Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 10:16 PM EDT

PDB ID	:	4XPA
Title	:	X-ray structure of Drosophila dopamine transporter bound to 3,4dichlorophe nethylamine
Authors	:	Aravind, P.; Wang, K.; Gouaux, E.
Deposited on	:	2015-01-16
Resolution	:	2.95 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:

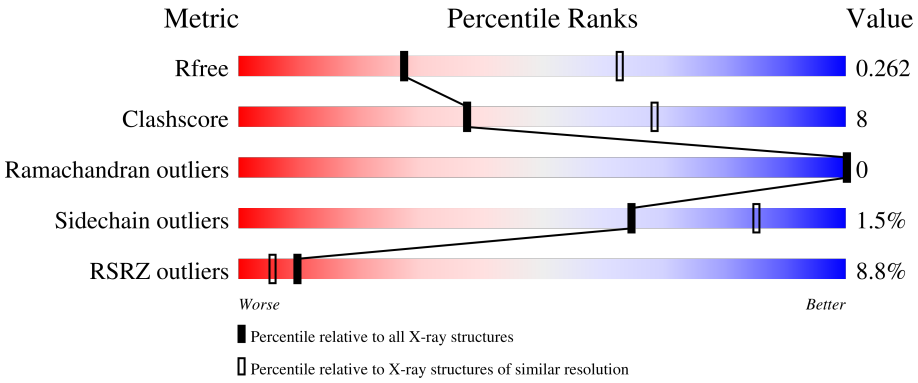
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	545	9% 77% 20%
2	L	237	8% 76% 14% 10%
3	H	240	7% 74% 17% 9%
4	B	2	50% 50%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7585 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 Transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	534	4231	2836	657	719	19	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	214	1629	1012	271	338	8	0	0	0

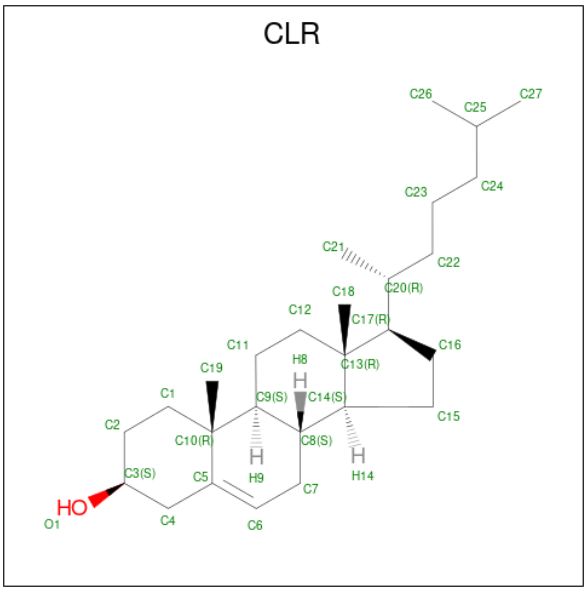
- Molecule 3 is a protein called Antibody fragment light chain-protein, 9D5-light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	219	1619	1019	274	318	8	0	0	0

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

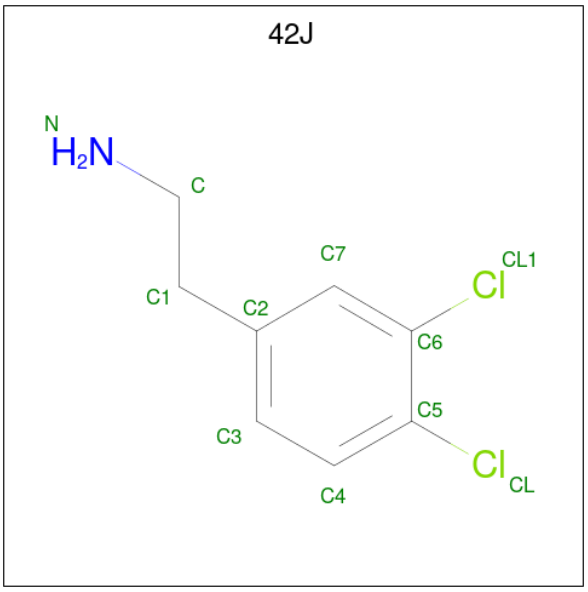
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
4	B	2	23	12	11	0	0	0

- 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
5	A	1	Total C O 28 27 1	0	0

- Molecule 6 is 2-(3,4-dichlorophenyl)ethanamine (three-letter code: 42J) (formula: $C_8H_9Cl_2N$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C Cl N 11 8 2 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

