



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:44 PM UTC

PDB ID : 4XPA / pdb_00004xpa
Title : X-ray structure of Drosophila dopamine transporter bound to 3,4dichlorophenethylamine
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 : 4-5-2 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

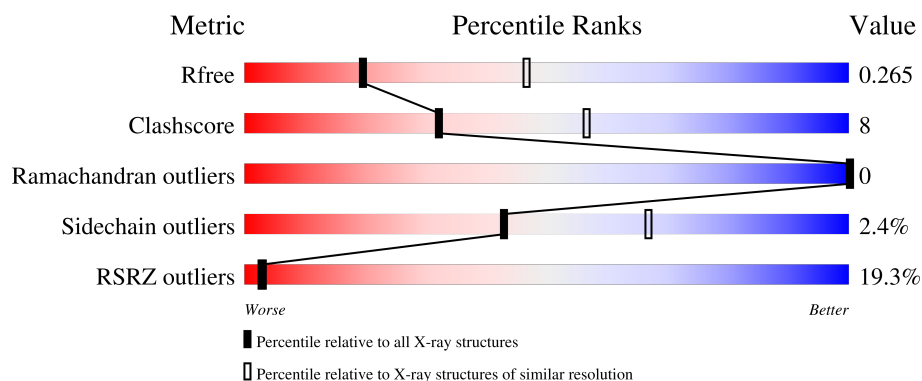
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	545	21% 76% 21% ..
2	L	237	11% 73% 16% • 10%
3	H	240	19% 72% 18% • 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
1	A	534	Total	C	N	O	S	0	1	0
			4231	2836	657	719	19			

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

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

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

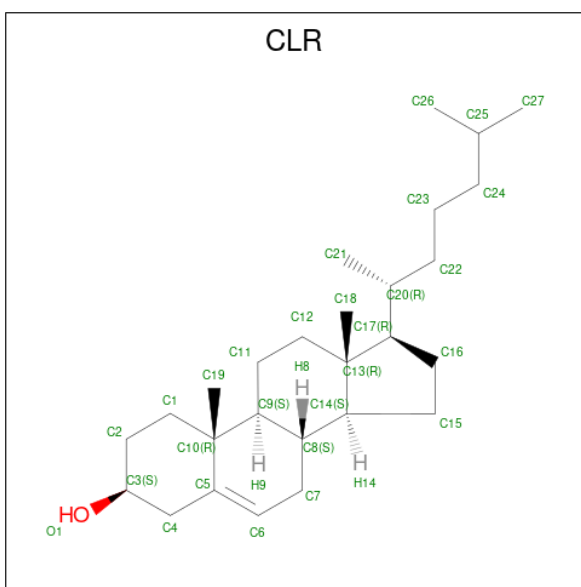
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1619	1019	274	318	8			

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



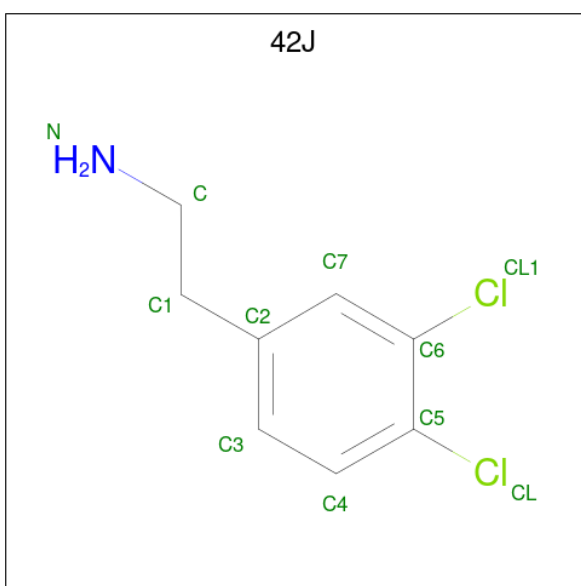
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	B	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



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

- Molecule 6 is 2-(3,4-dichlorophenyl)ethanamine (CCD ID: 42J) (formula: $C_8H_9Cl_2N$).



