:TYR:CD1	2.56	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	534/534 (100%)	506 (95%)	28 (5%)	0	100	100
2	L	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
3	H	217/219 (99%)	207 (95%)	10 (5%)	0	100	100
All	All	963/967 (100%)	916 (95%)	47 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	429/438 (98%)	417 (97%)	12 (3%)	43	69
2	L	182/187 (97%)	174 (96%)	8 (4%)	28	58
3	H	175/187 (94%)	173 (99%)	2 (1%)	73	84
All	All	786/812 (97%)	764 (97%)	22 (3%)	43	69

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	51	TRP

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Mol	Chain	Res	Type
1	A	148	CYS
1	A	153	ASN
1	A	254	LEU
1	A	255	TRP
1	A	261	SER
1	A	282	ARG
1	A	412	MET
1	A	436	GLU
1	A	589	ARG
1	A	598	ARG
2	L	26	SER
2	L	34	LEU
2	L	51	SER
2	L	64	SER
2	L	77	SER
2	L	92	PHE
2	L	177	SER
2	L	214	GLU
3	H	98	ARG
3	H	134	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	199	HIS

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)

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	$\#\|Z\| > 2$
4	GLC	B	1	4	12,12,12	0.55	0	17,17,17	1.50	5 (29%)
4	GLC	B	2	4	11,11,12	0.71	0	15,15,17	2.23	8 (53%)
4	GLC	C	1	4	12,12,12	0.71	0	17,17,17	1.82	4 (23%)
4	GLC	C	2	4	11,11,12	0.71	0	15,15,17	1.71	5 (33%)

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	GLC	B	1	4	-	2/2/22/22	0/1/1/1
4	GLC	B	2	4	-	1/2/19/22	0/1/1/1
4	GLC	C	1	4	-	2/2/22/22	0/1/1/1
4	GLC	C	2	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2	GLC	C1-O5-C5	3.44	116.86	112.19
4	C	1	GLC	O5-C1-C2	3.40	116.35	110.28
4	B	2	GLC	O2-C2-C1	3.28	115.86	109.15
4	C	1	GLC	O4-C4-C3	-3.24	102.87	110.35
4	C	1	GLC	O3-C3-C2	3.12	117.57	110.35
4	C	2	GLC	O5-C5-C6	2.94	111.82	107.20
4	B	1	GLC	O3-C3-C2	2.83	116.90	110.35
4	B	2	GLC	O2-C2-C3	-2.67	104.79	110.14
4	B	1	GLC	O4-C4-C3	-2.67	104.18	110.35
4	B	2	GLC	O5-C5-C6	2.58	111.24	107.20
4	B	2	GLC	O5-C1-C2	2.57	114.74	110.77
4	C	2	GLC	O2-C2-C1	2.56	114.39	109.15
4	C	1	GLC	O2-C2-C1	-2.43	103.53	109.16
4	C	2	GLC	O5-C1-C2	2.23	114.22	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2	GLC	C6-C5-C4	-2.15	107.96	113.00
4	B	2	GLC	O5-C5-C4	2.14	116.03	110.83
4	B	2	GLC	O3-C3-C2	-2.10	105.97	109.99
4	C	2	GLC	O3-C3-C2	-2.08	106.01	109.99
4	B	1	GLC	O5-C5-C6	2.03	111.49	106.44
4	C	2	GLC	O3-C3-C4	2.02	115.03	110.35
4	B	1	GLC	O2-C2-C1	-2.01	104.49	109.16
4	B	1	GLC	O1-C1-C2	-2.00	103.40	109.03

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	GLC	C4-C5-C6-O6
4	C	2	GLC	C4-C5-C6-O6
4	B	1	GLC	O5-C5-C6-O6
4	C	1	GLC	O5-C5-C6-O6
4	C	2	GLC	O5-C5-C6-O6
4	C	1	GLC	C4-C5-C6-O6
4	B	2	GLC	O5-C5-C6-O6

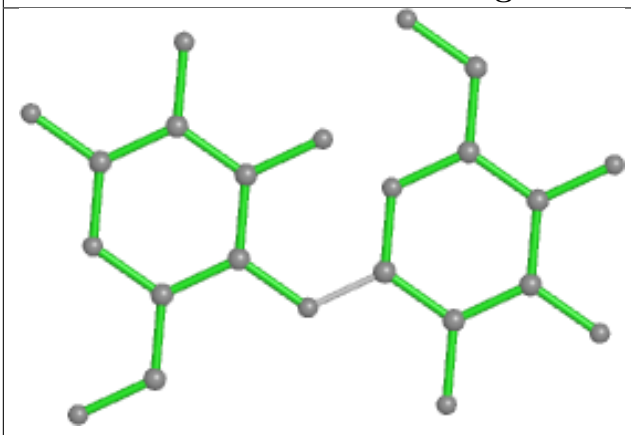
There are no ring outliers.