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

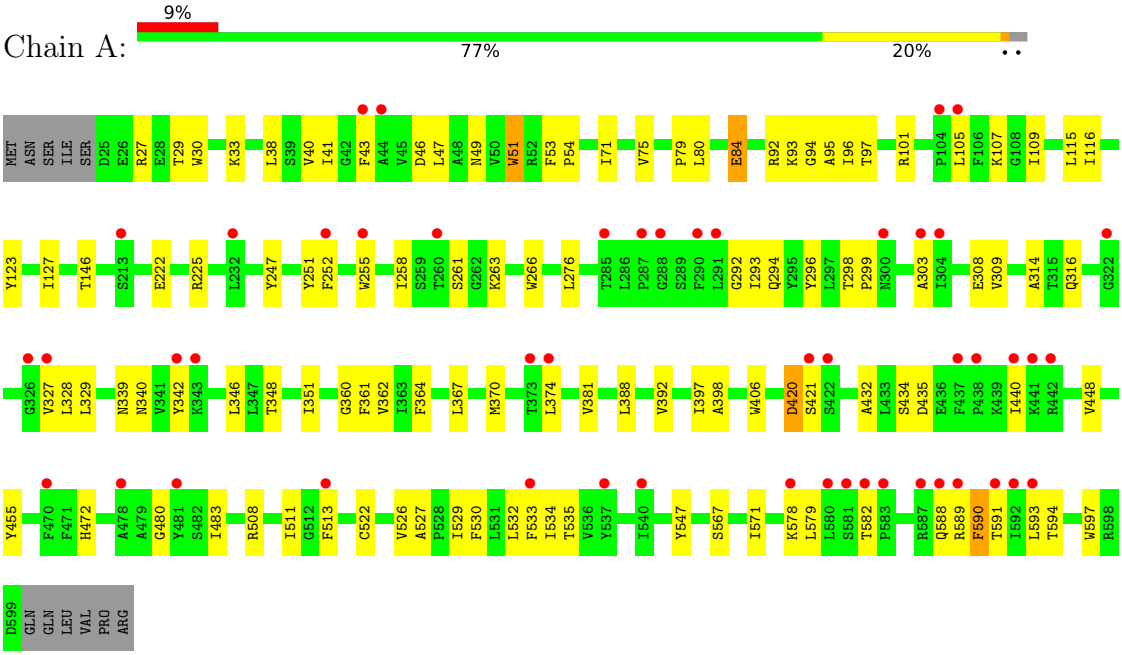
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	13	Total O 13 13	0	0

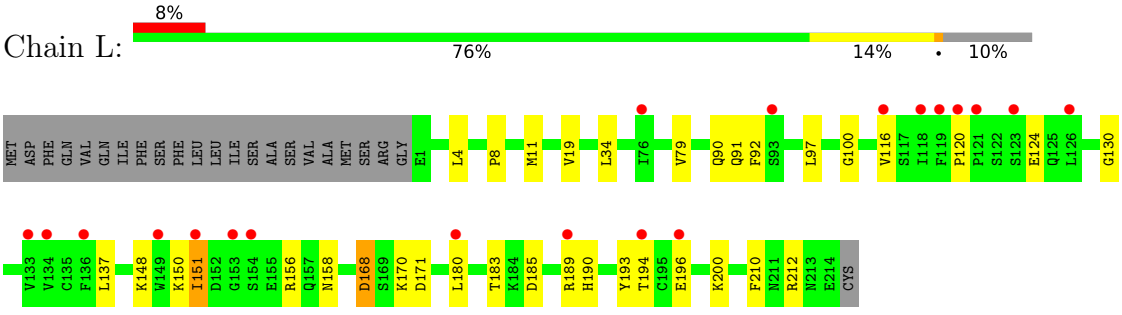
3 Residue-property plots (i)

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.

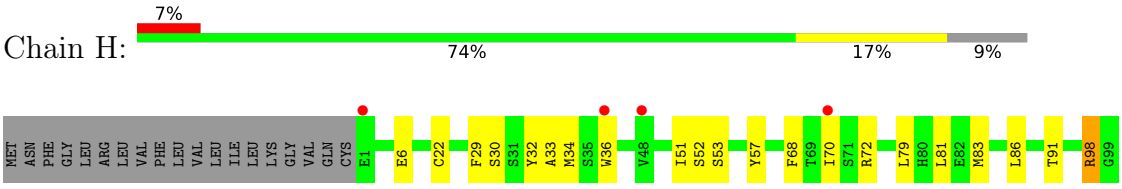
• Molecule 1: Transporter

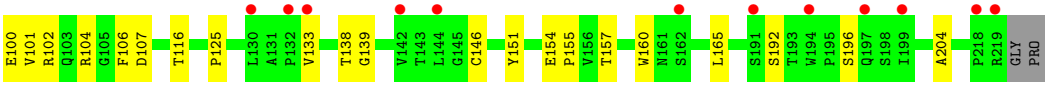


• Molecule 2: Antibody fragment heavy chain-protein, 9D5-heavy chain



• Molecule 3: Antibody fragment light chain-protein, 9D5-light chain





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

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.34Å 140.12Å 165.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.95 48.17 – 2.95	Depositor EDS
% Data completeness (in resolution range)	94.2 (48.17-2.95) 87.0 (48.17-2.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 2.96Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.230 , 0.255 0.232 , 0.262	Depositor DCC
R_{free} test set	2000 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å^2)	75.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 29.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7585	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: CLR, 42J, CL, NA, GLC, BGC

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	0.26	0/4376	0.45	0/5977
2	L	0.29	0/1667	0.45	0/2266
3	H	0.28	0/1658	0.46	0/2264
All	All	0.27	0/7701	0.45	0/10507

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	98	ARG	Peptide

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	4231	0	4156	67	0
2	L	1629	0	1538	25	0
3	H	1619	0	1546	27	0
4	B	23	0	21	0	0
5	A	56	0	92	3	0
6	A	11	0	9	0	0
7	A	1	0	0	0	0
8	A	2	0	0	0	0
9	A	13	0	0	0	0
All	All	7585	0	7362	115	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 8.