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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

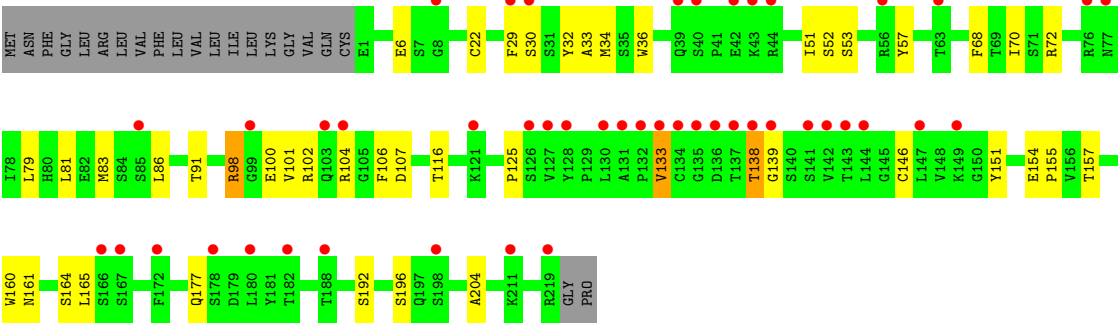
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 9 is water.

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



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



4 Data and refinement statistics

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) 86.9 (48.17-2.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.96Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.230 , 0.255 0.237 , 0.265	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)	0.29 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GLC, 42J, CLR, CL, 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	0.34	0/4376	0.76	1/5977 (0.0%)
2	L	0.35	0/1667	0.74	0/2266
3	H	0.33	0/1658	0.74	0/2264
All	All	0.34	0/7701	0.75	1/10507 (0.0%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	ALA	CB-CA-C	-5.04	110.74	116.54

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	29	0
3	H	1619	0	1546	29	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	120	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 (120) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:51:TRP:C	1:A:51:TRP:CD1	2.96	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
2:L:8:PRO:HD2	2:L:11:MET:HE2	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
2:L:162:ASN:HB3	2:L:176:MET:HE3	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
2:L:161:LEU:HD12	3:H:177:GLN:CD	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:H:161:ASN:O	3:H:164:SER:OG	2.32	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: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
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:95:TYR:HA	2:L:96:PRO:C	2.45	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 ⓘ

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%)	423 (97%)	12 (3%)	38	62
2	L	184/207 (89%)	180 (98%)	4 (2%)	45	69
3	H	175/205 (85%)	172 (98%)	3 (2%)	53	73
All	All	794/862 (92%)	775 (98%)	19 (2%)	43	67

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	GLU
1	A	123	TYR
1	A	236	LYS
1	A	306	LYS
1	A	308	GLU
1	A	317	VAL
1	A	329	LEU
1	A	383	THR
1	A	420	ASP
1	A	530	PHE
1	A	590	PHE
1	A	599	ASP
2	L	3	VAL
2	L	151	ILE
2	L	196	GLU
2	L	200	LYS
3	H	133	VAL
3	H	138	THR
3	H	165	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	150	ASN

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Mol	Chain	Res	Type
1	A	472	HIS
2	L	158	ASN
2	L	162	ASN
2	L	213	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
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	1.17	1 (6%)

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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	GLC	C1-O5-C5	3.86	117.36	112.19