1 monomer is involved in 1 short contact:

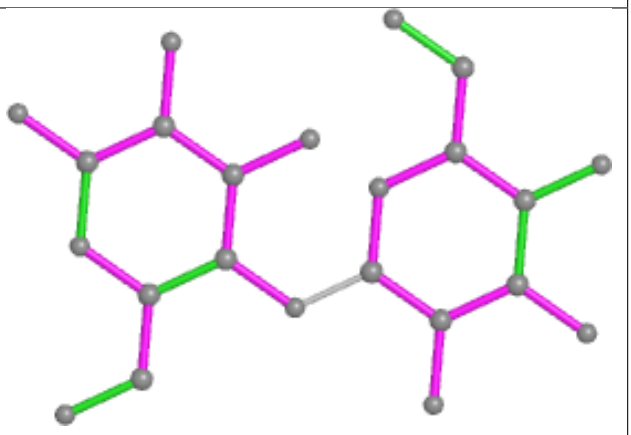
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	GLC	1	0

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

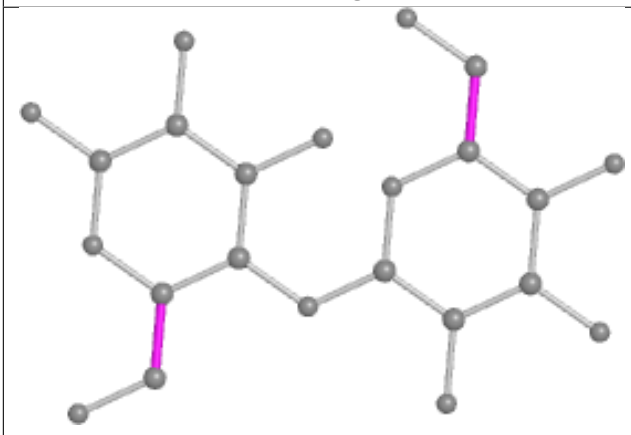
Oligosaccharide Chain B



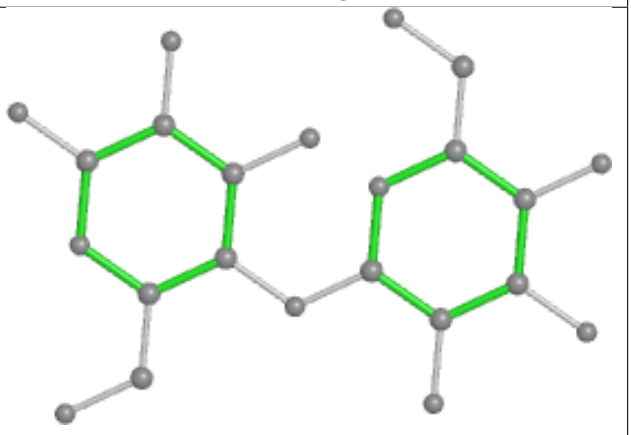
Bond lengths



Bond angles

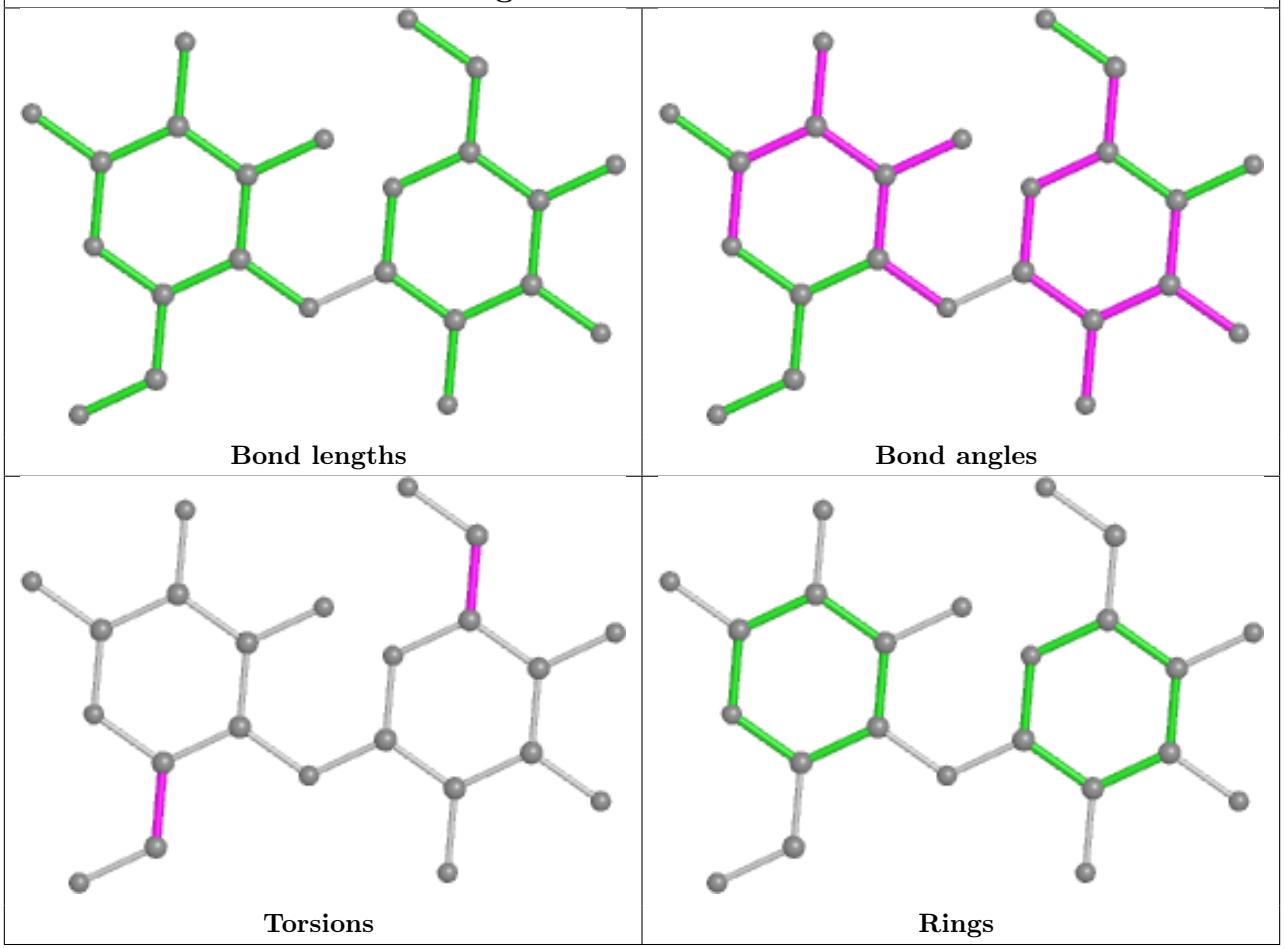


Torsions



Rings

Oligosaccharide Chain C



5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	CLR	A	601	-	31,31,31	0.63	0	48,48,48	1.57	10 (20%)
6	Y01	A	602	-	38,38,38	0.69	1 (2%)	57,57,57	1.74	15 (26%)
10	D10	A	609	-	9,9,9	0.34	0	8,8,8	0.29	0
9	F1U	A	608	-	18,20,20	2.01	4 (22%)	25,28,28	1.90	5 (20%)

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
5	CLR	A	601	-	-	1/10/68/68	0/4/4/4
6	Y01	A	602	-	-	7/19/77/77	0/4/4/4
10	D10	A	609	-	-	2/7/7/7	-
9	F1U	A	608	-	-	2/12/26/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	608	F1U	O18-C9	-4.41	1.36	1.43
9	A	608	F1U	C8-C9	-4.30	1.49	1.53
9	A	608	F1U	C15-C10	-2.90	1.34	1.39
6	A	602	Y01	CBH-CBF	-2.61	1.51	1.56
9	A	608	F1U	C11-C10	-2.55	1.35	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	608	F1U	C5-C4-C9	-5.60	104.60	110.73
6	A	602	Y01	CBI-CBG-CBD	-4.92	107.09	114.38