All (115) 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)
2:L:151:ILE:HG12	2:L:151:ILE:O	1.75	0.86
1:A:258:ILE:HA	1:A:261:SER:HB3	1.64	0.78
2:L:151:ILE:O	2:L:151:ILE:CG1	2.32	0.78
1:A:420:ASP:N	1:A:420:ASP:OD1	2.22	0.73
2:L:92:PHE:HD2	3:H:102:ARG:HA	1.52	0.72
3:H:138:THR:HG22	3:H:139:GLY:HA3	1.71	0.71
1:A:116:ILE:HG21	1:A:483:ILE:HD13	1.75	0.69
1:A:364:PHE:HA	1:A:367:LEU:HB2	1.74	0.69
1:A:370:MET:HG2	1:A:374:LEU:HD12	1.75	0.69
1:A:27:ARG:NH1	1:A:92:ARG:O	2.26	0.68
1:A:222:GLU:HB3	1:A:225:ARG:HD2	1.76	0.67
1:A:582:THR:O	1:A:589:ARG:NH2	2.28	0.66
1:A:146:THR:HG22	1:A:398:ALA:HB1	1.76	0.66
1:A:508:ARG:NE	3:H:100:GLU:O	2.30	0.65
3:H:157:THR:HB	3:H:204:ALA:HB3	1.79	0.64
1:A:43:PHE:HA	1:A:421:SER:HA	1.80	0.64
3:H:32:TYR:O	3:H:72:ARG:NH2	2.30	0.64
2:L:116:VAL:HG22	2:L:137:LEU:HD22	1.82	0.62
1:A:75:VAL:HB	1:A:526:VAL:HG11	1.81	0.62
1:A:95:ALA:HA	1:A:329:LEU:HD23	1.83	0.61
1:A:513:PHE:HB3	3:H:101:VAL:HG13	1.83	0.61
1:A:40:VAL:HG12	1:A:348:THR:HG21	1.82	0.60
1:A:107:LYS:HD3	1:A:578:LYS:HE3	1.85	0.58
3:H:98:ARG:NH1	3:H:107:ASP:OD2	2.37	0.58
3:H:29:PHE:O	3:H:72:ARG:NH2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:148:LYS:HB3	2:L:196:GLU:HG2	1.86	0.57
2:L:92:PHE:CD2	3:H:102:ARG:HA	2.39	0.56
3:H:34:MET:HB3	3:H:79:LEU:HD22	1.88	0.55
1:A:579:LEU:O	1:A:589:ARG:NH2	2.40	0.55
1:A:38:LEU:HD13	1:A:266:TRP:HA	1.89	0.54
2:L:90:GLN:HG2	2:L:91:GLN:N	2.23	0.54
1:A:340:ASN:HA	1:A:511:ILE:HG22	1.90	0.54
1:A:293:ILE:HD12	1:A:361:PHE:HD1	1.73	0.54
1:A:41:ILE:HD13	1:A:348:THR:HG23	1.89	0.53
1:A:94:GLY:HA3	1:A:432:ALA:HA	1.90	0.53
3:H:51:ILE:HD13	3:H:72:ARG:HB2	1.91	0.53
3:H:52:SER:HB3	3:H:57:TYR:HB2	1.91	0.53
3:H:68:PHE:HB3	3:H:81:LEU:HD11	1.91	0.52
2:L:92:PHE:HZ	3:H:106:PHE:CZ	2.28	0.52
1:A:46:ASP:N	1:A:49:ASN:OD1	2.29	0.52
2:L:92:PHE:CE1	2:L:97:LEU:HD13	2.45	0.51
1:A:251:TYR:CE1	1:A:448:VAL:HG23	2.45	0.51
2:L:124:GLU:OE1	2:L:124:GLU:N	2.40	0.51
1:A:53:PHE:HB3	1:A:54:PRO:HD3	1.93	0.50
1:A:296:TYR:CZ	1:A:360:GLY:HA3	2.46	0.50
2:L:150:LYS:HB2	2:L:194:THR:HB	1.93	0.50
2:L:156:ARG:NH1	2:L:158:ASN:O	2.45	0.50
1:A:252:PHE:HA	1:A:255:TRP:HB2	1.92	0.50
1:A:96:ILE:HG13	1:A:432:ALA:HB1	1.92	0.49
1:A:51:TRP:HH2	1:A:127:ILE:HD13	1.76	0.49
1:A:51:TRP:HA	1:A:388:LEU:HD23	1.92	0.49
1:A:75:VAL:O	1:A:79:PRO:HG2	2.11	0.49
2:L:4:LEU:HB2	2:L:100:GLY:HA2	1.94	0.49
2:L:130:GLY:HA2	2:L:183:THR:HA	1.94	0.49
1:A:303:ALA:HB1	1:A:309:VAL:HG21	1.94	0.49
1:A:47:LEU:HD13	1:A:127:ILE:HG21	1.95	0.49
2:L:190:HIS:O	2:L:212:ARG:HD3	2.12	0.49
1:A:27:ARG:HG2	1:A:92:ARG:HH11	1.78	0.49
1:A:80:LEU:HD11	1:A:527:ALA:HB1	1.94	0.49
1:A:109:ILE:HA	1:A:571:ILE:HG12	1.95	0.49
1:A:71:ILE:O	1:A:75:VAL:HG22	2.12	0.48
1:A:298:THR:HA	1:A:299:PRO:HD3	1.72	0.48
1:A:529:ILE:HG23	1:A:533:PHE:CE2	2.49	0.48
1:A:397:ILE:HG23	1:A:406:TRP:HB2	1.95	0.47
1:A:588:GLN:HA	1:A:591:THR:HG23	1.94	0.47
1:A:105:LEU:HB2	1:A:593:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HD22	1:A:362:VAL:HG21	1.97	0.47
5:A:701:CLR:H211	5:A:701:CLR:H232	1.74	0.47
2:L:168:ASP:OD2	2:L:170:LYS:HG2	2.15	0.46
3:H:192:SER:O	3:H:196:SER:OG	2.32	0.46
1:A:480:GLY:O	1:A:483:ILE:HG22	2.14	0.46
1:A:84:GLU:HB3	1:A:328:LEU:HB2	1.97	0.46
1:A:292:GLY:HA3	1:A:364:PHE:O	2.16	0.46
1:A:247:TYR:CZ	1:A:455:TYR:HB3	2.52	0.45
1:A:294:GLN:O	1:A:298:THR:OG1	2.26	0.45
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.98	0.45
3:H:101:VAL:HB	3:H:104:ARG:HB2	1.99	0.45
1:A:293:ILE:HD12	1:A:361:PHE:CD1	2.52	0.45
1:A:351:ILE:HD13	5:A:701:CLR:H151	2.00	0.45
1:A:115:LEU:HD23	1:A:567:SER:HA	1.99	0.44
3:H:91:THR:HG23	3:H:116:THR:HA	1.98	0.44
1:A:314:ALA:HB1	1:A:534:ILE:HD13	1.99	0.44
1:A:94:GLY:N	1:A:435:ASP:OD2	2.49	0.44
2:L:120:PRO:HD3	3:H:133:VAL:HG12	2.00	0.44
1:A:263:LYS:HD3	1:A:263:LYS:HA	1.85	0.44
2:L:8:PRO:HG2	2:L:11:MET:HB2	2.00	0.43
3:H:36:TRP:HD1	3:H:70:ILE:HD12	1.82	0.43
3:H:33:ALA:N	3:H:100:GLU:OE1	2.51	0.43
1:A:472:HIS:CD2	1:A:547:TYR:HB2	2.53	0.43
2:L:193:TYR:HB2	2:L:210:PHE:CE1	2.54	0.43
1:A:53:PHE:HB2	1:A:316:GLN:HE21	1.83	0.43
1:A:93:LYS:HB3	1:A:97:THR:HB	2.00	0.43
3:H:154:GLU:HG2	3:H:155:PRO:HA	2.01	0.43
2:L:19:VAL:HG13	2:L:79:VAL:HG21	2.01	0.42
1:A:101:ARG:HB3	1:A:597:TRP:HB2	2.01	0.42
3:H:22:CYS:HB3	3:H:79:LEU:HB3	2.02	0.42
1:A:590:PHE:O	1:A:594:THR:N	2.52	0.42
3:H:83:MET:HB3	3:H:86:LEU:HD21	2.01	0.42
5:A:701:CLR:H273	5:A:701:CLR:H231	1.88	0.42
1:A:532:LEU:O	1:A:535:THR:HG22	2.20	0.42
1:A:381:VAL:O	1:A:392:VAL:HG11	2.19	0.42
2:L:156:ARG:HH11	2:L:180:LEU:HD11	1.85	0.42
1:A:342:TYR:CZ	1:A:346:LEU:HD11	2.55	0.41
3:H:146:CYS:HB2	3:H:160:TRP:CH2	2.56	0.41
1:A:33:LYS:HZ3	1:A:339:ASN:CG	2.23	0.41
1:A:43:PHE:CG	1:A:327:VAL:HG11	2.56	0.41
1:A:434:SER:HA	1:A:440:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:185:ASP:HB3	2:L:189:ARG:HH21	1.85	0.41
2:L:120:PRO:HB3	2:L:210:PHE:CE2	2.55	0.41
1:A:522:CYS:HA	1:A:526:VAL:HB	2.03	0.40
2:L:170:LYS:HG3	2:L:171:ASP:H	1.85	0.40
3:H:6:GLU:OE1	3:H:6:GLU:N	2.50	0.40
1:A:29:THR:OG1	1:A:30:TRP:N	2.54	0.40
2:L:168:ASP:OD1	2:L:171:ASP:N	2.51	0.40
3:H:30:SER:O	3:H:53:SER:HB2	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	533/545 (98%)	513 (96%)	20 (4%)	0	100	100
2	L	212/237 (90%)	205 (97%)	7 (3%)	0	100	100
3	H	217/240 (90%)	213 (98%)	4 (2%)	0	100	100
All	All	962/1022 (94%)	931 (97%)	31 (3%)	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	435/450 (97%)	428 (98%)	7 (2%)	62 84
2	L	184/207 (89%)	180 (98%)	4 (2%)	52 79
3	H	175/205 (85%)	174 (99%)	1 (1%)	86 94
All	All	794/862 (92%)	782 (98%)	12 (2%)	65 85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	TRP
1	A	84	GLU
1	A	123	TYR
1	A	308	GLU
1	A	420	ASP
1	A	530	PHE
1	A	590	PHE
2	L	34	LEU
2	L	151	ILE
2	L	168	ASP
2	L	200	LYS
3	H	165	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BGC	B	1	4	12,12,12	0.48	0	17,17,17	0.80	0
4	GLC	B	2	4	11,11,12	0.24	0	15,15,17	1.27	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
4	BGC	B	1	4	-	0/2/22/22	0/1/1/1
4	GLC	B	2	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2	GLC	C1-O5-C5	3.81	117.36	112.19
4	B	2	GLC	O5-C5-C6	2.75	111.52	107.20

