



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:59 AM UTC

PDB ID : 4XPT / pdb_00004xpt
Title : X-ray structure of Drosophila dopamine transporter with subsiteB mutations D121G/S426M and EL2 deletion of 162-201 in complex with substrate analogue 3,4 dichlorophen ethylamine
Authors : Aravind, P.; Wang, K.; Gouaux, E.
Deposited on : 2015-01-17
Resolution : 3.36 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

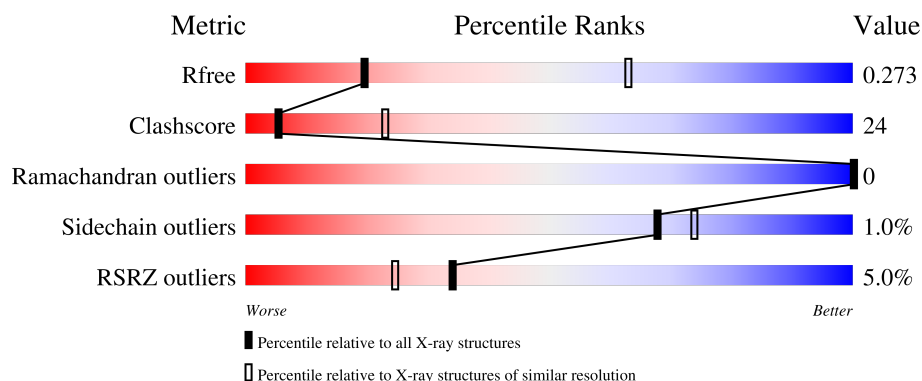
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	535	5% 53% 47% .
2	L	214	7% 65% 33% .
3	H	219	3% 69% 31%
4	B	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	C	2	 50% 50%
4	D	2	 50% 50%
4	E	2	 50% 50%
4	F	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GLC	B	2	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7685 atoms, of which 14 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 Dopamine transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	2	0
			4216	2826	657	713	20			

There are 44 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	415	ALA	LEU	engineered mutation	UNP Q7K4Y6
A	426	MET	SER	engineered mutation	UNP Q7K4Y6

- Molecule 2 is a protein called antibody fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1626	1011	271	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
			1623	1022	275	318	8			

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



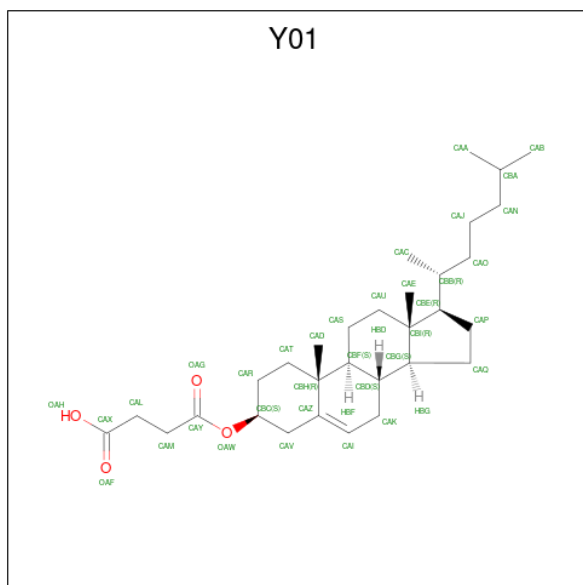
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	B	2	Total	C	O	0	0	0
			23	12	11			
4	C	2	Total	C	O	0	0	0
			23	12	11			

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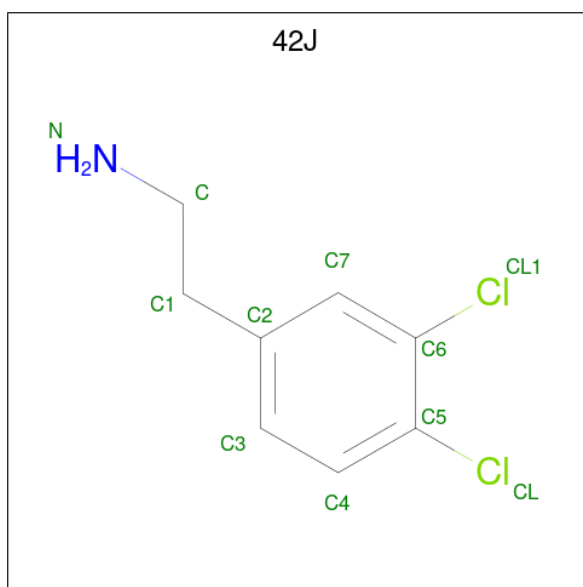
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	D	2	Total C O 23 12 11	0	0	0
4	E	2	Total C O 23 12 11	0	0	0
4	F	2	Total C O 23 12 11	0	0	0

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



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

- Molecule 6 is 2-(3,4-dichlorophenyl)ethanamine (CCD ID: 42J) (formula: $\text{C}_8\text{H}_9\text{Cl}_2\text{N}$).



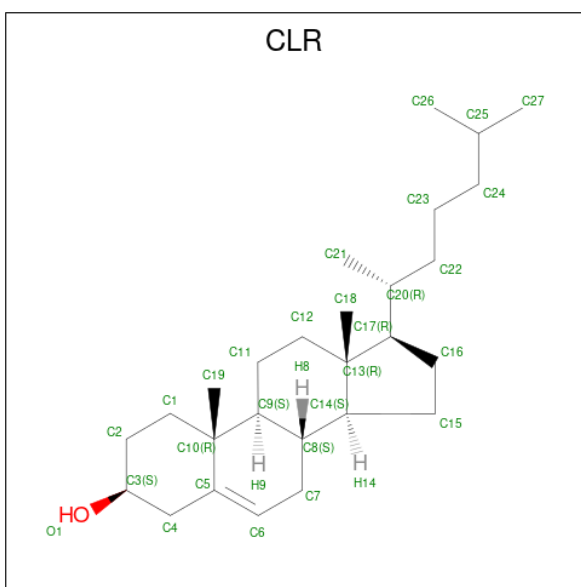
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	0	0
			11	8	2	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	
			28	8	14	1	5	0

- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



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

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

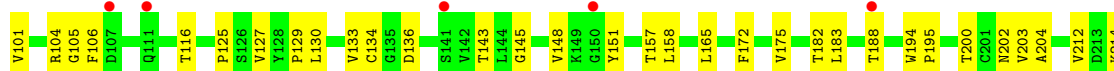
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		

- Molecule 10 is SODIUM ION (CCD ID: NA) (formula: Na).

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



- Molecule 3: antibody fragment heavy chain



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



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



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



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



- 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	96.61Å 139.15Å 166.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.60 – 3.36 38.60 – 3.36	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.60-3.36) 98.8 (38.60-3.36)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.232 , 0.273 0.236 , 0.273	Depositor DCC
R_{free} test set	1644 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	114.7	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7685	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, 42J, CLR, NAG, CL, Y01, NA, 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	0/4360	0.73	1/5958 (0.0%)
2	L	0.24	0/1664	0.67	0/2262
3	H	0.25	0/1662	0.72	1/2268 (0.0%)
All	All	0.25	0/7686	0.72	2/10488 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	136	ASP	CB-CA-C	-5.76	109.39	117.23
1	A	548	ALA	CB-CA-C	-5.22	110.53	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4216	0	4128	220	0
2	L	1626	0	1536	73	0
3	H	1623	0	1557	60	0
4	B	23	0	21	6	0
4	C	23	0	21	4	0
4	D	23	0	21	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	23	0	21	4	0
4	F	23	0	21	2	0
5	A	35	0	49	5	0
6	A	11	0	9	0	0
7	A	14	14	13	0	0
8	A	28	0	46	6	0
9	A	1	0	0	0	0
10	A	2	0	0	0	0
All	All	7671	14	7443	361	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 24.