5	A	601	CLR	C14-C8-C9	-4.27	103.38	109.09
9	A	608	F1U	C7-C8-C9	-3.98	108.66	112.52
6	A	602	Y01	CAK-CBD-CBG	-3.36	106.03	110.91
5	A	601	CLR	C13-C14-C8	-3.30	109.49	114.38
6	A	602	Y01	CAV-CAZ-CAI	-3.25	115.92	120.61
6	A	602	Y01	CAM-CAL-CAX	-3.12	106.88	113.60
5	A	601	CLR	C16-C17-C20	-2.99	107.51	112.15
6	A	602	Y01	CAO-CBB-CBE	-2.97	104.15	110.28
6	A	602	Y01	OAW-CAY-CAM	2.97	117.89	111.50
6	A	602	Y01	CAK-CBD-CBF	2.86	113.18	109.71
5	A	601	CLR	C19-C10-C9	-2.82	108.32	111.68
6	A	602	Y01	CAQ-CBG-CBD	-2.77	114.52	119.08
6	A	602	Y01	CBG-CBI-CBE	-2.74	96.83	100.07
9	A	608	F1U	C1-N02-C3	-2.66	104.02	111.01
5	A	601	CLR	C22-C20-C17	-2.56	105.00	110.28
6	A	602	Y01	CBI-CBE-CBB	-2.54	115.50	119.49
6	A	602	Y01	CAD-CBH-CBF	-2.47	108.74	111.68
9	A	608	F1U	C8-C7-C6	-2.32	107.78	111.37
5	A	601	CLR	C18-C13-C14	-2.21	107.59	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	601	CLR	C9-C10-C5	2.18	113.07	109.65
5	A	601	CLR	C7-C8-C14	-2.17	107.76	110.91
5	A	601	CLR	C4-C5-C6	-2.16	117.50	120.61
9	A	608	F1U	C10-C9-C4	2.12	114.43	111.67
6	A	602	Y01	CBD-CAK-CAI	-2.10	109.71	112.73
6	A	602	Y01	CAL-CAM-CAY	-2.08	107.37	113.43
6	A	602	Y01	CAV-CAZ-CBH	2.05	119.14	116.42
6	A	602	Y01	OAH-CAX-CAL	2.05	120.61	114.03
5	A	601	CLR	C13-C17-C20	-2.05	116.28	119.49