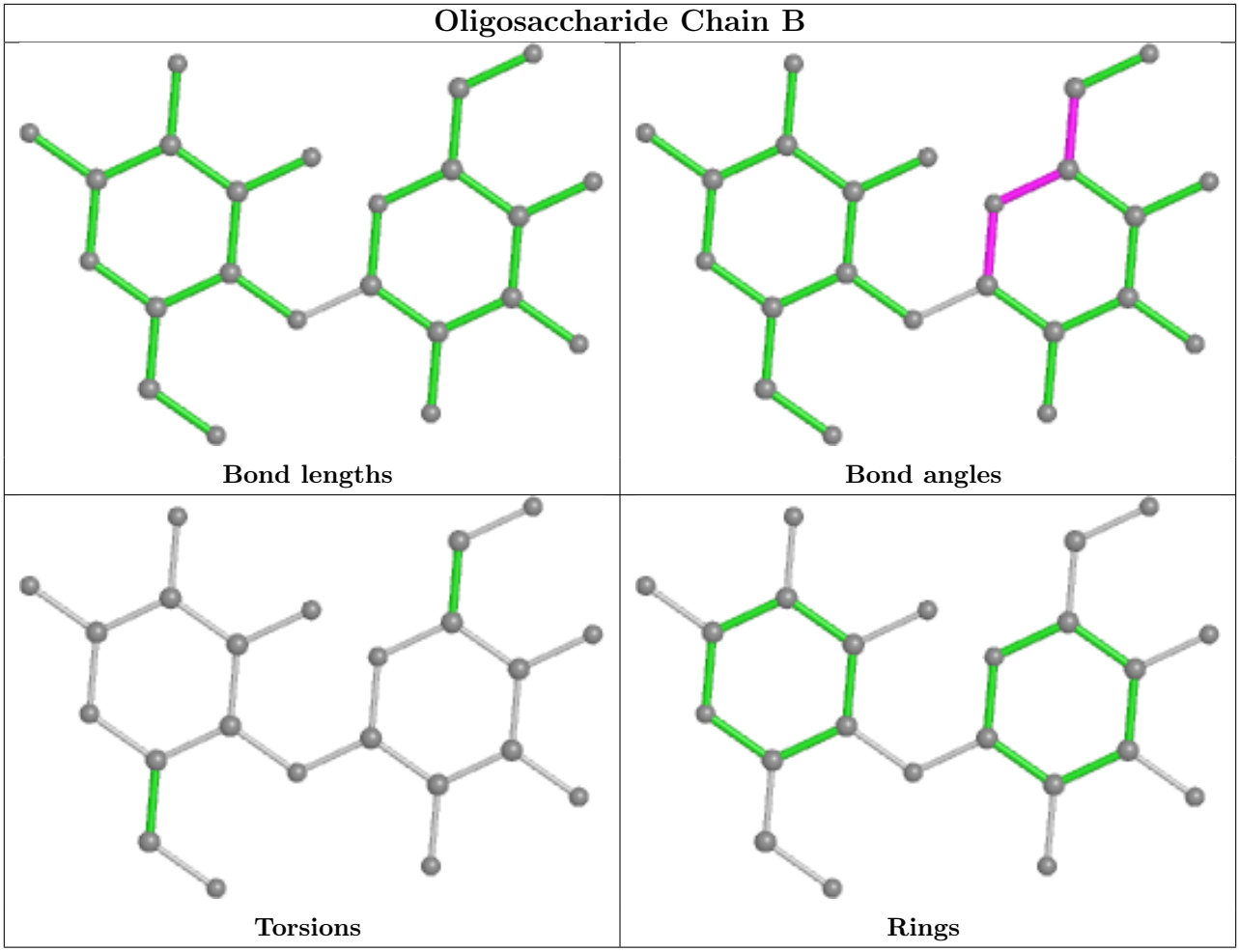
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
6	42J	A	703	-	10,11,11	1.21	2 (20%)	13,14,14	0.62	0
5	CLR	A	702	-	31,31,31	0.65	0	48,48,48	1.09	2 (4%)
5	CLR	A	701	-	31,31,31	0.65	0	48,48,48	1.22	5 (10%)