All (361) 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)
4:C:1:BGC:H3	4:C:2:GLC:H3	1.34	1.10
4:B:1:BGC:H3	4:B:2:GLC:H3	1.25	1.10
1:A:204:HIS:HB2	1:A:205:VAL:HA	1.36	1.07
1:A:202:VAL:HG21	3:H:42:GLU:HG2	1.37	1.05
4:B:1:BGC:H3	4:B:2:GLC:C3	1.98	0.94
1:A:570:MET:HE2	1:A:570:MET:HA	1.53	0.90
3:H:51:ILE:HD13	3:H:72:ARG:HB2	1.51	0.90
2:L:197:ALA:HB3	2:L:206:ILE:HB	1.54	0.90
1:A:370:MET:HG2	1:A:374:LEU:HD12	1.56	0.86
4:C:1:BGC:H3	4:C:2:GLC:C3	2.06	0.85
1:A:258:ILE:HA	1:A:261:SER:HB3	1.61	0.83
1:A:204:HIS:HB2	1:A:205:VAL:CA	2.12	0.79
2:L:148:LYS:N	2:L:196:GLU:OE1	2.13	0.79
3:H:130:LEU:HD12	3:H:145:GLY:HA3	1.65	0.78
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.66	0.77
2:L:92:PHE:CE2	3:H:105:GLY:HA2	2.21	0.75
1:A:95:ALA:HA	1:A:329:LEU:HD23	1.69	0.74
1:A:251:TYR:HE1	1:A:448:VAL:HG23	1.51	0.74
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.69	0.74
1:A:205:VAL:HB	1:A:206:GLU:CA	2.18	0.74
1:A:80:LEU:HD13	1:A:487:VAL:HG11	1.70	0.73
2:L:107:MET:HE2	2:L:107:MET:HA	1.69	0.73
3:H:129:PRO:HD3	3:H:214:LYS:HE3	1.71	0.73
1:A:597:TRP:CD1	1:A:598[A]:ARG:HG2	2.24	0.73
1:A:205:VAL:HB	1:A:206:GLU:CB	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:HG12	1:A:571:ILE:HD12	1.71	0.71
1:A:597:TRP:HD1	1:A:598[A]:ARG:HG2	1.54	0.71
1:A:205:VAL:CB	1:A:206:GLU:HA	2.20	0.70
1:A:115:LEU:HD11	1:A:567:SER:HB3	1.73	0.70
1:A:367:LEU:HA	1:A:370:MET:HE2	1.74	0.70
8:A:609:CLR:H183	8:A:609:CLR:H212	1.74	0.69
3:H:127:VAL:HG12	3:H:148:VAL:HG22	1.73	0.69
1:A:116:ILE:HG21	1:A:483:ILE:HD11	1.73	0.69
1:A:364:PHE:HA	1:A:367:LEU:HB2	1.76	0.68
2:L:214:GLU:HG2	3:H:134:CYS:HB2	1.74	0.68
3:H:165:LEU:H	3:H:165:LEU:HD23	1.58	0.68
1:A:72[A]:MET:HG2	1:A:314:ALA:HA	1.74	0.67
1:A:263:LYS:HA	1:A:266:TRP:CD1	2.30	0.67
2:L:196:GLU:HG2	2:L:197:ALA:N	2.09	0.67
1:A:113:VAL:HG23	1:A:324:GLY:O	1.93	0.66
1:A:72[B]:MET:HE2	1:A:310:TRP:CE3	2.30	0.66
1:A:340:ASN:HA	1:A:511:ILE:HG22	1.78	0.66
1:A:598[A]:ARG:HH11	1:A:598[A]:ARG:HA	1.61	0.65
4:C:1:BGC:H3	4:C:2:GLC:C2	2.23	0.65
1:A:43:PHE:HA	1:A:421:SER:HA	1.79	0.65
2:L:143:LYS:H	2:L:143:LYS:HD2	1.61	0.65
1:A:72[B]:MET:HE2	1:A:310:TRP:HE3	1.61	0.64
1:A:507:ILE:HD12	1:A:515:PRO:CG	2.27	0.64
2:L:162:ASN:HB3	2:L:176:MET:HE2	1.80	0.64
1:A:146:THR:HG22	1:A:398:ALA:HB1	1.79	0.63
4:C:1:BGC:C3	4:C:2:GLC:H3	2.22	0.63
1:A:71:ILE:O	1:A:75:VAL:HG22	1.99	0.63
1:A:251:TYR:CE1	1:A:448:VAL:HG23	2.33	0.63
1:A:370:MET:SD	1:A:396:ALA:HB2	2.39	0.63
1:A:481:TYR:CE2	1:A:538:GLY:HA3	2.34	0.63
4:D:1:BGC:O6	4:D:1:BGC:O1	2.14	0.63
3:H:40:SER:HB2	3:H:41:PRO:HD2	1.81	0.62
1:A:51:TRP:HH2	1:A:127:ILE:HD13	1.63	0.62
1:A:571:ILE:HB	1:A:572:PRO:HD3	1.82	0.62
2:L:34:LEU:HD13	2:L:72:TYR:CD1	2.35	0.62
1:A:78:ILE:HB	1:A:79:PRO:HD3	1.82	0.61
1:A:318:PHE:O	1:A:323:PRO:HD2	2.00	0.61
1:A:134:PHE:HB3	1:A:411:PHE:CE2	2.36	0.61
1:A:80:LEU:HD13	1:A:487:VAL:CG1	2.31	0.61
1:A:158:ARG:HG3	1:A:202:VAL:HG11	1.83	0.61
1:A:434:SER:HB3	1:A:441:LYS:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:91:THR:HG23	3:H:116:THR:HA	1.82	0.60
1:A:219:TYR:O	1:A:222:GLU:HG3	2.02	0.60
1:A:206:GLU:CB	2:L:9:ALA:HB1	2.32	0.60
1:A:507:ILE:HD12	1:A:515:PRO:HG3	1.83	0.59
1:A:599:ASP:OD1	1:A:599:ASP:N	2.35	0.59
1:A:480:GLY:C	1:A:482:SER:H	2.11	0.59
2:L:188:GLU:O	2:L:212:ARG:NH2	2.35	0.59
1:A:351:ILE:HD13	8:A:609:CLR:H72	1.85	0.59
4:E:1:BGC:O6	4:E:1:BGC:O1	2.17	0.59
1:A:155:PRO:HG3	2:L:163:SER:HA	1.84	0.58
1:A:62:GLY:HA2	1:A:296:TYR:O	2.03	0.58
1:A:293:ILE:HD12	1:A:361:PHE:HD1	1.68	0.58
2:L:214:GLU:CG	3:H:134:CYS:HB2	2.32	0.58
1:A:94:GLY:N	1:A:435:ASP:OD2	2.36	0.58
3:H:51:ILE:HG13	3:H:58:ILE:CD1	2.32	0.58
4:B:1:BGC:C3	4:B:2:GLC:H3	2.16	0.58
2:L:124:GLU:OE1	2:L:124:GLU:N	2.36	0.58
1:A:105:LEU:HB2	1:A:593:LEU:HB3	1.86	0.58
4:D:1:BGC:HA	4:D:1:BGC:H6	1.48	0.58
1:A:40:VAL:HG12	1:A:348:THR:HG21	1.84	0.57
1:A:155:PRO:HG3	2:L:162:ASN:O	2.05	0.57
1:A:304:ILE:HD11	1:A:310:TRP:CZ2	2.38	0.57
1:A:351:ILE:CD1	8:A:609:CLR:H72	2.34	0.57
1:A:53:PHE:HB3	1:A:54:PRO:HD3	1.87	0.57
1:A:296:TYR:CZ	1:A:360:GLY:HA3	2.40	0.57
1:A:589:ARG:O	1:A:593:LEU:HG	2.04	0.57
1:A:75:VAL:HB	1:A:526:VAL:HG11	1.87	0.57
2:L:185:ASP:O	2:L:189:ARG:HG3	2.04	0.57
1:A:571:ILE:HB	1:A:572:PRO:CD	2.36	0.56
1:A:121:GLY:O	1:A:125:ASN:ND2	2.37	0.56
1:A:260:THR:O	1:A:264:VAL:HG23	2.06	0.56
1:A:271:PHE:HB3	1:A:272:PRO:HD3	1.88	0.56
2:L:167:GLN:HA	2:L:174:TYR:CE1	2.41	0.56
4:E:1:BGC:H3	4:E:2:GLC:O5	2.04	0.56
1:A:75:VAL:O	1:A:79:PRO:HG2	2.05	0.55
1:A:596:PRO:HD2	1:A:599:ASP:HB2	1.88	0.55
2:L:199:HIS:ND1	2:L:201:THR:HG23	2.21	0.55
3:H:101:VAL:HB	3:H:104:ARG:HG2	1.87	0.55
1:A:145:TRP:HB2	1:A:212:ALA:HA	1.88	0.55
1:A:312:ASP:HA	1:A:315:THR:HG22	1.89	0.55
1:A:420:ASP:N	1:A:420:ASP:OD1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ILE:HD11	1:A:528:PRO:HB3	1.89	0.55
1:A:393:TYR:HB3	1:A:394:PRO:HD3	1.88	0.55
1:A:263:LYS:HA	1:A:266:TRP:HD1	1.69	0.55
1:A:308:GLU:O	1:A:311:VAL:HG12	2.06	0.55
2:L:193:TYR:HB2	2:L:210:PHE:CE1	2.41	0.55
1:A:47:LEU:HD13	1:A:127:ILE:HG21	1.88	0.55
1:A:51:TRP:CH2	1:A:127:ILE:HD13	2.42	0.55
3:H:51:ILE:CD1	3:H:72:ARG:HB2	2.31	0.55
1:A:99:TRP:CZ2	1:A:490:GLU:HG2	2.42	0.54
1:A:378:ILE:HA	1:A:381:VAL:CG2	2.37	0.54
1:A:75:VAL:HG23	1:A:76:GLY:N	2.22	0.54
1:A:522:CYS:HA	1:A:526:VAL:HB	1.89	0.54
1:A:553:PRO:HB2	1:A:555:TRP:CD1	2.43	0.54
4:B:1:BGC:H3	4:B:2:GLC:C2	2.35	0.54
1:A:41:ILE:HD11	1:A:348:THR:HA	1.89	0.54
1:A:33:LYS:NZ	1:A:344:ASP:OD2	2.41	0.54
1:A:588:GLN:O	1:A:592:ILE:HG12	2.08	0.54
1:A:427:GLU:OE2	1:A:431:THR:OG1	2.25	0.54
1:A:498:TYR:CE2	1:A:502:ARG:HG2	2.43	0.54
2:L:62:ARG:HD2	2:L:83:ASP:OD2	2.07	0.54
3:H:30:SER:O	3:H:53:SER:HB2	2.08	0.54
1:A:591:THR:O	1:A:595:THR:HG23	2.08	0.54
1:A:245:ILE:O	1:A:249:ILE:HG13	2.08	0.53
1:A:115:LEU:CD1	1:A:567:SER:HB3	2.37	0.53
1:A:393:TYR:CE2	1:A:397:ILE:HD11	2.44	0.53
2:L:8:PRO:CG	2:L:11:MET:HE2	2.39	0.53
2:L:49:ILE:HG12	2:L:55:LEU:HD23	1.90	0.53
1:A:546:THR:HG22	1:A:551:VAL:HG13	1.91	0.53
2:L:161:LEU:HD13	3:H:182:THR:HB	1.91	0.53
1:A:295:TYR:CE1	1:A:378:ILE:HG21	2.44	0.53
4:B:1:BGC:O2	4:B:2:GLC:O5	2.18	0.53
1:A:134:PHE:HB3	1:A:411:PHE:CD2	2.43	0.52
1:A:378:ILE:HA	1:A:381:VAL:HG22	1.90	0.52
3:H:32:TYR:O	3:H:72:ARG:NH2	2.36	0.52
3:H:68:PHE:CE1	3:H:83:MET:HB3	2.44	0.52
1:A:49:ASN:ND2	1:A:356:SER:OG	2.43	0.52
4:E:2:GLC:O6	4:E:2:GLC:O3	2.23	0.52
1:A:73:LEU:HA	1:A:317:VAL:HG11	1.90	0.52
1:A:143:LEU:HD13	1:A:145:TRP:CZ2	2.44	0.52
1:A:297:LEU:HD11	1:A:361:PHE:CZ	2.45	0.52
1:A:580:LEU:HA	1:A:589:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:VAL:HB	1:A:206:GLU:HA	1.83	0.51
5:A:601:Y01:HAU2	5:A:601:Y01:HAC1	1.91	0.51
1:A:72[A]:MET:HG2	1:A:314:ALA:CA	2.40	0.51
1:A:489:PHE:CD2	1:A:571:ILE:HG21	2.45	0.51
2:L:188:GLU:HA	2:L:212:ARG:NH1	2.25	0.51
2:L:214:GLU:OE2	3:H:133:VAL:HB	2.10	0.51
3:H:157:THR:HB	3:H:204:ALA:HB3	1.92	0.51
1:A:202:VAL:HG21	3:H:42:GLU:CG	2.26	0.51
1:A:393:TYR:CD2	1:A:397:ILE:HD11	2.46	0.51
1:A:54:PRO:HB3	1:A:360:GLY:HA2	1.93	0.51
1:A:115:LEU:HD11	1:A:567:SER:CB	2.41	0.51
1:A:123:TYR:O	1:A:126:VAL:HG12	2.10	0.51
2:L:196:GLU:OE2	2:L:198:THR:OG1	2.21	0.51
1:A:481:TYR:HE2	1:A:538:GLY:HA3	1.76	0.51
3:H:48:VAL:HG13	3:H:64:VAL:HG21	1.91	0.51
1:A:268:THR:OG1	1:A:420:ASP:HB3	2.11	0.50
1:A:524:ARG:HG2	1:A:525:PHE:CD1	2.46	0.50
1:A:572:PRO:O	1:A:576:ILE:HG12	2.10	0.50
1:A:41:ILE:HD13	1:A:348:THR:HG23	1.93	0.50
1:A:545:LEU:HG	1:A:552:TYR:CD1	2.45	0.50
1:A:481:TYR:CD1	4:F:2:GLC:H2	2.46	0.50
1:A:387:GLY:O	1:A:391:VAL:HB	2.12	0.50
2:L:143:LYS:H	2:L:143:LYS:CD	2.21	0.50
1:A:161:GLU:HB2	1:A:376:VAL:HG21	1.93	0.50
1:A:517:ARG:O	1:A:521:VAL:HG23	2.12	0.50
1:A:444:ARG:O	1:A:448:VAL:HG22	2.12	0.50
3:H:158:LEU:HA	3:H:202:ASN:O	2.12	0.50
3:H:183:LEU:C	3:H:183:LEU:HD23	2.37	0.50
2:L:90:GLN:CD	2:L:92:PHE:HE1	2.20	0.49
2:L:12:SER:HA	2:L:106:GLU:O	2.11	0.49
1:A:342:TYR:CZ	1:A:346:LEU:HD11	2.47	0.49
1:A:507:ILE:HD12	1:A:515:PRO:HG2	1.94	0.49
3:H:34:MET:SD	3:H:98:ARG:HB3	2.53	0.49
2:L:188:GLU:HA	2:L:212:ARG:CZ	2.43	0.49
1:A:236:LYS:NZ	1:A:236:LYS:HB3	2.28	0.49
2:L:188:GLU:HG2	2:L:212:ARG:HH12	1.78	0.49
1:A:158:ARG:HB3	1:A:159:PRO:HD2	1.94	0.49