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	608	F1U	C4-C3-N02-C1
6	A	602	Y01	CAX-CAL-CAM-CAY
6	A	602	Y01	CAO-CAJ-CAN-CBA
6	A	602	Y01	CAN-CAJ-CAO-CBB
10	A	609	D10	C4-C5-C6-C7
6	A	602	Y01	CAM-CAY-OAW-CBC
6	A	602	Y01	OAG-CAY-OAW-CBC
10	A	609	D10	C5-C6-C7-C8
6	A	602	Y01	CAJ-CAN-CBA-CAA
9	A	608	F1U	C4-C3-N02-C19
6	A	602	Y01	CAJ-CAN-CBA-CAB
5	A	601	CLR	C20-C22-C23-C24

There are no ring outliers.

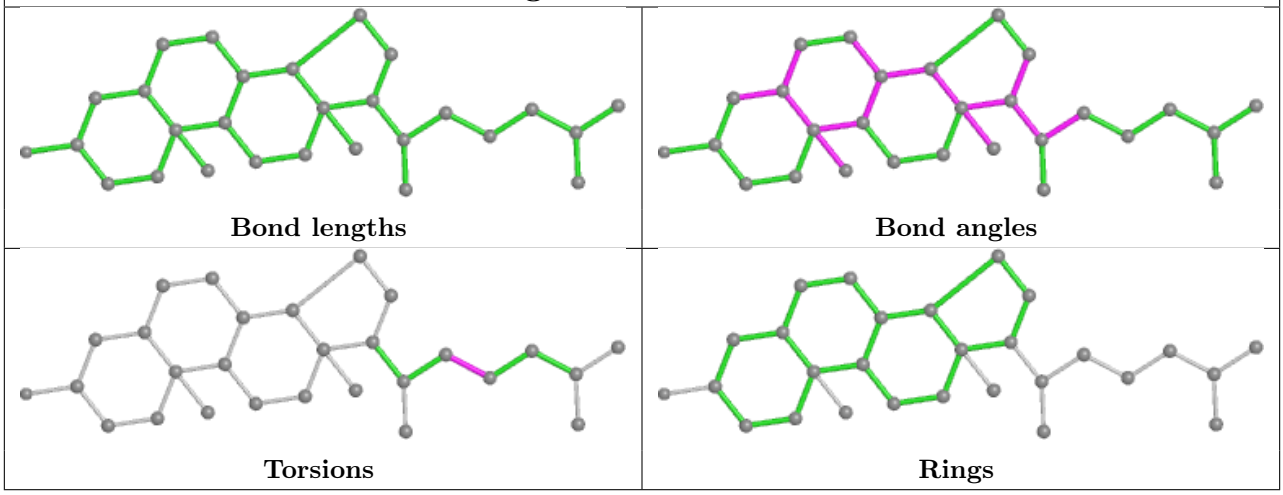
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	CLR	1	0
6	A	602	Y01	2	0
9	A	608	F1U	1	0