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
6	42J	A	703	-	-	2/3/3/3	0/1/1/1
5	CLR	A	702	-	-	7/10/68/68	0/4/4/4
5	CLR	A	701	-	-	1/10/68/68	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703	42J	C5-CL	2.72	1.80	1.73
6	A	703	42J	C6-CL1	2.60	1.79	1.73

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	702	CLR	C4-C5-C10	3.55	121.14	116.42
5	A	701	CLR	C4-C5-C10	3.22	120.70	116.42
5	A	701	CLR	C7-C8-C9	2.99	113.33	109.71
5	A	702	CLR	C13-C17-C20	-2.63	115.37	119.49
5	A	701	CLR	C7-C6-C5	-2.39	120.65	125.06
5	A	701	CLR	C14-C8-C9	-2.24	106.09	109.09
5	A	701	CLR	C10-C5-C6	-2.19	119.55	122.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	703	42J	N-C-C1-C2
5	A	702	CLR	C21-C20-C22-C23
5	A	702	CLR	C13-C17-C20-C22
5	A	702	CLR	C17-C20-C22-C23
5	A	702	CLR	C13-C17-C20-C21
5	A	702	CLR	C16-C17-C20-C22
5	A	702	CLR	C16-C17-C20-C21
5	A	702	CLR	C22-C23-C24-C25
5	A	701	CLR	C21-C20-C22-C23
6	A	703	42J	C-C1-C2-C3

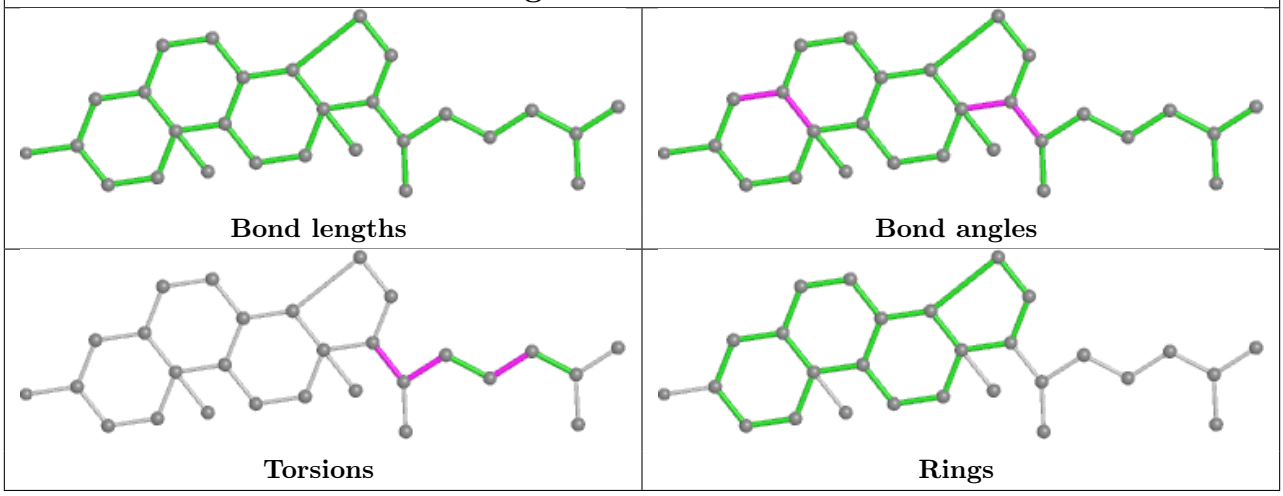
There are no ring outliers.