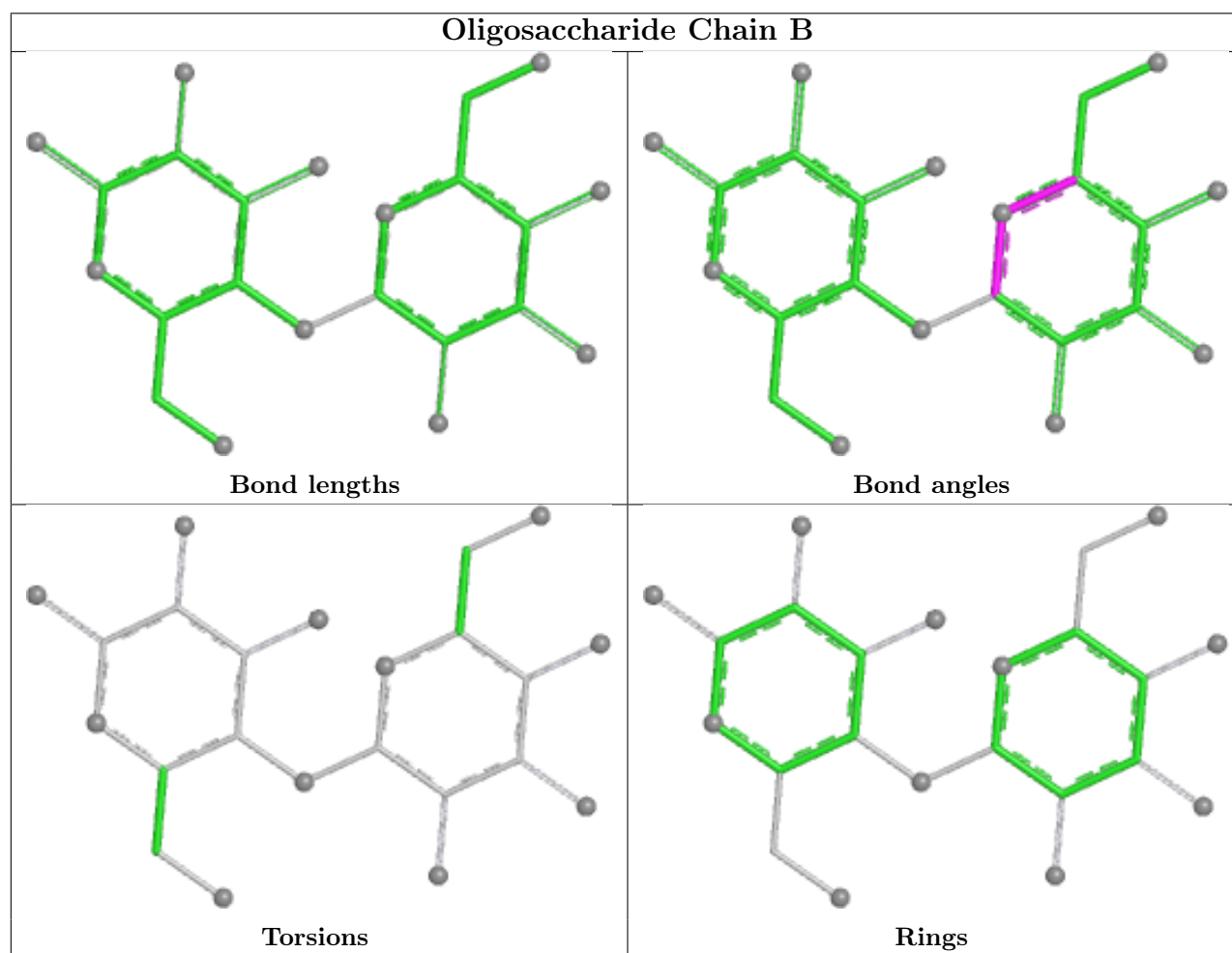
There are no chirality outliers.

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
5	CLR	A	701	-	31,31,31	0.67	0	48,48,48	1.27	6 (12%)
5	CLR	A	702	-	31,31,31	0.67	0	48,48,48	1.12	3 (6%)
6	42J	A	703	-	11,11,11	1.17	2 (18%)	14,14,14	0.66	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLR	A	701	-	-	1/10/68/68	0/4/4/4
5	CLR	A	702	-	-	7/10/68/68	0/4/4/4
6	42J	A	703	-	-	3/3/3/3	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703	42J	C5-CL	2.74	1.80	1.73
6	A	703	42J	C6-CL1	2.61	1.79	1.73

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	702	CLR	C4-C5-C10	3.68	121.14	116.42
5	A	701	CLR	C4-C5-C10	3.34	120.70	116.42
5	A	701	CLR	C7-C8-C9	3.12	113.33	109.72
5	A	702	CLR	C13-C17-C20	-2.67	115.37	119.50
5	A	701	CLR	C7-C6-C5	-2.59	120.65	125.02
5	A	701	CLR	C10-C5-C6	-2.32	119.55	122.93
5	A	701	CLR	C14-C8-C9	-2.29	106.09	109.09
5	A	701	CLR	C13-C14-C8	-2.11	111.42	114.41
5	A	702	CLR	C8-C7-C6	-2.02	109.96	112.76

There are no chirality outliers.

All (11) torsion outliers are listed below:

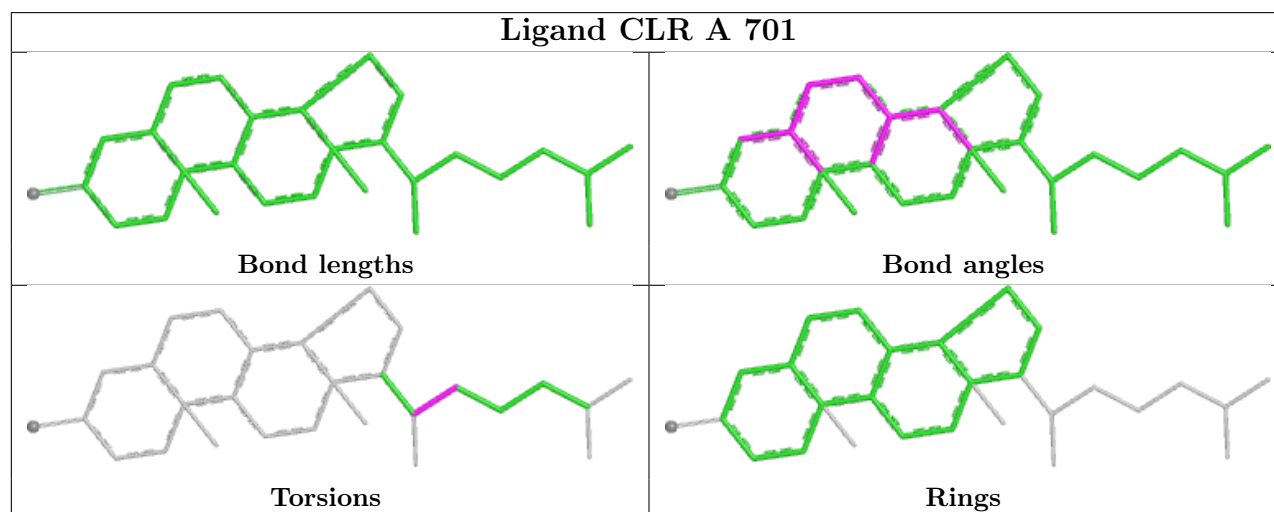
Mol	Chain	Res	Type	Atoms
6	A	703	42J	N-C-C1-C2
5	A	702	CLR	C21-C20-C22-C23
5	A	702	CLR	C13-C17-C20-C22
5	A	702	CLR	C17-C20-C22-C23
5	A	702	CLR	C13-C17-C20-C21
5	A	702	CLR	C16-C17-C20-C21
5	A	702	CLR	C16-C17-C20-C22
5	A	702	CLR	C22-C23-C24-C25
6	A	703	42J	C-C1-C2-C3
5	A	701	CLR	C21-C20-C22-C23
6	A	703	42J	C-C1-C2-C7

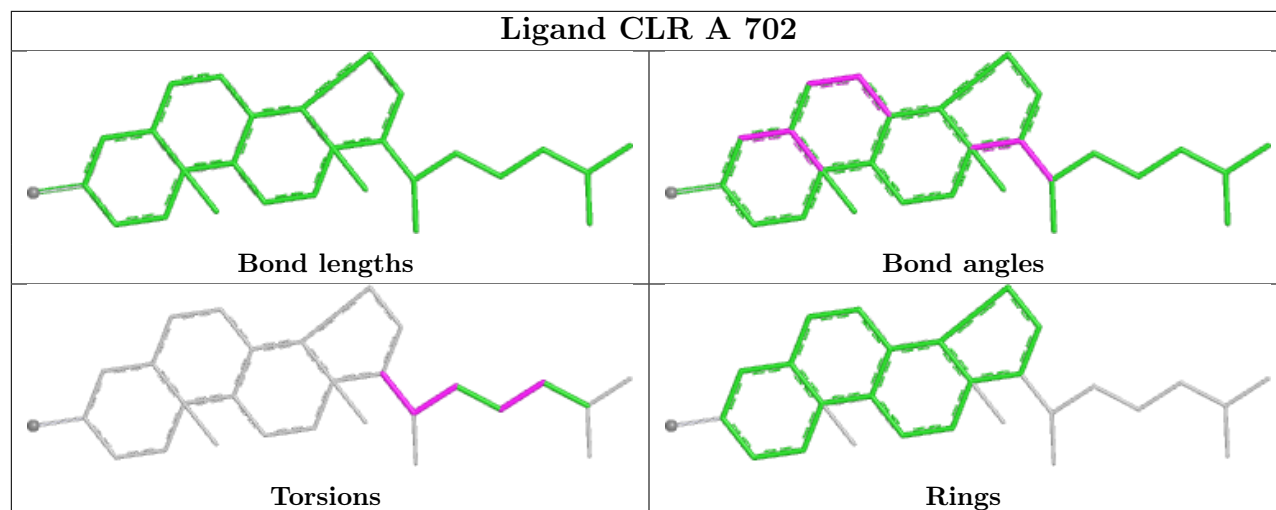
There are no ring outliers.