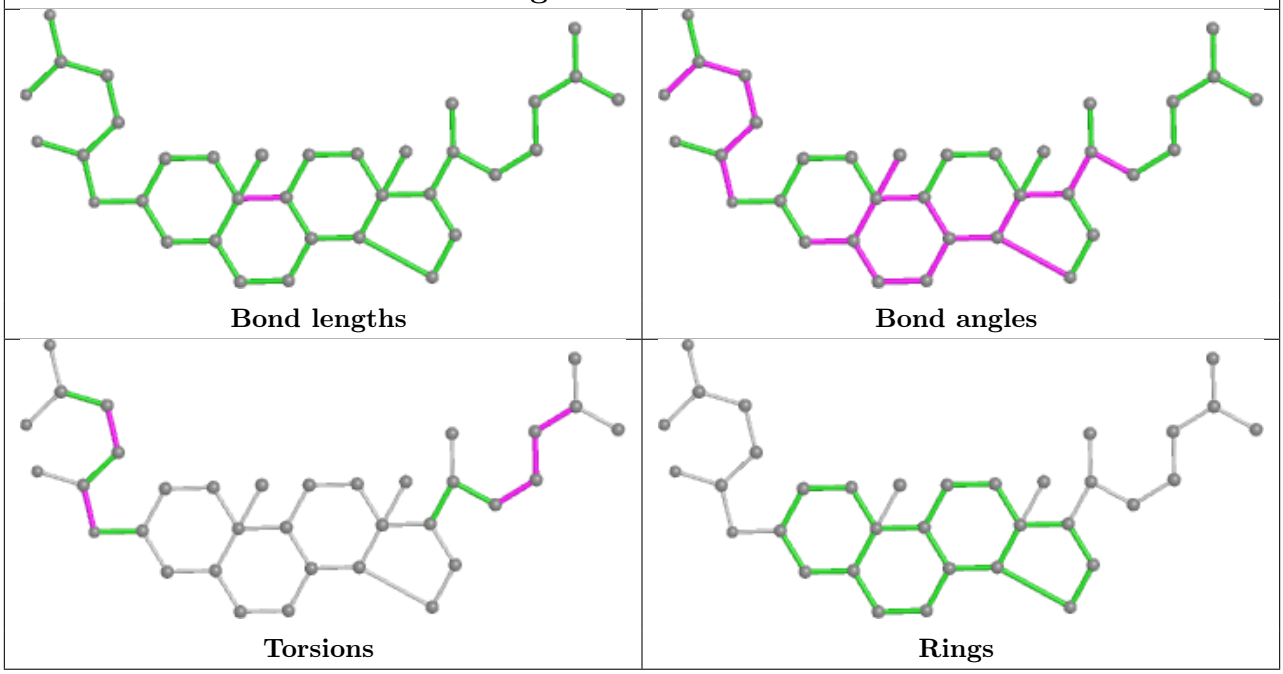
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