1 monomer is involved in 3 short contacts:

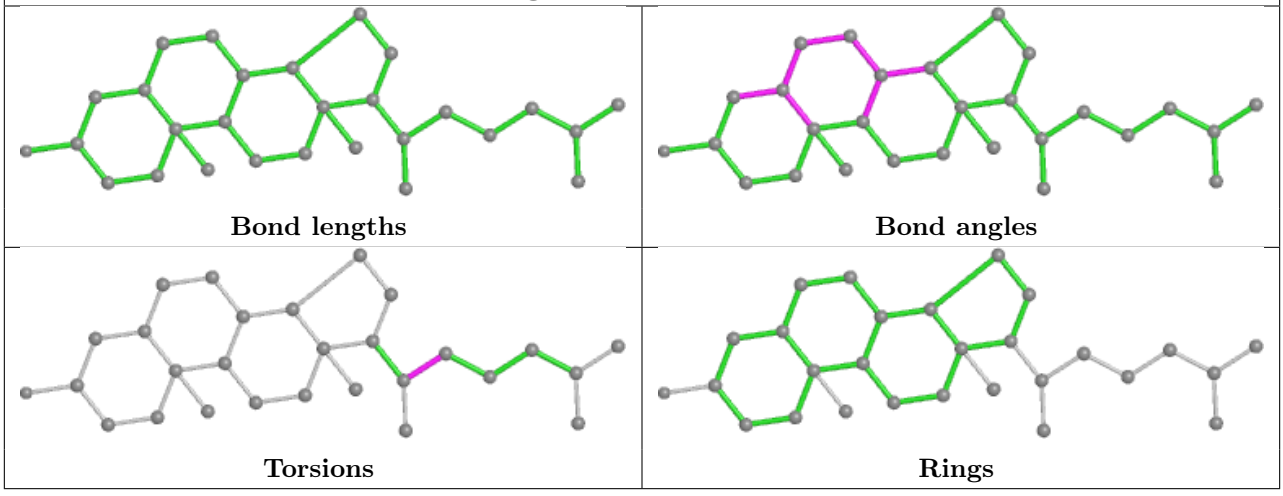
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	CLR	3	0

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 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 702



Ligand CLR A 701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	534/545 (97%)	0.62	49 (9%)	9	5	60, 79, 109, 136	0
2	L	214/237 (90%)	0.51	20 (9%)	8	5	54, 73, 100, 120	0
3	H	219/240 (91%)	0.41	16 (7%)	15	8	58, 74, 109, 146	0
All	All	967/1022 (94%)	0.55	85 (8%)	10	5	54, 77, 107, 146	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	583	PRO	5.4
1	A	582	THR	5.1
3	H	133	VAL	5.1
1	A	537	TYR	4.8
1	A	290	PHE	4.8
2	L	119	PHE	4.5
2	L	149	TRP	4.4
1	A	578	LYS	4.1
2	L	133	VAL	4.1
1	A	255	TRP	3.8
1	A	441	LYS	3.7
2	L	118	ILE	3.6
1	A	481	TYR	3.6
2	L	154	SER	3.5
1	A	105	LEU	3.5
2	L	189	ARG	3.5
2	L	134	VAL	3.4
3	H	142	VAL	3.4
2	L	153	GLY	3.3
3	H	162	SER	3.3
1	A	588	GLN	3.3
1	A	304	ILE	3.3
1	A	287	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	104	PRO	3.2
3	H	144	LEU	3.2
1	A	581	SER	3.2
1	A	438	PRO	3.1
1	A	540	ILE	3.1
2	L	194	THR	3.0
1	A	440	ILE	3.0
1	A	592	ILE	2.9
2	L	120	PRO	2.9
1	A	343	LYS	2.9
3	H	197	GLN	2.8
1	A	252	PHE	2.8
1	A	589	ARG	2.8
2	L	126	LEU	2.8
2	L	180	LEU	2.8
1	A	288	GLY	2.7
2	L	121	PRO	2.7
3	H	199	ILE	2.7
1	A	303	ALA	2.7
3	H	130	LEU	2.6
3	H	219	ARG	2.6
3	H	218	PRO	2.5
1	A	300	ASN	2.5
1	A	587	ARG	2.5
1	A	327	VAL	2.5
1	A	421	SER	2.4
1	A	437	PHE	2.4
1	A	285	THR	2.4
1	A	44	ALA	2.4
1	A	442	ARG	2.4
3	H	48	VAL	2.4
1	A	374	LEU	2.4
1	A	580	LEU	2.3
3	H	1	GLU	2.3
1	A	43	PHE	2.3
2	L	93	SER	2.3
1	A	593	LEU	2.3
1	A	260	THR	2.3
1	A	591	THR	2.3
1	A	422	SER	2.2
3	H	70	ILE	2.2
2	L	136	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	232	LEU	2.2
1	A	513	PHE	2.2
2	L	123	SER	2.2
1	A	326	GLY	2.2
3	H	194	TRP	2.2
1	A	373	THR	2.1
2	L	76	ILE	2.1
3	H	191	SER	2.1
1	A	478	ALA	2.1
1	A	322	GLY	2.1
1	A	291	LEU	2.1
2	L	116	VAL	2.1
1	A	533	PHE	2.1
3	H	36	TRP	2.1
3	H	132	PRO	2.1
2	L	196	GLU	2.0
1	A	213	SER	2.0
1	A	470	PHE	2.0
1	A	342	TYR	2.0
2	L	151	ILE	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)