3:H:125:PRO:CB	3:H:151:TYR:HB3	2.42	0.49
2:L:116:VAL:HG21	2:L:197:ALA:HB2	1.94	0.48
2:L:192:SER:HB3	2:L:211:ASN:ND2	2.28	0.48
2:L:120:PRO:HB3	2:L:210:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2:GLC:H2	4:B:2:GLC:H62	1.95	0.48
1:A:160:PHE:O	1:A:161:GLU:HG2	2.14	0.48
1:A:236:LYS:NZ	1:A:238:ASP:OD1	2.46	0.48
3:H:143:THR:OG1	3:H:188:THR:HG22	2.13	0.48
2:L:148:LYS:HB2	2:L:148:LYS:HE2	1.50	0.48
2:L:4:LEU:HB2	2:L:100:GLY:HA2	1.96	0.48
2:L:3:VAL:HG22	2:L:26:SER:HB3	1.95	0.48
1:A:88:GLY:O	1:A:333:SER:HA	2.14	0.48
1:A:519:TRP:CH2	5:A:601:Y01:HAI	2.49	0.48
1:A:109:ILE:O	1:A:113:VAL:HG12	2.14	0.48
1:A:87:LEU:HD11	1:A:494:VAL:HG21	1.96	0.48
1:A:241:LEU:O	1:A:245:ILE:HG13	2.14	0.48
1:A:354:ALA:O	1:A:358:ILE:HG12	2.14	0.48
2:L:165:THR:HG23	3:H:172:PHE:CD2	2.49	0.48
3:H:44:ARG:O	3:H:44:ARG:HG3	2.14	0.48
4:D:1:BGC:H3	4:D:2:GLC:O5	2.14	0.48
1:A:63:GLY:HA2	1:A:66:LEU:HG	1.96	0.47
1:A:72[A]:MET:HE2	1:A:314:ALA:HB1	1.94	0.47
1:A:115:LEU:HD11	1:A:567:SER:CA	2.44	0.47
1:A:282:ARG:O	1:A:286:LEU:HG	2.13	0.47
1:A:75:VAL:HG23	1:A:76:GLY:H	1.79	0.47
1:A:67:VAL:HB	1:A:68:PRO:CD	2.45	0.47
1:A:155:PRO:HG2	2:L:164:TRP:H	1.79	0.47
1:A:204:HIS:NE2	1:A:209:GLN:OE1	2.47	0.47
1:A:209:GLN:HB2	1:A:214:GLU:HG3	1.96	0.47
1:A:511:ILE:HD12	1:A:513:PHE:CZ	2.49	0.47
1:A:205:VAL:HG12	1:A:206:GLU:HA	1.96	0.47
1:A:363:ILE:O	1:A:367:LEU:HD13	2.15	0.47
1:A:420:ASP:HA	1:A:423:PHE:CD2	2.50	0.47
2:L:38:GLN:HG3	2:L:87:TYR:CE2	2.50	0.47
2:L:40:LYS:NZ	2:L:82:GLU:O	2.46	0.47
2:L:116:VAL:O	2:L:208:LYS:HE3	2.14	0.47
2:L:137:LEU:HD12	2:L:137:LEU:N	2.29	0.47
3:H:127:VAL:CG2	3:H:212:VAL:HG11	2.45	0.47
1:A:133:ARG:HH12	1:A:137:ALA:HB2	1.79	0.47
1:A:151:ILE:HG22	2:L:160:VAL:HG21	1.97	0.47
1:A:244:LEU:HB2	1:A:456:PHE:CE1	2.50	0.47
3:H:29:PHE:O	3:H:72:ARG:NH2	2.46	0.47
3:H:98:ARG:O	3:H:98:ARG:HG3	2.13	0.47
1:A:370:MET:O	1:A:376:VAL:HG12	2.15	0.47
1:A:565:GLY:O	1:A:569:VAL:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:125:PRO:HB3	3:H:151:TYR:CB	2.41	0.47
1:A:67:VAL:HB	1:A:68:PRO:HD3	1.96	0.46
1:A:575:ALA:O	1:A:579:LEU:HB2	2.15	0.46
5:A:601:Y01:HAE2	5:A:601:Y01:HBB	1.66	0.46
8:A:609:CLR:C21	8:A:609:CLR:H121	2.45	0.46
1:A:210:SER:H	1:A:213:SER:HB3	1.79	0.46
1:A:271:PHE:CE2	1:A:412:MET:HG3	2.50	0.46
3:H:22:CYS:HB3	3:H:79:LEU:HB3	1.96	0.46
3:H:129:PRO:CD	3:H:214:LYS:HE3	2.43	0.46
1:A:109:ILE:HG12	1:A:571:ILE:CD1	2.41	0.46
1:A:579:LEU:HA	1:A:593:LEU:HD11	1.96	0.46
1:A:133:ARG:NH1	1:A:137:ALA:HB2	2.30	0.46
1:A:298:THR:HA	1:A:299:PRO:HD3	1.69	0.46
1:A:251:TYR:OH	1:A:449:ALA:HB2	2.15	0.46
2:L:188:GLU:HG2	2:L:212:ARG:NH1	2.31	0.46
1:A:69:TYR:HA	1:A:313:ALA:HB1	1.97	0.46
1:A:84:GLU:OE2	1:A:324:GLY:N	2.42	0.46
1:A:272:PRO:HA	1:A:413:MET:HG3	1.96	0.46
3:H:216:ILE:N	3:H:216:ILE:HD12	2.30	0.46
1:A:53:PHE:CD2	1:A:356:SER:HB3	2.51	0.46
1:A:327:VAL:HG22	1:A:424:GLY:O	2.16	0.46
3:H:72:ARG:HD3	3:H:74:ASN:HD21	1.81	0.46
3:H:87:ARG:NE	3:H:89:GLU:OE2	2.42	0.45
1:A:112:ALA:O	1:A:116:ILE:HG13	2.17	0.45
1:A:33:LYS:NZ	1:A:339:ASN:OD1	2.38	0.45
1:A:96:ILE:HG13	1:A:432:ALA:HB1	1.98	0.45
2:L:24:ARG:HA	2:L:70:THR:O	2.15	0.45
1:A:378:ILE:HD12	1:A:381:VAL:CG2	2.46	0.45
3:H:127:VAL:CG1	3:H:203:VAL:HG21	2.47	0.45
1:A:38:LEU:HD21	8:A:609:CLR:C19	2.47	0.45
1:A:587:ARG:O	1:A:591:THR:HG23	2.17	0.45
2:L:143:LYS:HE3	2:L:143:LYS:HB3	1.56	0.45
3:H:35:SER:OG	3:H:50:GLU:HG3	2.17	0.45
1:A:426:MET:HE2	1:A:426:MET:HA	1.98	0.45
2:L:161:LEU:C	2:L:161:LEU:HD23	2.41	0.45
1:A:205:VAL:CG1	1:A:206:GLU:HA	2.46	0.44
1:A:282:ARG:HD2	1:A:406:TRP:CZ2	2.52	0.44
1:A:393:TYR:O	1:A:397:ILE:HG13	2.18	0.44
1:A:482:SER:O	1:A:485:VAL:HG22	2.18	0.44
3:H:200:THR:HA	3:H:215:LYS:HA	1.99	0.44
1:A:202:VAL:CG2	3:H:42:GLU:HG2	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:167:GLN:HB2	2:L:174:TYR:OH	2.16	0.44
2:L:123:SER:O	2:L:127:THR:HG23	2.18	0.44
1:A:570:MET:HA	1:A:570:MET:CE	2.35	0.44
3:H:194:TRP:CG	3:H:195:PRO:HA	2.53	0.44
1:A:553:PRO:HG2	1:A:556:ALA:HB2	1.98	0.44
1:A:590:PHE:O	1:A:594:THR:HG23	2.18	0.44
4:D:2:GLC:HO6	4:D:2:GLC:C3	2.29	0.44
8:A:609:CLR:H212	8:A:609:CLR:H121	1.98	0.44
2:L:74:LEU:C	2:L:74:LEU:HD23	2.43	0.44
3:H:6:GLU:OE1	3:H:6:GLU:N	2.48	0.44
1:A:294:GLN:O	1:A:298:THR:OG1	2.28	0.44
1:A:559:LEU:O	1:A:563:ILE:HG13	2.19	0.43
2:L:95:TYR:HA	2:L:96:PRO:C	2.42	0.43
3:H:60:TYR:CE1	3:H:70:ILE:HG22	2.53	0.43
3:H:98:ARG:HA	3:H:99:GLY:HA3	1.63	0.43
1:A:252:PHE:HA	1:A:255:TRP:HB2	1.99	0.43
2:L:196:GLU:HA	2:L:206:ILE:O	2.17	0.43
3:H:52:SER:HB2	3:H:57:TYR:HB2	2.00	0.43
4:F:1:BGC:O2	4:F:2:GLC:O5	2.32	0.43
2:L:34:LEU:HD13	2:L:72:TYR:CG	2.54	0.43
1:A:123:TYR:CE2	1:A:475:ASP:HA	2.54	0.43
1:A:123:TYR:HB3	1:A:474:LEU:HD12	2.01	0.43
1:A:497:ILE:N	1:A:497:ILE:HD12	2.34	0.43
5:A:601:Y01:HAP1	5:A:601:Y01:HAO1	1.67	0.43
1:A:89:GLN:HA	1:A:332:ALA:O	2.19	0.43
1:A:330:ALA:O	1:A:333:SER:OG	2.23	0.43
2:L:161:LEU:HD11	3:H:175:VAL:HB	1.99	0.43
1:A:292:GLY:HA3	1:A:364:PHE:O	2.19	0.43
2:L:121:PRO:HG2	2:L:187:TYR:CE1	2.54	0.43
1:A:489:PHE:CE2	1:A:571:ILE:HG21	2.53	0.43
2:L:139:ASN:N	2:L:174:TYR:O	2.51	0.43
1:A:242:CYS:O	1:A:246:VAL:HG23	2.18	0.42
1:A:144:PRO:HB2	1:A:215:TYR:CE1	2.54	0.42
1:A:378:ILE:HD12	1:A:381:VAL:HG23	2.01	0.42
2:L:141:TYR:CG	2:L:142:PRO:HA	2.54	0.42
4:E:1:BGC:H3	4:E:2:GLC:H62	2.01	0.42
1:A:73:LEU:O	1:A:78:ILE:HG13	2.18	0.42
1:A:156:ASN:HB3	1:A:208:PHE:CD2	2.54	0.42
1:A:104:PRO:HD2	1:A:593:LEU:O	2.19	0.42
2:L:197:ALA:N	2:L:206:ILE:O	2.49	0.42
1:A:52:ARG:O	1:A:55:TYR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:TYR:HB2	1:A:364:PHE:CZ	2.55	0.42
1:A:275:VAL:HG13	1:A:409:ILE:HD12	2.02	0.42
2:L:199:HIS:CE1	2:L:201:THR:HG23	2.55	0.42
1:A:327:VAL:HG22	1:A:428:ALA:HB2	2.02	0.42
1:A:534:ILE:HG13	1:A:535:THR:N	2.33	0.42
3:H:158:LEU:C	3:H:158:LEU:HD23	2.44	0.42
1:A:157:CYS:HB2	1:A:214:GLU:OE1	2.20	0.42
1:A:532:LEU:O	1:A:535:THR:HG22	2.20	0.42
1:A:565:GLY:O	1:A:569:VAL:HG22	2.19	0.42
1:A:412:MET:O	1:A:416:THR:HG23	2.20	0.42
3:H:127:VAL:HG11	3:H:203:VAL:HG21	2.02	0.42
1:A:370:MET:HE1	1:A:392:VAL:CG1	2.50	0.41
2:L:122:SER:CB	3:H:129:PRO:HD2	2.50	0.41
3:H:127:VAL:HG21	3:H:212:VAL:HG11	2.01	0.41
2:L:47:LEU:HB2	3:H:106:PHE:O	2.20	0.41
2:L:137:LEU:HD13	2:L:176:MET:HG2	2.02	0.41
1:A:493:ALA:HA	1:A:497:ILE:HD13	2.02	0.41
1:A:135:PHE:O	1:A:138:SER:HB2	2.21	0.41
1:A:303:ALA:O	1:A:309:VAL:HG21	2.20	0.41
1:A:580:LEU:HA	1:A:589:ARG:NH2	2.33	0.41
2:L:195:CYS:SG	2:L:196:GLU:N	2.94	0.41
3:H:129:PRO:HB3	3:H:214:LYS:HZ3	1.85	0.41
3:H:165:LEU:HG	3:H:165:LEU:O	2.19	0.41
1:A:109:ILE:HA	1:A:571:ILE:CD1	2.51	0.41
1:A:474:LEU:O	1:A:478:ALA:HB3	2.21	0.41
1:A:502:ARG:NH2	1:A:599:ASP:OD2	2.53	0.41
3:H:51:ILE:HG12	3:H:55:GLY:HA2	2.02	0.41
1:A:65:PHE:C	1:A:68:PRO:HD2	2.45	0.41
2:L:137:LEU:HD22	2:L:145:ILE:HD13	2.01	0.41
3:H:2:VAL:HG13	3:H:27:PHE:CD1	2.56	0.41
3:H:34:MET:HB3	3:H:79:LEU:HD22	2.02	0.41
1:A:115:LEU:HD11	1:A:567:SER:HA	2.03	0.41
1:A:203:GLY:HA3	1:A:204:HIS:HA	1.84	0.41
1:A:322:GLY:N	1:A:323:PRO:CD	2.84	0.41
1:A:492:ILE:O	1:A:496:TRP:HB2	2.21	0.41
1:A:524:ARG:HG2	1:A:525:PHE:CE1	2.55	0.41
2:L:148:LYS:HD3	2:L:196:GLU:CD	2.46	0.41
2:L:164:TRP:CH2	2:L:176:MET:HE1	2.56	0.41
1:A:488:PHE:CE1	1:A:532:LEU:HB2	2.56	0.41
2:L:92:PHE:HE2	3:H:105:GLY:HA2	1.78	0.40
2:L:125:GLN:HG2	2:L:130:GLY:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:107:MET:HE2	2:L:107:MET:CA	2.44	0.40
1:A:377:ARG:HB2	1:A:380:ASP:OD2	2.21	0.40
1:A:422:SER:O	1:A:426:MET:HG2	2.22	0.40
5:A:601:Y01:HAS2	5:A:601:Y01:HAE1	1.92	0.40
2:L:13:THR:C	2:L:108:LYS:HG2	2.46	0.40
2:L:24:ARG:HH21	2:L:71:SER:CB	2.35	0.40
2:L:52:THR:HG23	2:L:72:TYR:HD2	1.85	0.40
1:A:306:LYS:O	1:A:309:VAL:HG22	2.22	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	535/535 (100%)	511 (96%)	24 (4%)	0	100	100
2	L	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
3	H	217/219 (99%)	213 (98%)	4 (2%)	0	100	100
All	All	964/968 (100%)	928 (96%)	36 (4%)	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	429/439 (98%)	424 (99%)	5 (1%)	63	72
2	L	183/187 (98%)	179 (98%)	4 (2%)	45	63
3	H	176/187 (94%)	176 (100%)	0	100	100
All	All	788/813 (97%)	779 (99%)	9 (1%)	68	73