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 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	534/545 (97%)	1.21	116 (21%) 2 2	51, 79, 109, 136	1 (0%)
2	L	214/237 (90%)	0.79	25 (11%) 9 8	54, 73, 100, 120	0
3	H	219/240 (91%)	1.04	46 (21%) 2 2	58, 74, 109, 146	0
All	All	967/1022 (94%)	1.08	187 (19%) 3 3	51, 77, 107, 146	1 (0%)

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	537	TYR	7.9
1	A	481	TYR	7.1
1	A	480	GLY	6.4
1	A	290	PHE	6.3
1	A	513	PHE	6.1
1	A	123	TYR	6.1
1	A	325	PHE	5.8
1	A	478	ALA	5.7
1	A	586	LEU	5.7
1	A	343	LYS	5.5
1	A	585	SER	5.4
1	A	124	TYR	5.4
1	A	479	ALA	5.3
1	A	72[A]	MET	5.2
2	L	133	VAL	5.1
1	A	599	ASP	5.1
2	L	119	PHE	4.9
1	A	304	ILE	4.8
3	H	137	THR	4.7
2	L	101	SER	4.7
1	A	578	LYS	4.6
2	L	120	PRO	4.5
3	H	133	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	122	PHE	4.3
2	L	121	PRO	4.2
1	A	206	GLU	4.2
3	H	128	TYR	4.2
1	A	68	PRO	4.2
1	A	205	VAL	4.1
1	A	425	GLY	4.1
1	A	592	ILE	4.1
3	H	219	ARG	4.1
1	A	310	TRP	4.0
1	A	590	PHE	4.0
2	L	201	THR	4.0
3	H	44	ARG	4.0
1	A	583	PRO	4.0
1	A	227	GLU	4.0
3	H	166	SER	3.9
1	A	76	GLY	3.9
1	A	204	HIS	3.9
1	A	577	PHE	3.8
3	H	180	LEU	3.8
3	H	39	GLN	3.8
1	A	142	SER	3.7
2	L	154	SER	3.7
1	A	582	THR	3.7
1	A	588	GLN	3.7
1	A	501	ASN	3.7
1	A	534	ILE	3.7
1	A	515	PRO	3.7
1	A	324	GLY	3.7
3	H	149	LYS	3.6
1	A	584	GLY	3.6
2	L	123	SER	3.6
2	L	153	GLY	3.5
1	A	533	PHE	3.5
1	A	119	TYR	3.5
1	A	141	ASN	3.5
3	H	56	ARG	3.5
1	A	540	ILE	3.4
1	A	120	VAL	3.4
3	H	178	SER	3.4
1	A	117	ALA	3.4
3	H	138	THR	3.4