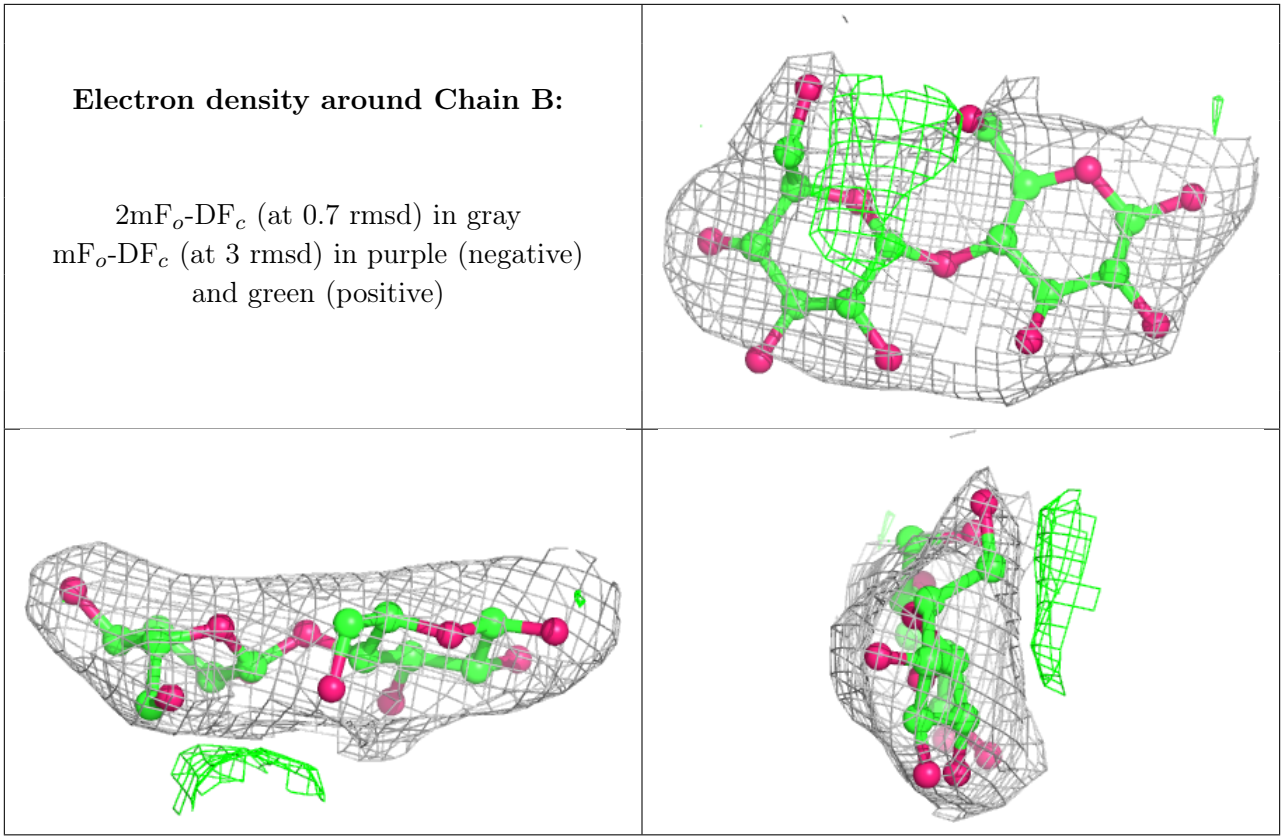
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	BGC	B	1	12/12	0.87	0.15	69,90,94,102	0
4	GLC	B	2	11/12	0.95	0.18	79,88,95,100	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)