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	VAL
1	A	236	LYS
1	A	598[A]	ARG
1	A	598[B]	ARG
1	A	599	ASP
2	L	143	LYS
2	L	148	LYS
2	L	196	GLU
2	L	214	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	150	ASN
1	A	224	ASN
1	A	352	ASN
1	A	443	ASN
1	A	520	GLN
2	L	162	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

10 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	0.49	0	17,17,17	0.74	0
4	GLC	B	2	4	11,11,12	0.48	0	15,15,17	1.00	1 (6%)
4	BGC	C	1	4	12,12,12	0.51	0	17,17,17	0.75	1 (5%)
4	GLC	C	2	4	11,11,12	0.39	0	15,15,17	0.73	0
4	BGC	D	1	4	12,12,12	0.53	0	17,17,17	1.00	2 (11%)
4	GLC	D	2	4	11,11,12	0.31	0	15,15,17	0.80	0
4	BGC	E	1	4	12,12,12	0.57	0	17,17,17	1.05	1 (5%)
4	GLC	E	2	4	11,11,12	0.32	0	15,15,17	0.76	0
4	BGC	F	1	4	12,12,12	0.55	0	17,17,17	1.14	1 (5%)
4	GLC	F	2	4	11,11,12	0.26	0	15,15,17	0.39	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
4	BGC	B	1	4	-	2/2/22/22	0/1/1/1
4	GLC	B	2	4	-	2/2/19/22	0/1/1/1
4	BGC	C	1	4	-	1/2/22/22	0/1/1/1
4	GLC	C	2	4	-	2/2/19/22	0/1/1/1
4	BGC	D	1	4	-	2/2/22/22	0/1/1/1
4	GLC	D	2	4	-	0/2/19/22	0/1/1/1
4	BGC	E	1	4	-	0/2/22/22	0/1/1/1
4	GLC	E	2	4	-	0/2/19/22	0/1/1/1
4	BGC	F	1	4	-	1/2/22/22	0/1/1/1
4	GLC	F	2	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	BGC	O5-C5-C6	2.34	112.24	106.44
4	D	1	BGC	C1-O5-C5	2.31	118.12	113.65
4	B	2	GLC	C1-C2-C3	2.31	113.00	109.64
4	F	1	BGC	C4-C3-C2	2.16	114.62	110.83
4	E	1	BGC	O5-C5-C6	2.01	111.41	106.44
4	C	1	BGC	O4-C4-C3	2.00	115.09	110.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

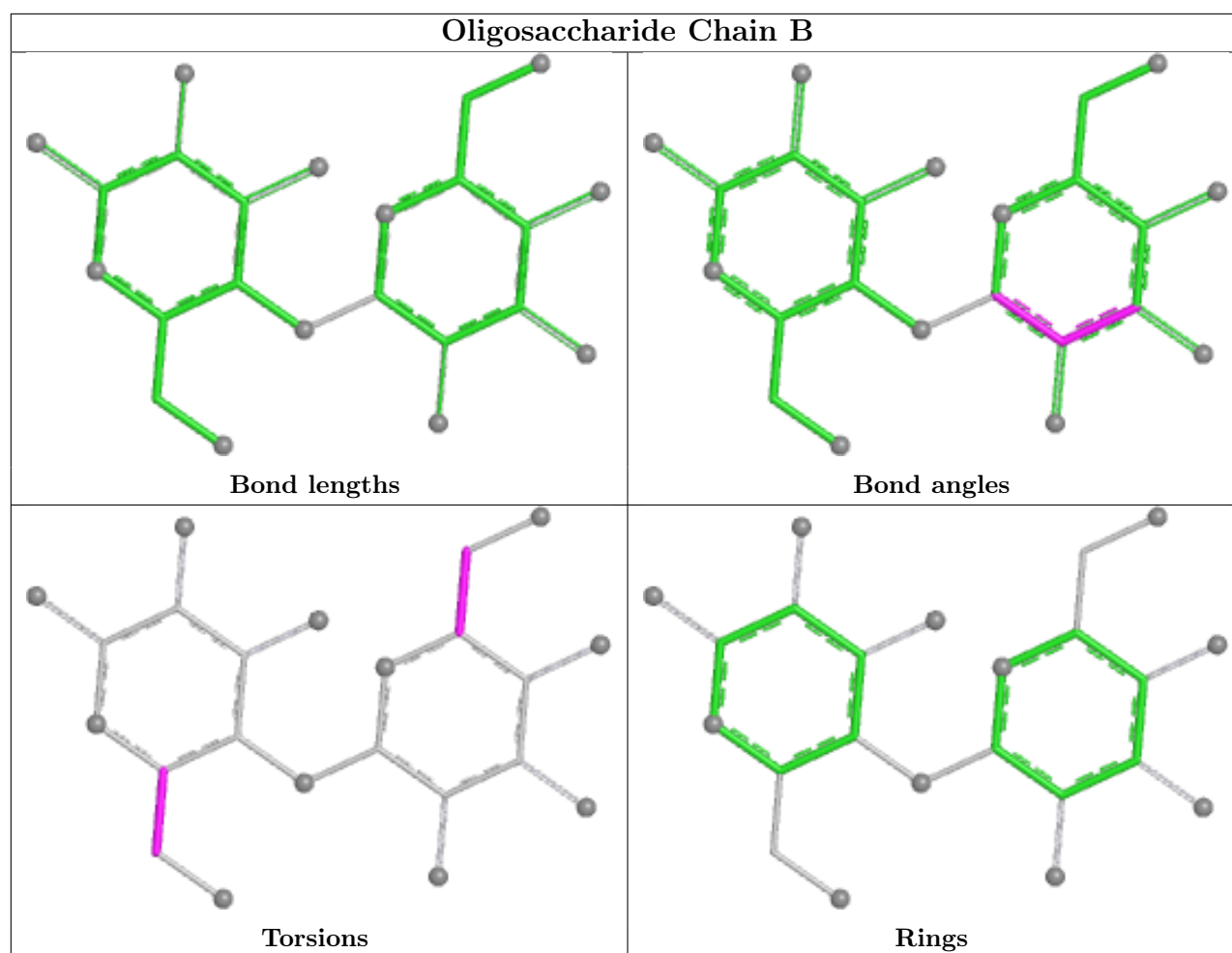
Mol	Chain	Res	Type	Atoms
4	C	2	GLC	C4-C5-C6-O6
4	C	2	GLC	O5-C5-C6-O6
4	B	2	GLC	O5-C5-C6-O6
4	B	1	BGC	O5-C5-C6-O6
4	D	1	BGC	C4-C5-C6-O6
4	D	1	BGC	O5-C5-C6-O6
4	B	1	BGC	C4-C5-C6-O6
4	F	1	BGC	O5-C5-C6-O6
4	C	1	BGC	O5-C5-C6-O6
4	B	2	GLC	C4-C5-C6-O6