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Mol	Chain	Res	Type	RSRZ
3	H	103	GLN	3.4
2	L	134	VAL	3.4
3	H	43	LYS	3.4
1	A	319	PHE	3.4
3	H	172	PHE	3.4
1	A	476	ARG	3.3
1	A	598	ARG	3.3
1	A	208	PHE	3.3
2	L	149	TRP	3.3
3	H	126	SER	3.3
3	H	136	ASP	3.2
2	L	164	TRP	3.2
1	A	438	PRO	3.2
1	A	268	THR	3.2
1	A	530	PHE	3.2
1	A	455	TYR	3.1
3	H	30	SER	3.1
1	A	69	TYR	3.1
1	A	66	LEU	3.1
2	L	180	LEU	3.1
3	H	104	ARG	3.1
1	A	535	THR	3.0
3	H	135	GLY	2.9
3	H	42	GLU	2.9
1	A	121	ASP	2.9
3	H	211	LYS	2.9
1	A	315	THR	2.9
1	A	63	GLY	2.9
1	A	145	TRP	2.9
2	L	41	SER	2.9
3	H	8	GLY	2.8
1	A	255	TRP	2.8
1	A	296	TYR	2.8
1	A	500	THR	2.8
1	A	340	ASN	2.8
3	H	198	SER	2.8
1	A	371	ALA	2.7
1	A	261	SER	2.7
3	H	147	LEU	2.7
2	L	136	PHE	2.7
1	A	372	HIS	2.7
1	A	71	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	437	PHE	2.6
2	L	9	ALA	2.6
3	H	131	ALA	2.6
3	H	127	VAL	2.6
3	H	143	THR	2.6
3	H	182	THR	2.6
1	A	344	ASP	2.6
1	A	597	TRP	2.5
1	A	82	TYR	2.5
1	A	143	LEU	2.5
1	A	302	SER	2.5
1	A	482	SER	2.5
3	H	142	VAL	2.5
1	A	589	ARG	2.5
1	A	31	SER	2.5
3	H	188	THR	2.5
1	A	441	LYS	2.5
1	A	60	ASN	2.5
1	A	463	CYS	2.4
1	A	39	SER	2.4
2	L	93	SER	2.4
2	L	214	GLU	2.4
2	L	152	ASP	2.4
3	H	141	SER	2.4
1	A	67	VAL	2.4
1	A	574	VAL	2.4
3	H	99	GLY	2.4
2	L	181	THR	2.4
1	A	73	LEU	2.4
2	L	92	PHE	2.3
1	A	543	GLU	2.3
1	A	75	VAL	2.3
1	A	313	ALA	2.3
1	A	140	THR	2.3
3	H	63	THR	2.3
1	A	331	TYR	2.3
1	A	118	PHE	2.3
3	H	29	PHE	2.3
1	A	399	THR	2.3
1	A	502	ARG	2.3
3	H	76	ARG	2.3
1	A	230	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	146	THR	2.2
1	A	70	GLY	2.2
1	A	483	ILE	2.2
2	L	118	ILE	2.2
1	A	591	THR	2.2
3	H	40	SER	2.2
3	H	167	SER	2.2
1	A	115	LEU	2.2
3	H	139	GLY	2.2
1	A	477	TYR	2.2
3	H	85	SER	2.2
3	H	144	LEU	2.2
1	A	307	ALA	2.2
1	A	573	ALA	2.2
3	H	132	PRO	2.1
2	L	203	THR	2.1
3	H	134	CYS	2.1
1	A	252	PHE	2.1
1	A	357	PHE	2.1
3	H	130	LEU	2.1
1	A	496	TRP	2.1
1	A	303	ALA	2.1
2	L	156	ARG	2.1
1	A	576	ILE	2.1
3	H	121	LYS	2.1
1	A	433	LEU	2.1
1	A	77	GLY	2.1
1	A	429	ILE	2.1
1	A	342	TYR	2.1
1	A	54	PRO	2.0
1	A	299	PRO	2.0
3	H	77	ASN	2.0
2	L	130	GLY	2.0
1	A	595	THR	2.0
1	A	269	ALA	2.0
1	A	519	TRP	2.0
1	A	581	SER	2.0
1	A	436	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

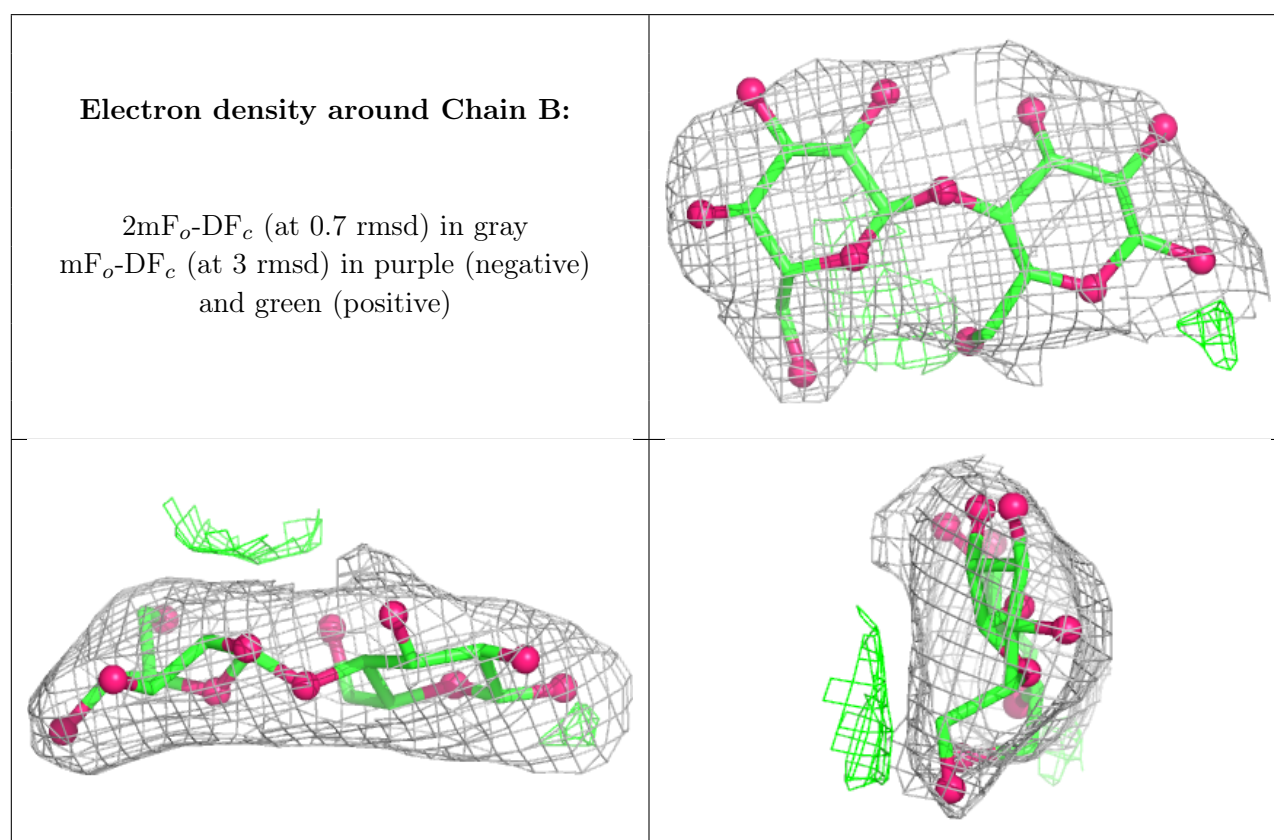
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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	BGC	B	1	12/12	-	-	69,90,94,102	0
4	GLC	B	2	11/12	-	-	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.