6.4 Ligands

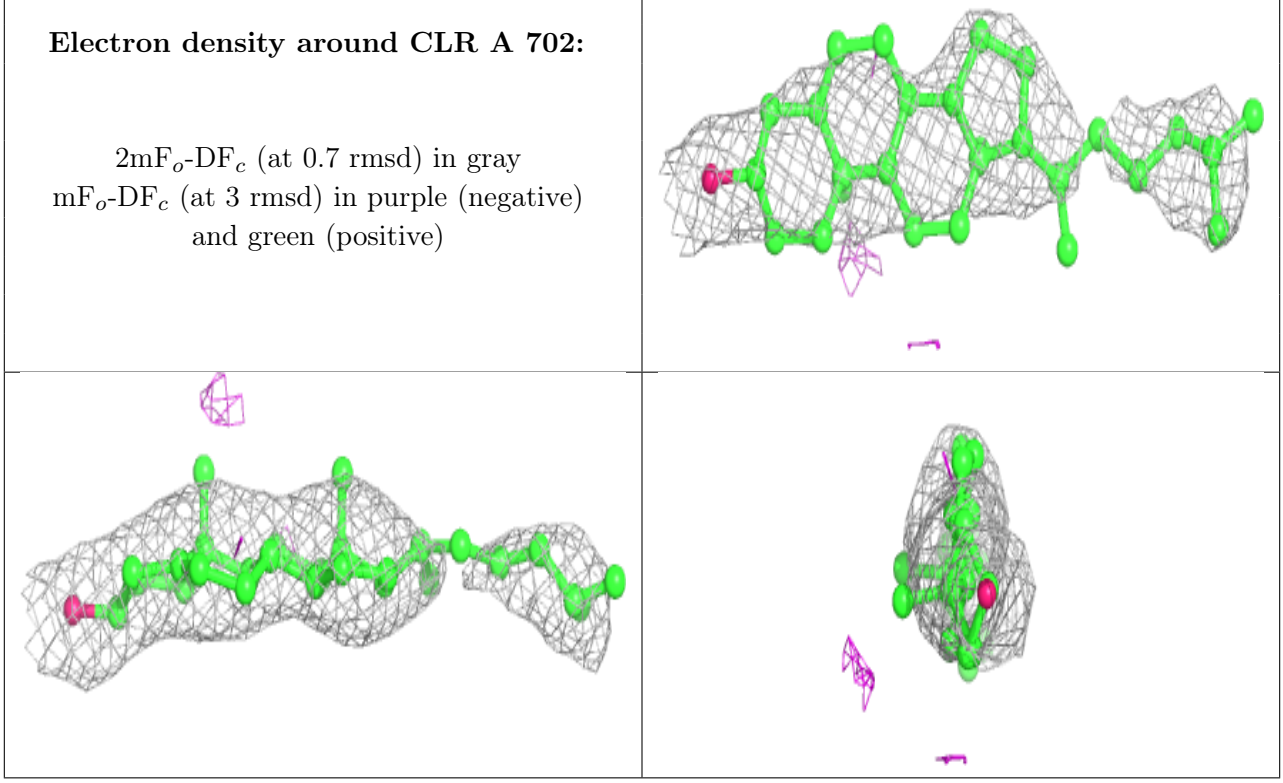
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
8	NA	A	706	1/1	0.63	0.21	86,86,86,86	0
8	NA	A	705	1/1	0.75	0.12	73,73,73,73	0
5	CLR	A	702	28/28	0.86	0.37	79,93,102,104	0
5	CLR	A	701	28/28	0.91	0.59	65,88,99,102	0
6	42J	A	703	11/11	0.91	0.22	65,75,87,90	0
7	CL	A	704	1/1	0.95	0.15	71,71,71,71	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.

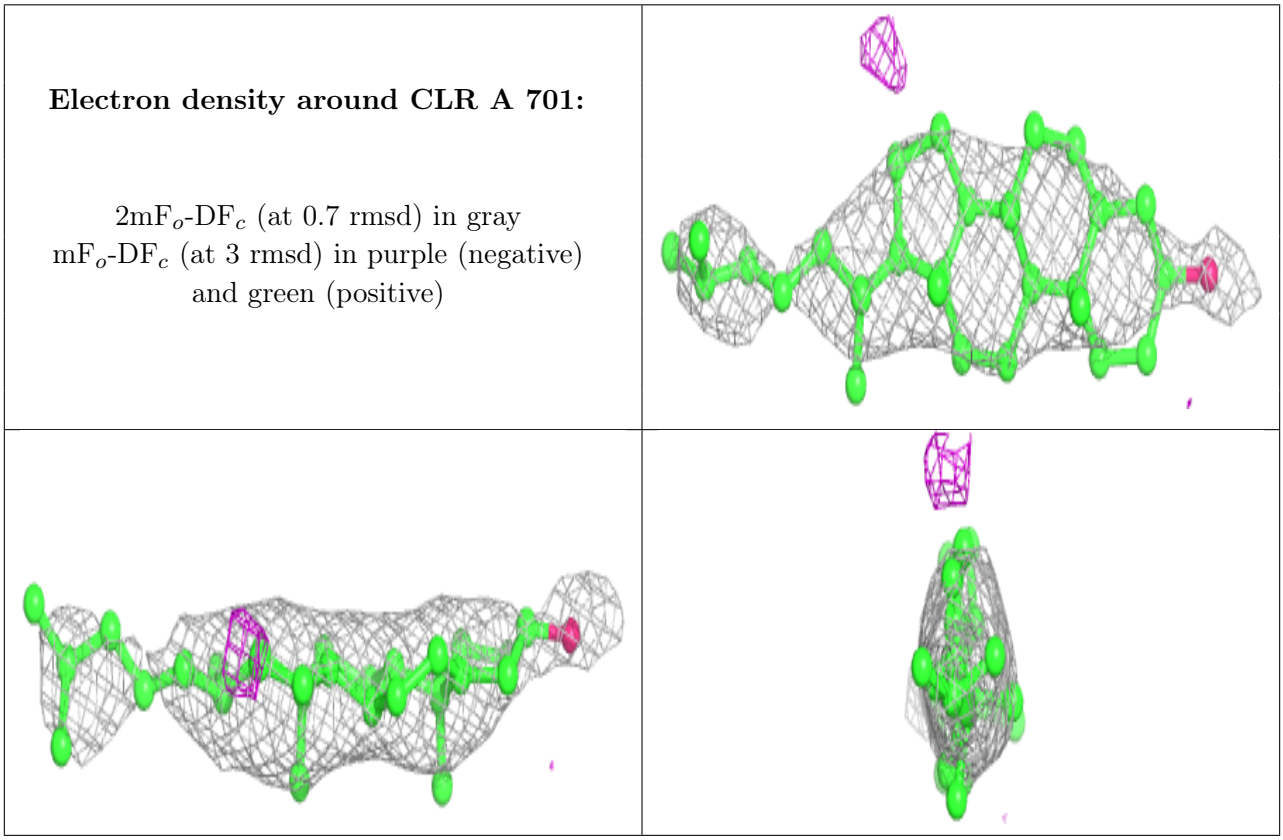
Electron density around CLR A 702:

$2mF_o$-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 701:

$2mF_o$-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.