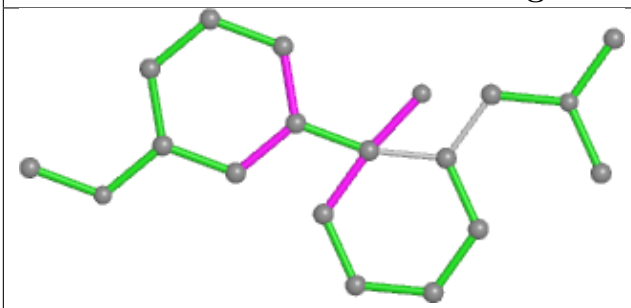
Ligand CLR A 601



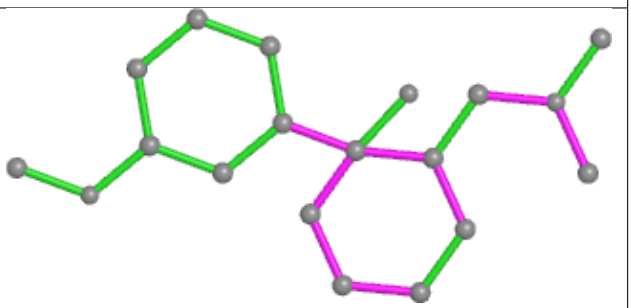
Ligand Y01 A 602



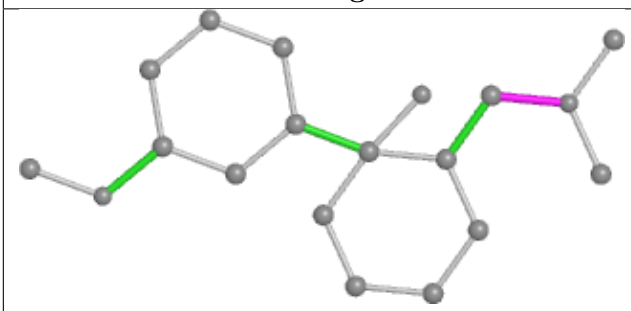
Ligand F1U A 608



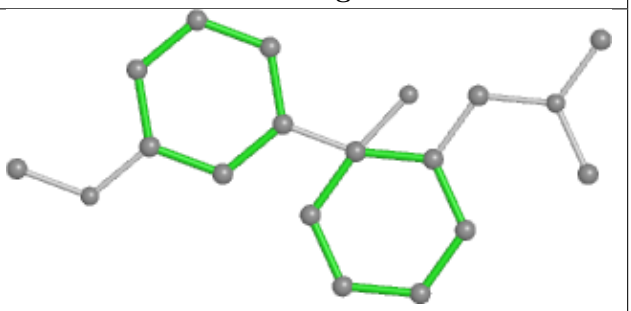
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	534/534 (100%)	-0.25	1 (0%)	95	95	70, 88, 110, 133	0
2	L	214/214 (100%)	-0.19	4 (1%)	66	64	67, 87, 110, 130	0
3	H	219/219 (100%)	-0.26	2 (0%)	84	84	72, 86, 116, 140	0
All	All	967/967 (100%)	-0.24	7 (0%)	87	88	67, 87, 111, 140	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	68	SER	3.0
3	H	138	THR	2.6
2	L	64	SER	2.4
2	L	130	GLY	2.4
3	H	139	GLY	2.4
1	A	583	PRO	2.2
2	L	53	SER	2.0

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
4	GLC	B	1	12/12	0.86	0.26	102,110,120,121	0

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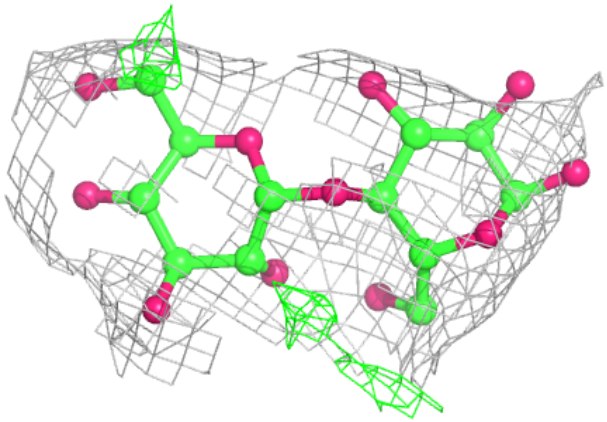
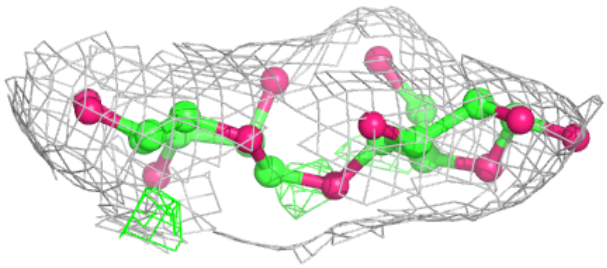
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GLC	C	1	12/12	0.86	0.31	108,132,148,148	0
4	GLC	B	2	11/12	0.92	0.12	79,102,114,116	0
4	GLC	C	2	11/12	0.92	0.23	99,117,126,126	0

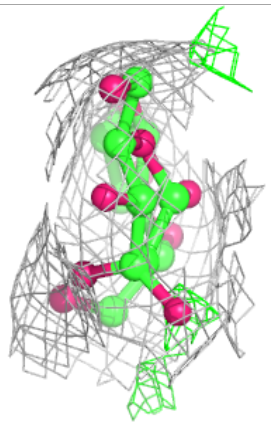
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