6.4 Ligands ⓘ

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

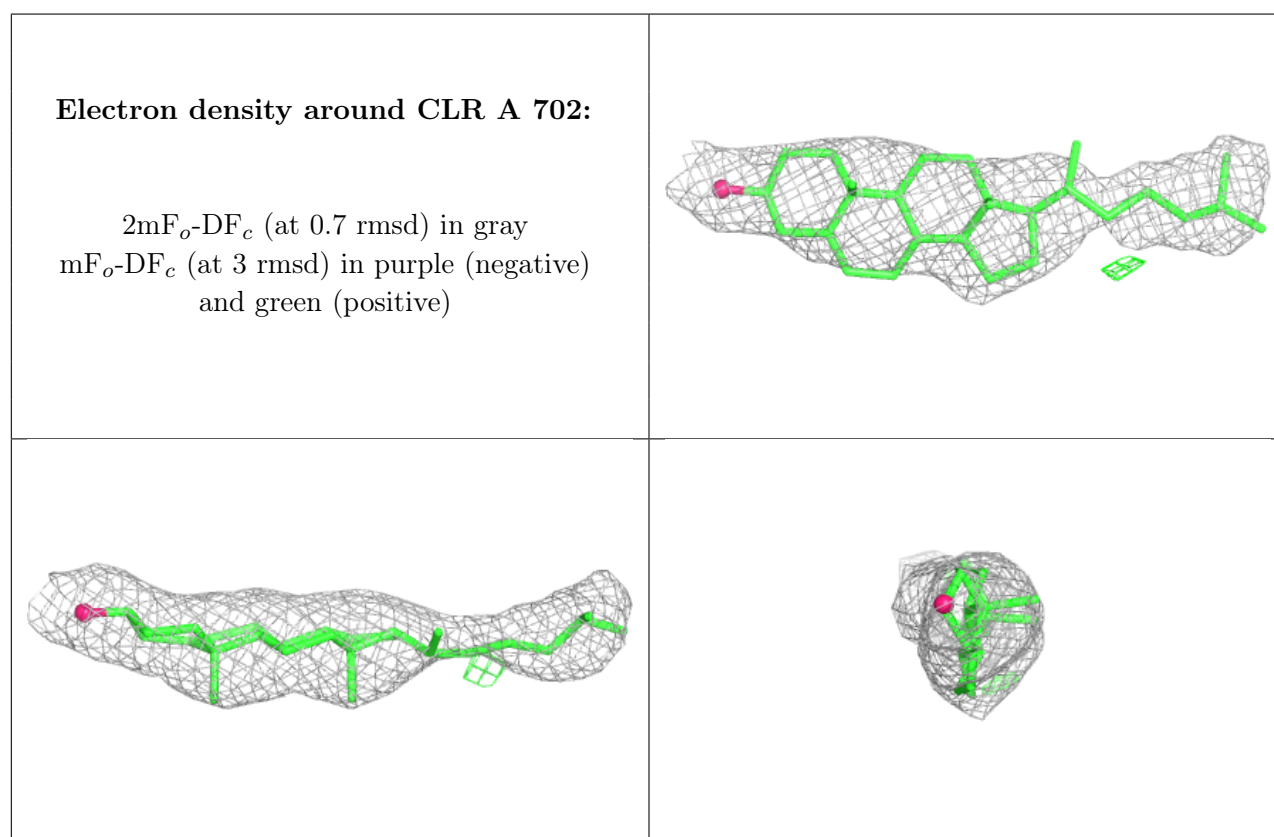
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CLR	A	702	28/28	0.87	0.22	79,93,102,104	0