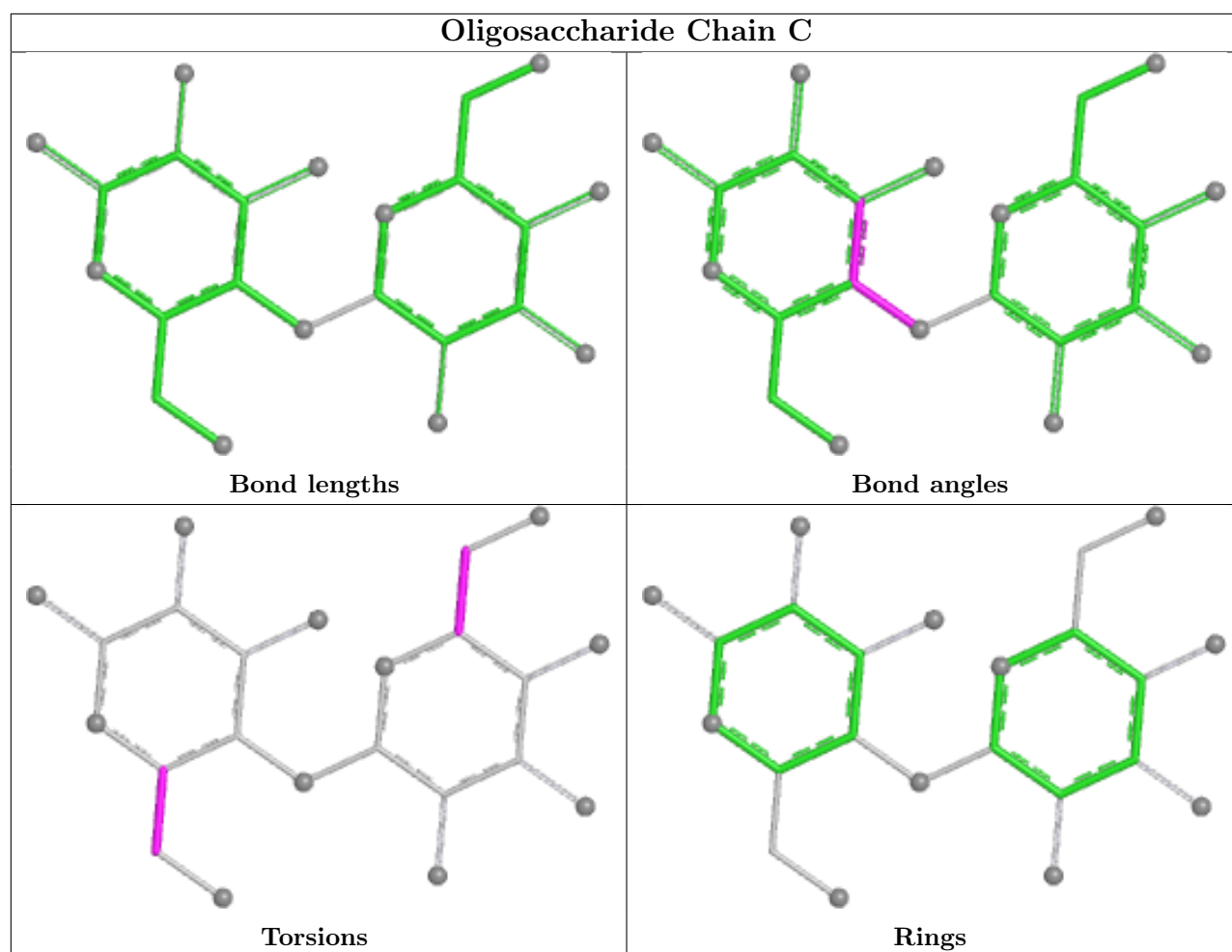
There are no ring outliers.

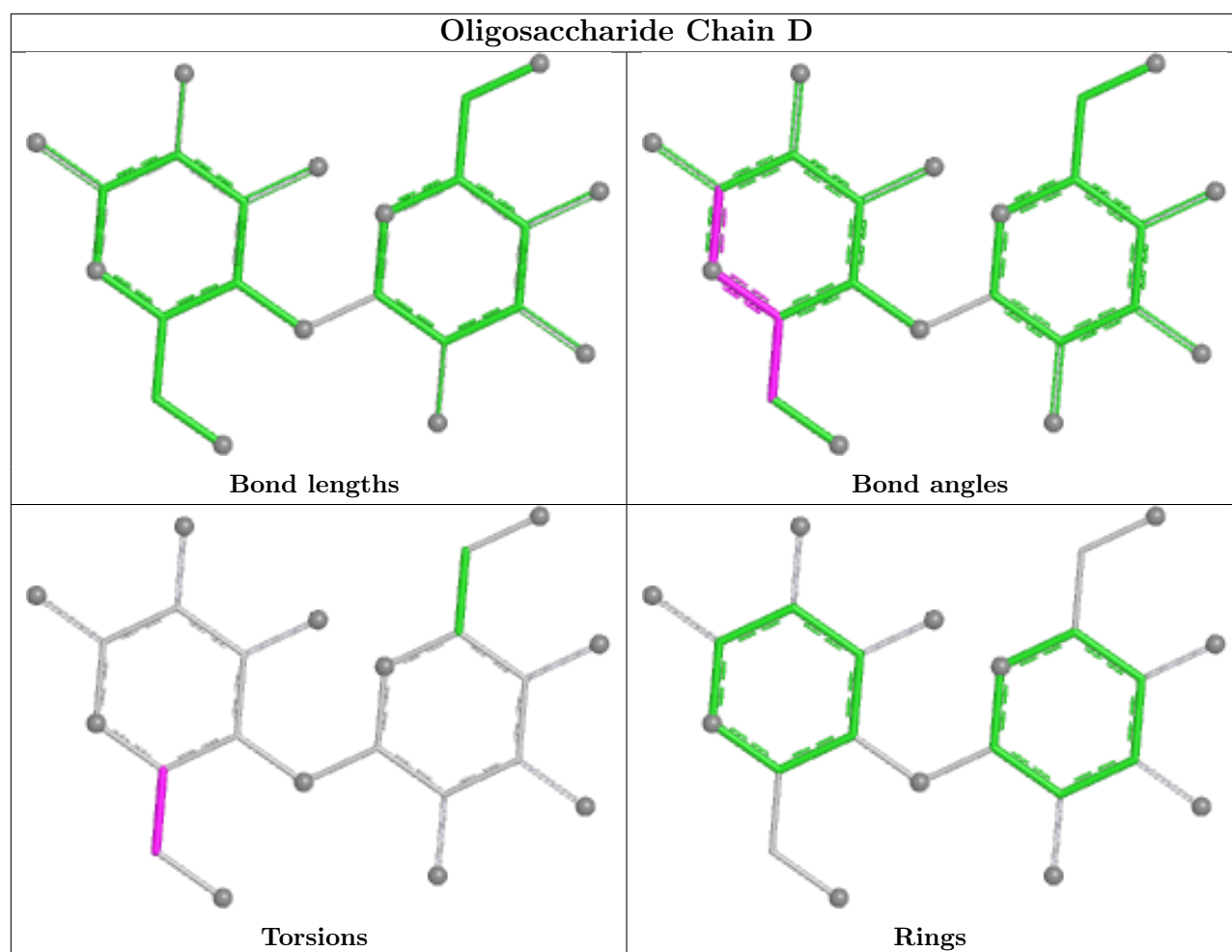
10 monomers are involved in 20 short contacts:

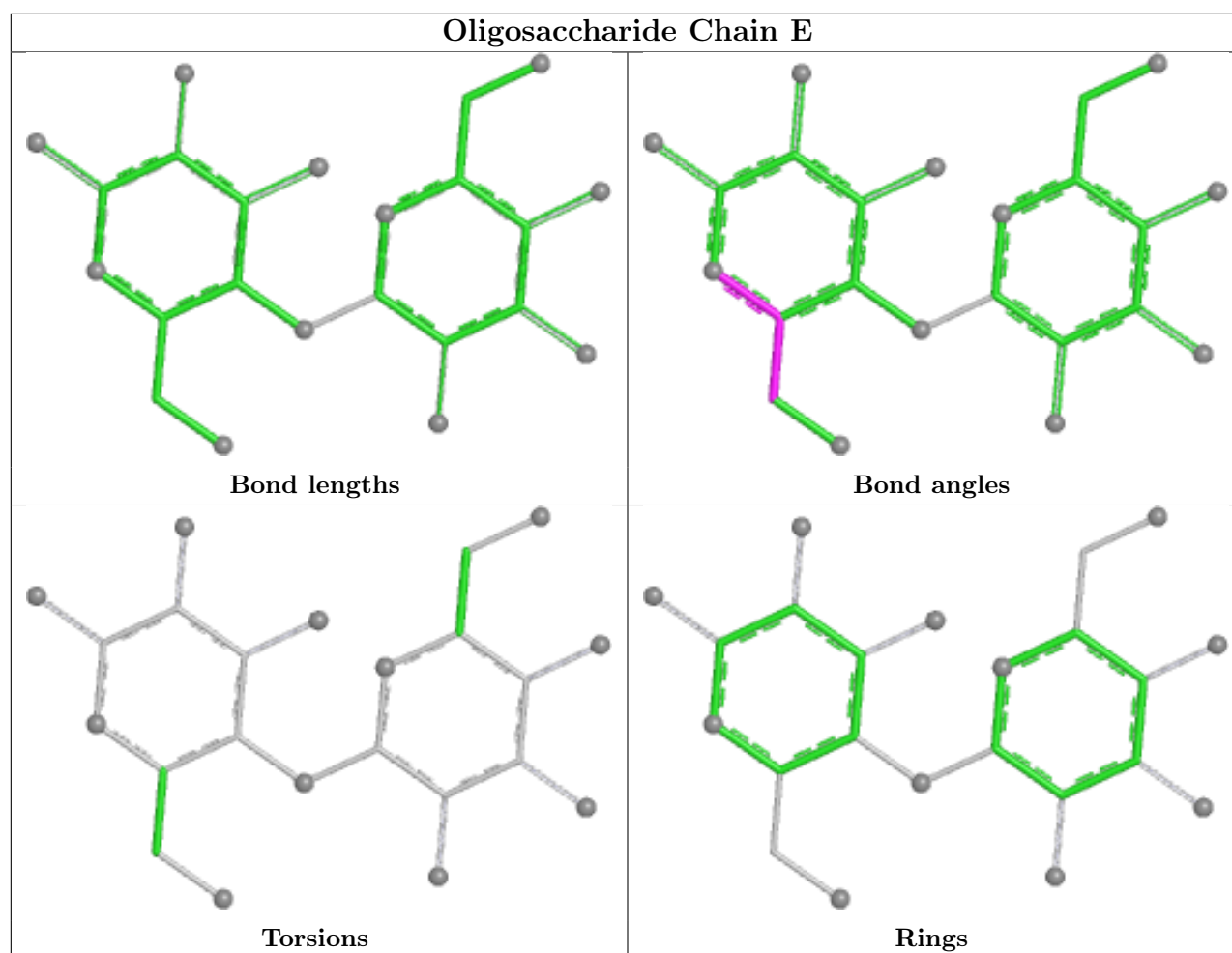
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	BGC	5	0
4	D	2	GLC	2	0
4	C	2	GLC	4	0
4	D	1	BGC	3	0
4	B	2	GLC	6	0
4	E	2	GLC	3	0
4	F	2	GLC	2	0
4	E	1	BGC	3	0
4	C	1	BGC	4	0
4	F	1	BGC	1	0

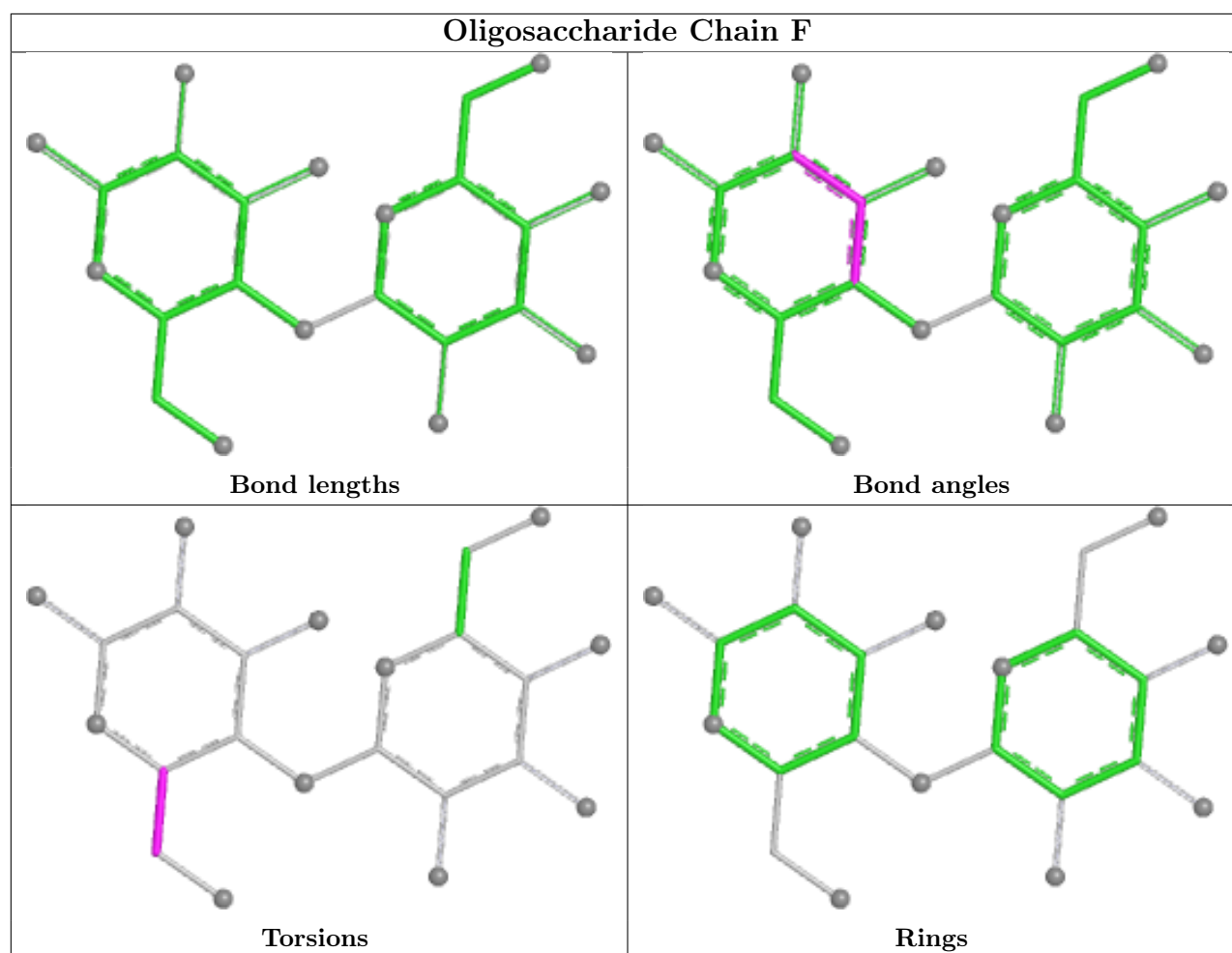
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











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	Y01	A	601	-	38,38,38	4.47	14 (36%)	57,57,57	2.03	15 (26%)
6	42J	A	602	-	11,11,11	1.17	2 (18%)	14,14,14	0.68	0
7	NAG	A	603	1	14,14,15	0.61	0	17,19,21	0.48	0
8	CLR	A	609	-	31,31,31	0.77	1 (3%)	48,48,48	1.20	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
5	Y01	A	601	-	-	7/19/77/77	0/4/4/4
6	42J	A	602	-	-	2/3/3/3	0/1/1/1
7	NAG	A	603	1	-	0/6/23/26	0/1/1/1
8	CLR	A	609	-	-	2/10/68/68	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	Y01	CAI-CAZ	18.18	1.70	1.33
5	A	601	Y01	CBB-CBE	-10.46	1.36	1.54
5	A	601	Y01	CBH-CBF	8.09	1.68	1.56
5	A	601	Y01	CAU-CBI	-7.24	1.41	1.54
5	A	601	Y01	CAP-CBE	5.72	1.66	1.54
5	A	601	Y01	CAU-CAS	5.63	1.64	1.53
5	A	601	Y01	CAK-CBD	5.55	1.62	1.53
5	A	601	Y01	CBI-CBE	4.96	1.64	1.55
5	A	601	Y01	CBH-CAZ	-4.83	1.43	1.52
5	A	601	Y01	OAW-CAY	3.25	1.43	1.34
5	A	601	Y01	CAO-CBB	2.85	1.61	1.54
5	A	601	Y01	CAQ-CBG	2.83	1.60	1.54
6	A	602	42J	C5-CL	2.67	1.79	1.73
6	A	602	42J	C6-CL1	2.64	1.79	1.73
5	A	601	Y01	CBD-CBF	-2.16	1.49	1.53
5	A	601	Y01	CAE-CBI	-2.07	1.50	1.54
8	A	609	CLR	C10-C9	-2.05	1.52	1.56

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	Y01	CBI-CBE-CBB	-5.74	110.64	119.50
5	A	601	Y01	CBH-CAZ-CAI	-4.28	116.67	122.93
5	A	601	Y01	CAU-CBI-CBG	4.20	113.53	107.25
5	A	601	Y01	OAW-CAY-CAM	3.92	119.97	111.48
5	A	601	Y01	CAE-CBI-CAU	-3.79	105.02	110.61
5	A	601	Y01	CAK-CAI-CAZ	-3.78	118.64	125.02
8	A	609	CLR	C4-C5-C10	3.67	121.12	116.42
5	A	601	Y01	CBG-CBI-CBE	3.66	104.30	100.10
5	A	601	Y01	CAE-CBI-CBE	-3.45	105.43	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	Y01	CAU-CBI-CBE	3.40	121.61	116.60
5	A	601	Y01	CAE-CBI-CBG	-3.29	105.71	111.68
5	A	601	Y01	CAK-CBD-CBF	2.95	113.13	109.72
8	A	609	CLR	C13-C17-C20	-2.87	115.06	119.50
5	A	601	Y01	CAD-CBH-CBF	-2.78	108.54	111.66
5	A	601	Y01	CAS-CBF-CBH	-2.52	109.98	113.08
8	A	609	CLR	C13-C14-C8	-2.44	110.94	114.41
5	A	601	Y01	CAC-CBB-CBE	-2.44	109.22	112.88
8	A	609	CLR	C10-C5-C6	-2.37	119.46	122.93
5	A	601	Y01	CBF-CBH-CAZ	2.36	113.11	109.65
8	A	609	CLR	C11-C12-C13	-2.27	108.91	112.74

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	609	CLR	C17-C20-C22-C23
8	A	609	CLR	C21-C20-C22-C23
5	A	601	Y01	CAM-CAY-OAW-CBC
5	A	601	Y01	OAG-CAY-OAW-CBC
5	A	601	Y01	CAX-CAL-CAM-CAY
6	A	602	42J	C-C1-C2-C3
6	A	602	42J	C-C1-C2-C7
5	A	601	Y01	CAC-CBB-CBE-CBI
5	A	601	Y01	CAM-CAL-CAX-OAH
5	A	601	Y01	CAM-CAL-CAX-OAF
5	A	601	Y01	CAO-CAJ-CAN-CBA