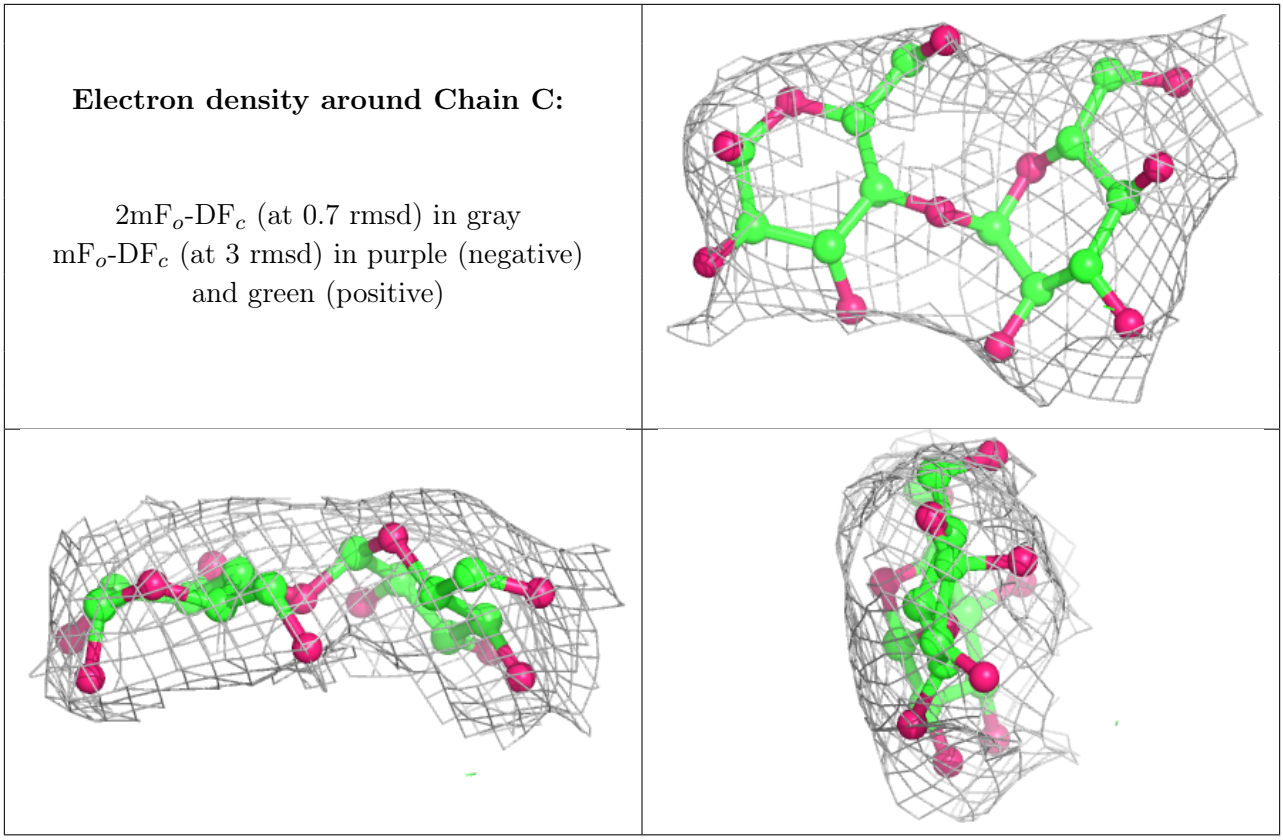






Electron density around Chain C:

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



6.4 Ligands

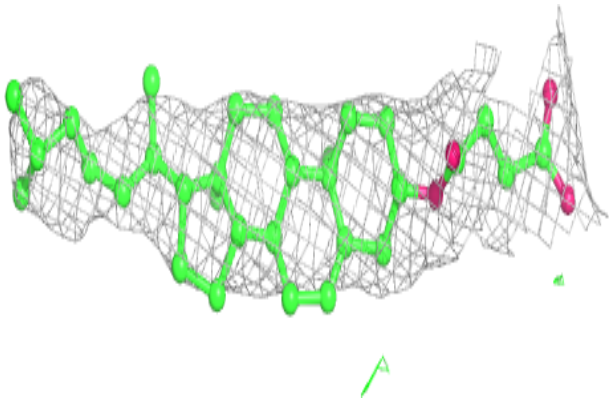
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

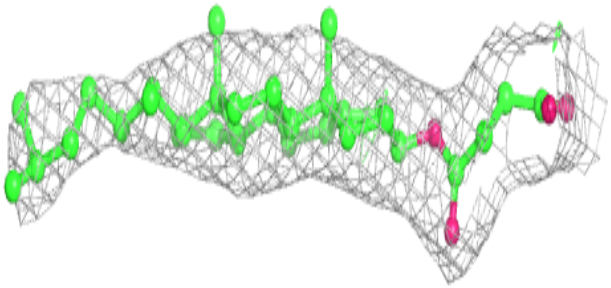
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	D10	A	609	10/10	0.80	0.28	64,90,95,96	0
6	Y01	A	602	35/35	0.90	0.29	78,95,132,134	0
5	CLR	A	601	28/28	0.92	0.36	64,85,99,100	0
9	F1U	A	608	19/19	0.95	0.29	75,86,99,109	0
7	NA	A	604	1/1	0.95	0.22	85,85,85,85	0
7	NA	A	603	1/1	0.97	0.12	85,85,85,85	0
8	CL	A	605	1/1	0.97	0.09	80,80,80,80	0

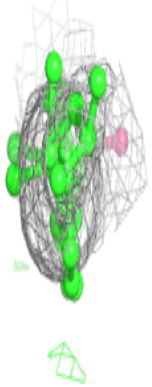
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around Y01 A 602:

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

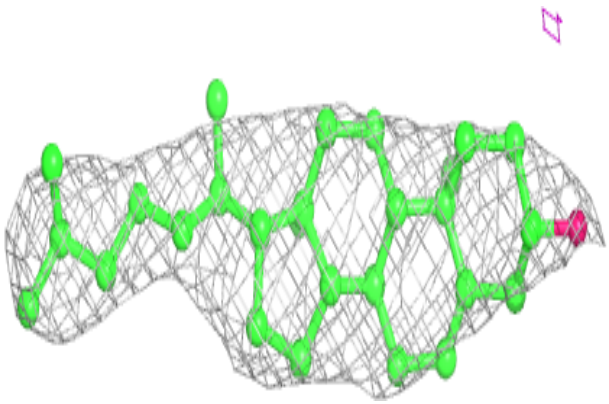


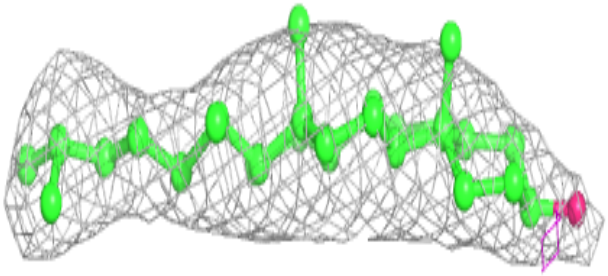


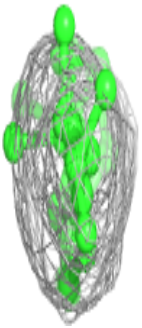


Electron density around CLR A 601:

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

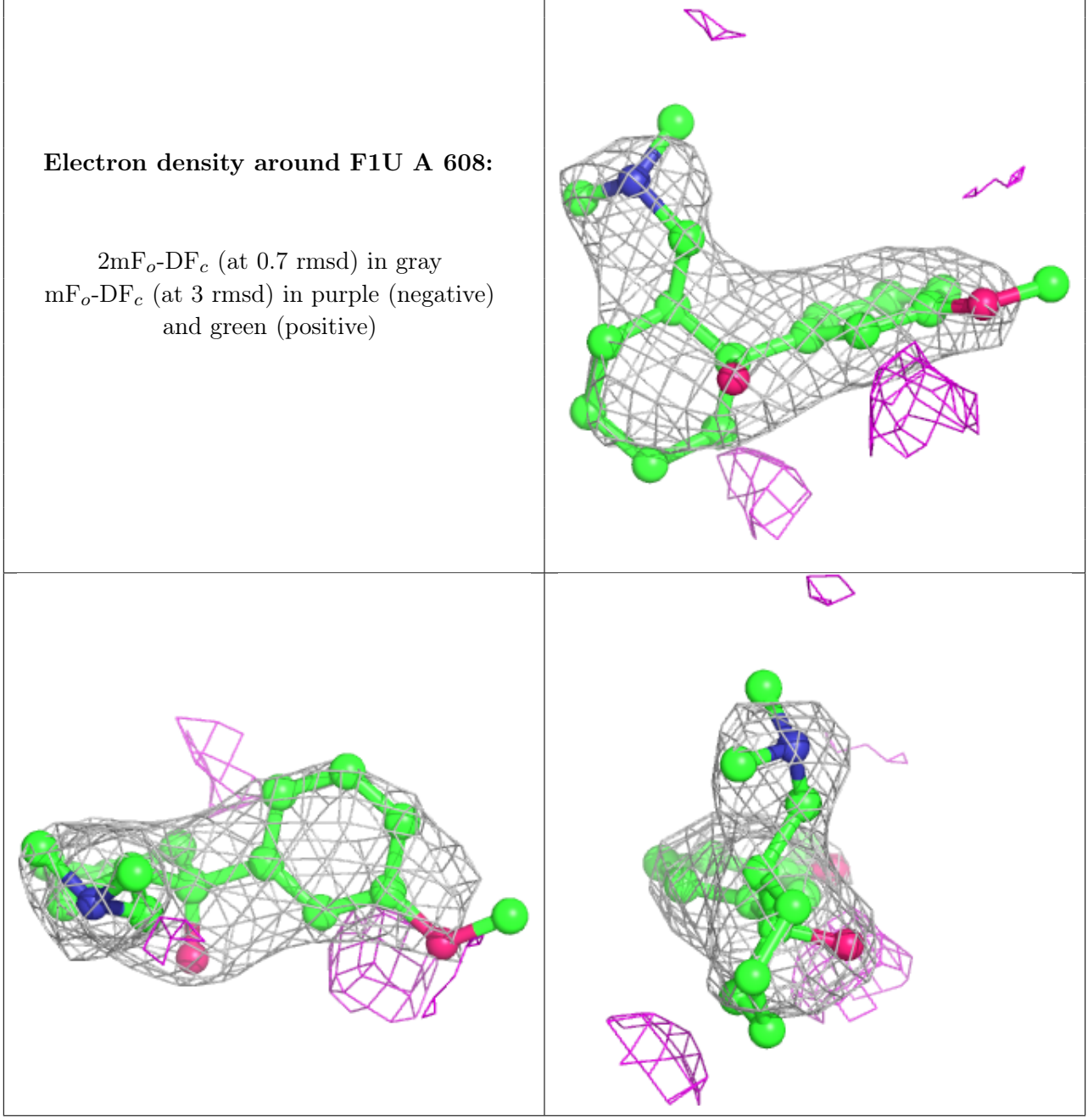






Electron density around F1U A 608:

$2mF_o$-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.