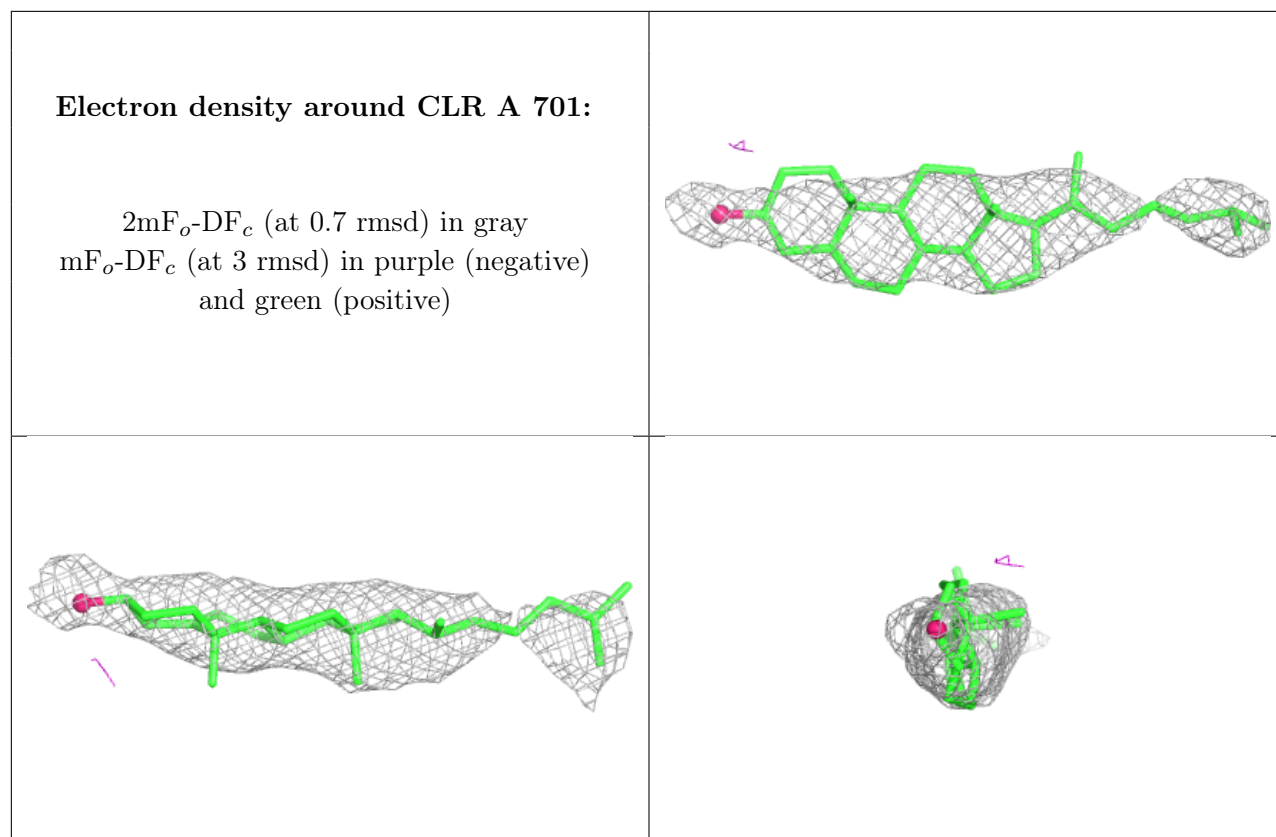
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CL	A	704	1/1	0.89	0.14	71,71,71,71	0
6	42J	A	703	11/11	0.91	0.16	65,75,87,90	0
8	NA	A	706	1/1	0.92	0.08	86,86,86,86	0
5	CLR	A	701	28/28	0.93	0.17	65,88,99,102	0
8	NA	A	705	1/1	0.96	0.08	73,73,73,73	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.