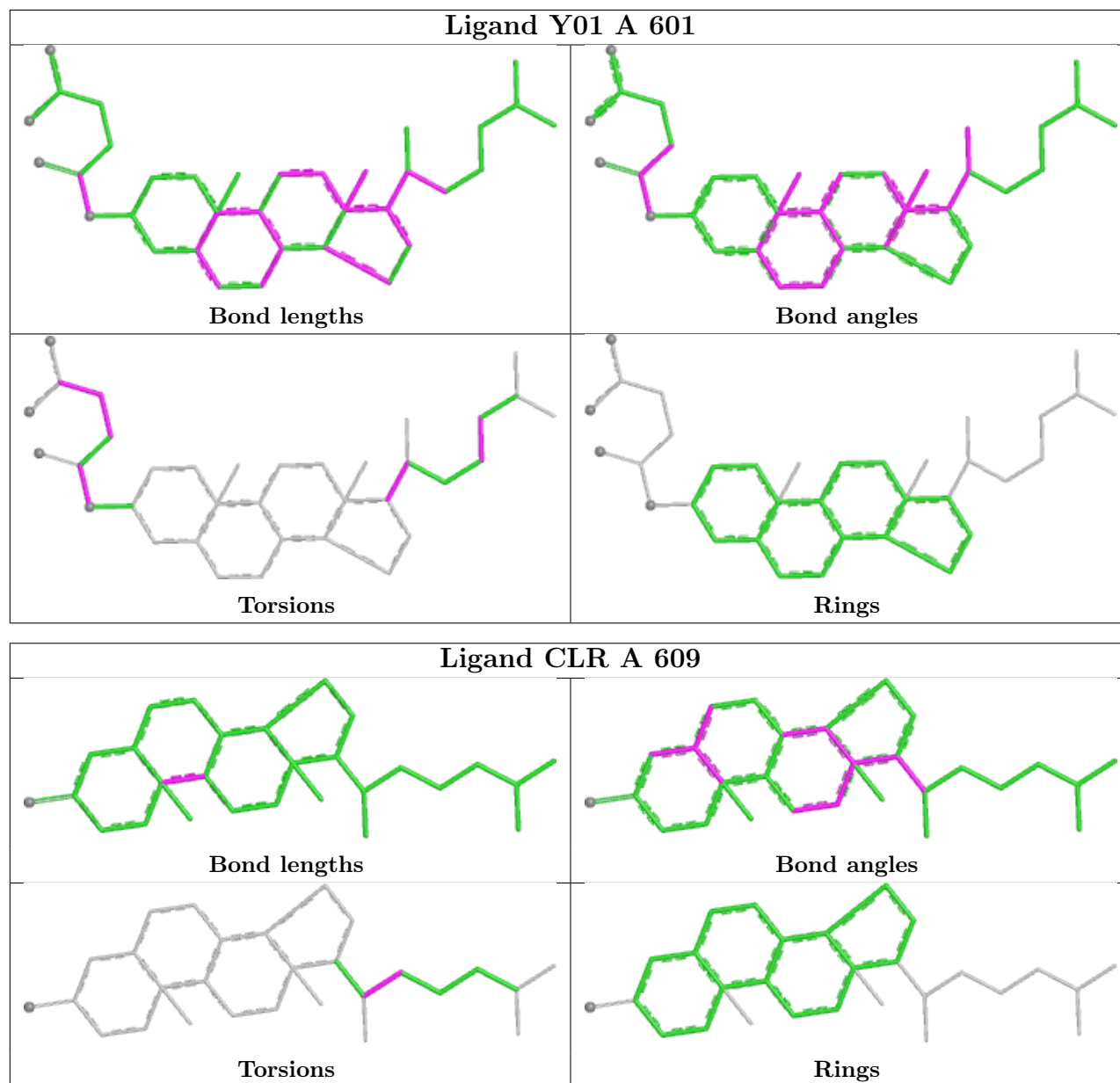
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	Y01	5	0
8	A	609	CLR	6	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	535/535 (100%)	0.36	28 (5%) 33 23	72, 101, 140, 171	2 (0%)
2	L	214/214 (100%)	0.28	14 (6%) 25 18	71, 96, 132, 176	0
3	H	219/219 (100%)	0.19	6 (2%) 56 41	75, 96, 143, 194	0
All	All	968/968 (100%)	0.30	48 (4%) 34 24	71, 99, 141, 194	2 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	ALA	7.6
1	A	305	TYR	5.7
2	L	153	GLY	5.0
1	A	304	ILE	4.6
1	A	537	TYR	4.3
2	L	92	PHE	4.0
1	A	501	ASN	3.9
1	A	205	VAL	3.7
2	L	154	SER	3.7
1	A	322	GLY	3.7
1	A	301	PHE	3.7
1	A	250	CYS	3.7
1	A	227	GLU	3.4
2	L	90	GLN	3.1
3	H	111	GLN	3.1
1	A	308	GLU	3.1
1	A	300	ASN	3.1
1	A	219	TYR	3.0
1	A	206	GLU	3.0
2	L	197	ALA	2.9
3	H	141	SER	2.8
2	L	149	TRP	2.8
2	L	196	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	534	ILE	2.5
1	A	310	TRP	2.5
1	A	299	PRO	2.4
1	A	479	ALA	2.4
2	L	157	GLN	2.4
1	A	325	PHE	2.4
2	L	174	TYR	2.4
3	H	188	THR	2.3
3	H	219	ARG	2.3
2	L	148	LYS	2.3
2	L	101	SER	2.3
1	A	319	PHE	2.3
2	L	147	VAL	2.2
3	H	107	ASP	2.2
1	A	111	TYR	2.2
1	A	229	ILE	2.2
1	A	437	PHE	2.2
1	A	147	SER	2.1
1	A	255	TRP	2.1
1	A	306	LYS	2.1
1	A	598[A]	ARG	2.1
1	A	51	TRP	2.1
2	L	99	PHE	2.0
2	L	158	ASN	2.0
3	H	150	GLY	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.

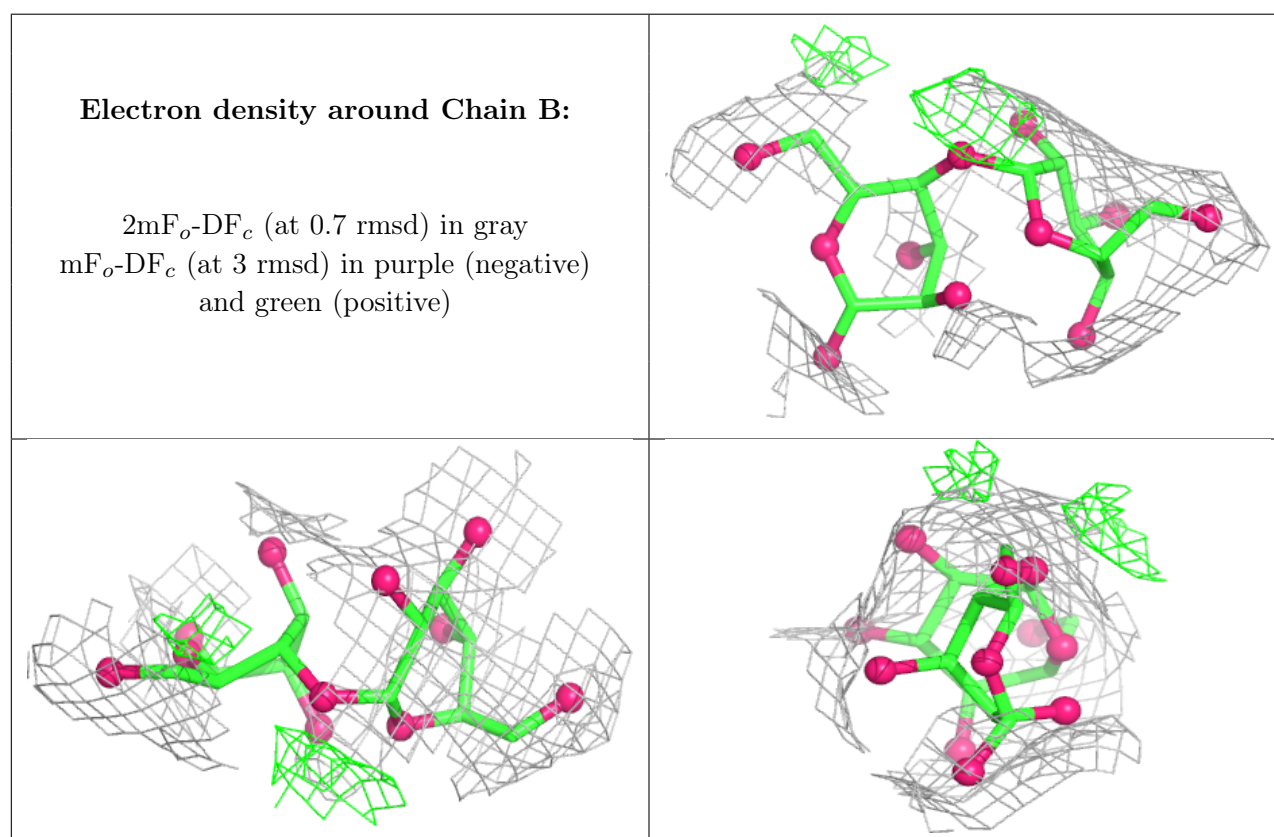
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BGC	B	1	12/12	-	-	146,172,178,189	0
4	GLC	B	2	11/12	-	-	152,173,176,178	0
4	BGC	C	1	12/12	-	-	176,186,189,192	0

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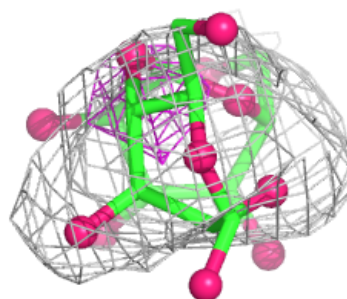
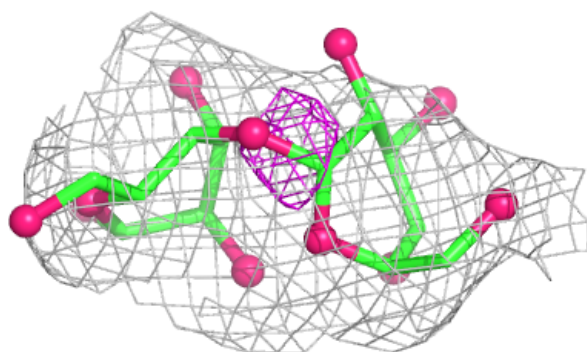
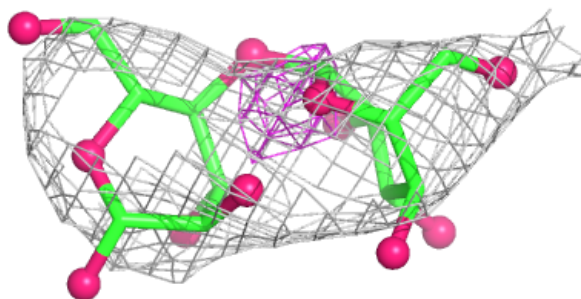
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GLC	C	2	11/12	-	-	131,176,182,187	0
4	BGC	D	1	12/12	0.50	0.13	150,162,173,177	0
4	GLC	D	2	11/12	0.58	0.12	142,160,169,170	0
4	GLC	F	2	11/12	0.67	0.16	158,188,198,200	0
4	BGC	E	1	12/12	0.70	0.11	183,197,202,205	0
4	BGC	F	1	12/12	0.74	0.15	166,194,198,201	0
4	GLC	E	2	11/12	0.83	0.15	157,170,186,186	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.

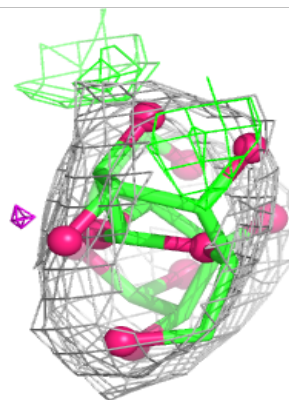
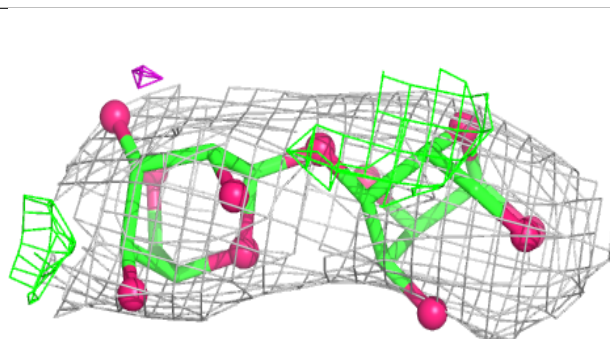
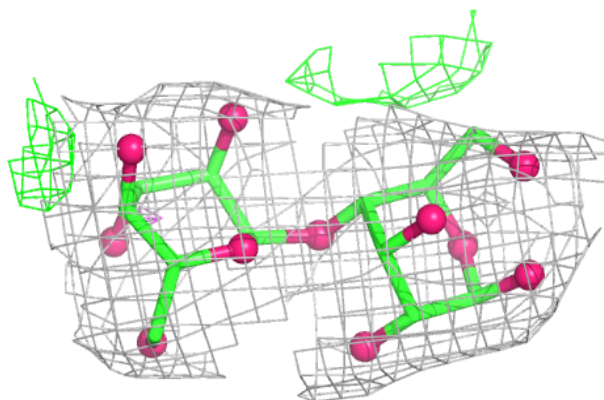


Electron density around Chain C:

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

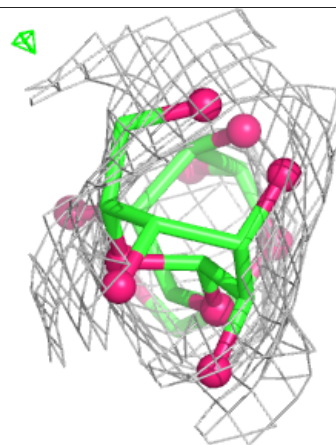
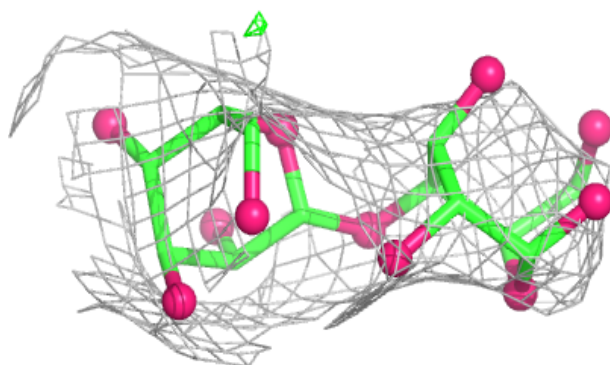
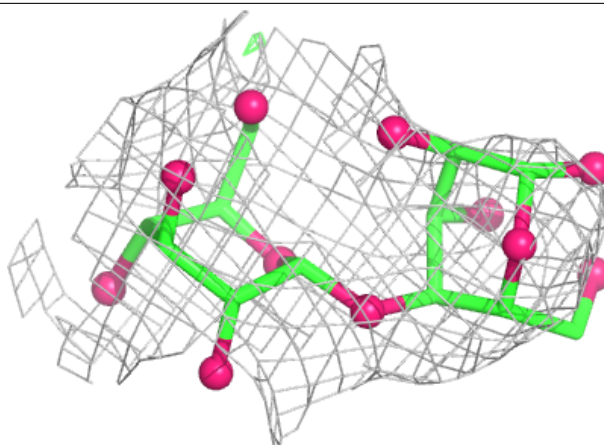
**Electron density around Chain D:**

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

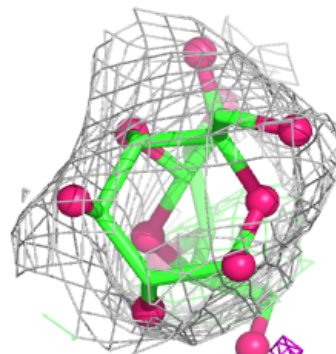
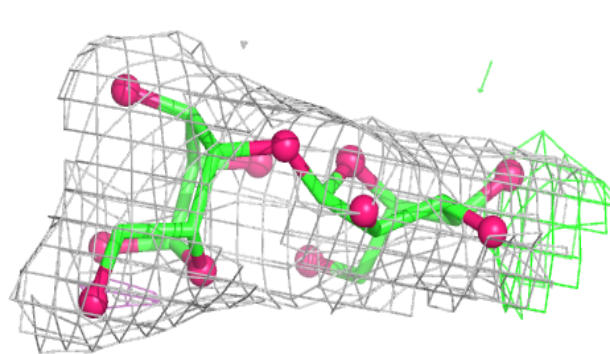
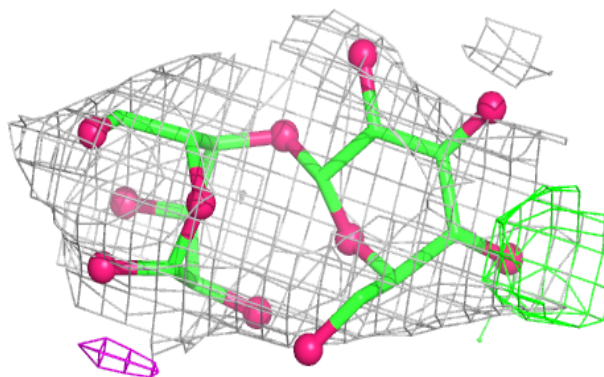


Electron density around Chain E:

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

**Electron density around Chain F:**

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



6.4 Ligands [i](#)

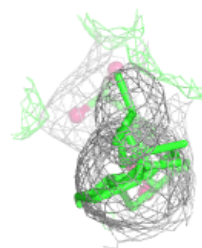
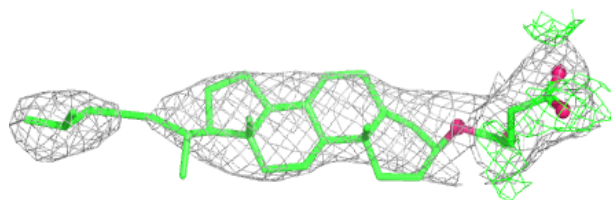
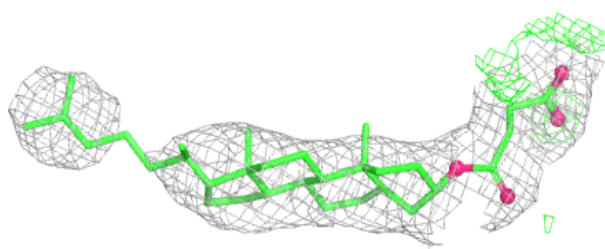
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

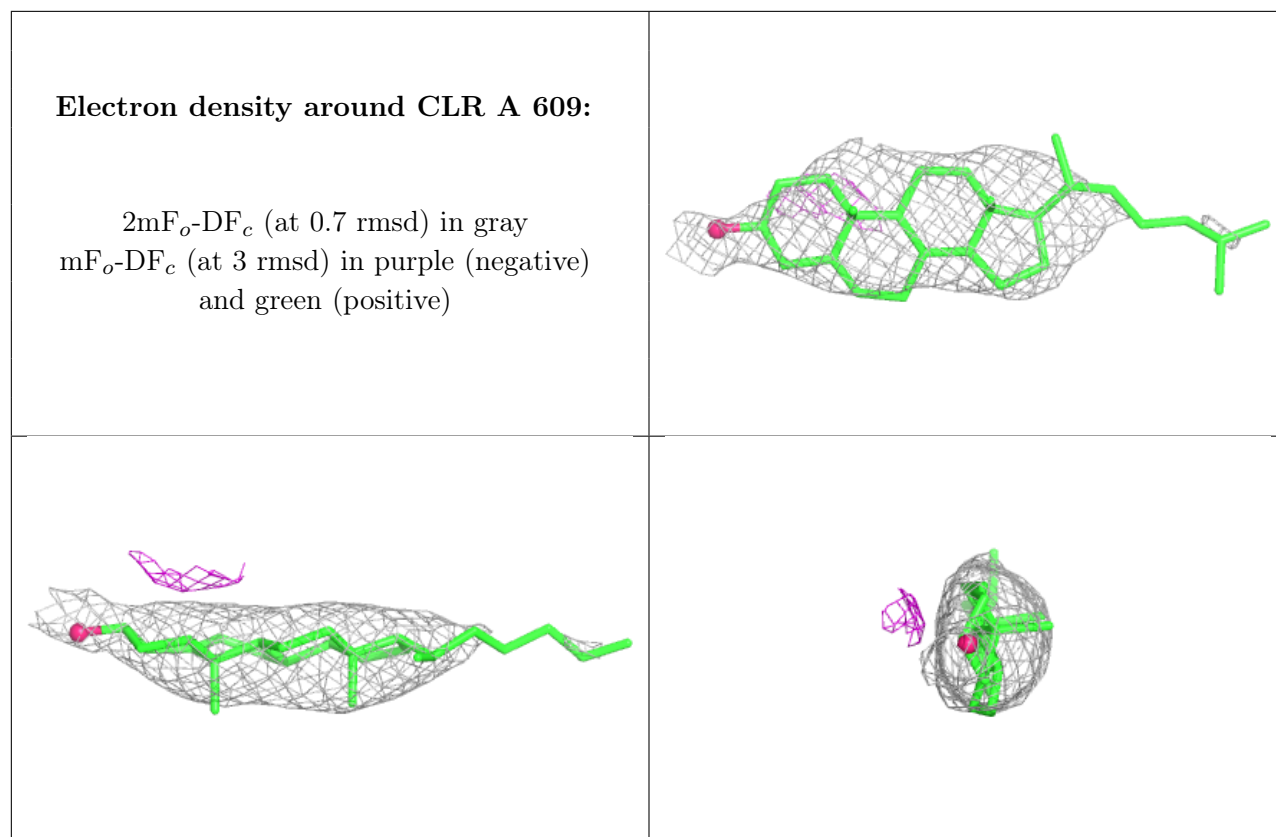
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	603	14/15	0.50	0.16	138,173,203,208	0
5	Y01	A	601	35/35	0.85	0.18	84,121,135,139	0
10	NA	A	612	1/1	0.88	0.14	91,91,91,91	0
10	NA	A	611	1/1	0.90	0.12	89,89,89,89	0
6	42J	A	602	11/11	0.91	0.14	85,90,105,122	0
8	CLR	A	609	28/28	0.92	0.14	92,102,108,110	0
9	CL	A	610	1/1	0.93	0.15	101,101,101,101	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 601:

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.