



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 13, 2023 – 10:49 AM EDT

PDB ID : 8DV4
Title : Crystal structure of the BC8B TCR-CD1b-PI complex
Authors : Farquhar, R.; Rossjohn, J.; Shahine, A.
Deposited on : 2022-07-28
Resolution : 2.40 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 : 2.32.2
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) : 2.32.2

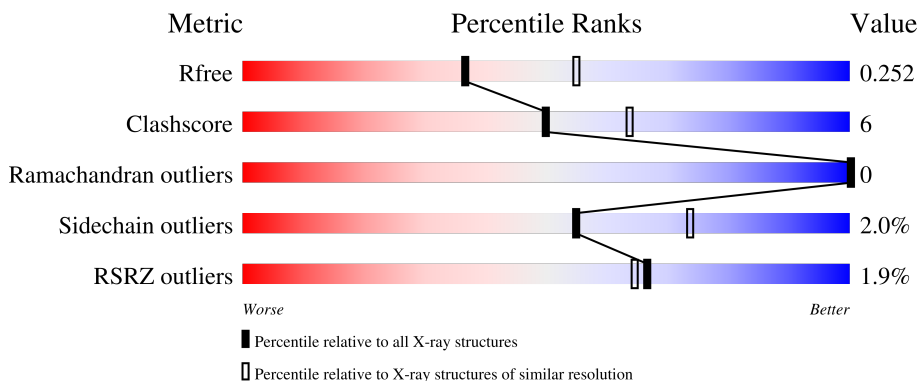
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	300	 2% 76% 14% 9%
2	B	99	 84% 15%
3	D	207	 3% 74% 17% 9%
4	E	245	 89% 11%
5	C	3	 67% 33%

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Mol	Chain	Length	Quality of chain
6	F	4	 25% 75%

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
10	NAG	A	604	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 6742 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 T-cell surface glycoprotein CD1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	2107	1354	356	387	10	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	GLY	-	expression tag	UNP P29016
A	280	SER	-	expression tag	UNP P29016
A	281	GLY	-	expression tag	UNP P29016
A	282	LEU	-	expression tag	UNP P29016
A	283	ASN	-	expression tag	UNP P29016
A	284	ASP	-	expression tag	UNP P29016
A	285	ILE	-	expression tag	UNP P29016
A	286	PHE	-	expression tag	UNP P29016
A	287	GLU	-	expression tag	UNP P29016
A	288	ALA	-	expression tag	UNP P29016
A	289	GLN	-	expression tag	UNP P29016
A	290	LYS	-	expression tag	UNP P29016
A	291	ILE	-	expression tag	UNP P29016
A	292	GLU	-	expression tag	UNP P29016
A	293	TRP	-	expression tag	UNP P29016
A	294	HIS	-	expression tag	UNP P29016
A	295	GLU	-	expression tag	UNP P29016
A	296	HIS	-	expression tag	UNP P29016
A	297	HIS	-	expression tag	UNP P29016
A	298	HIS	-	expression tag	UNP P29016
A	299	HIS	-	expression tag	UNP P29016
A	300	HIS	-	expression tag	UNP P29016
A	301	HIS	-	expression tag	UNP P29016

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	98	807	515	138	152	2	0	1	0

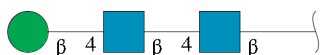
- Molecule 3 is a protein called T-cell receptor alpha variable TRAV9-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	189	1409	888	224	290	7	0	0	0

- Molecule 4 is a protein called T-cell receptor beta variable TRBV6-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	244	1921	1220	329	362	10	0	2	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	C	3	39	22	2	15	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	F	4	50	28	2	20	0	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



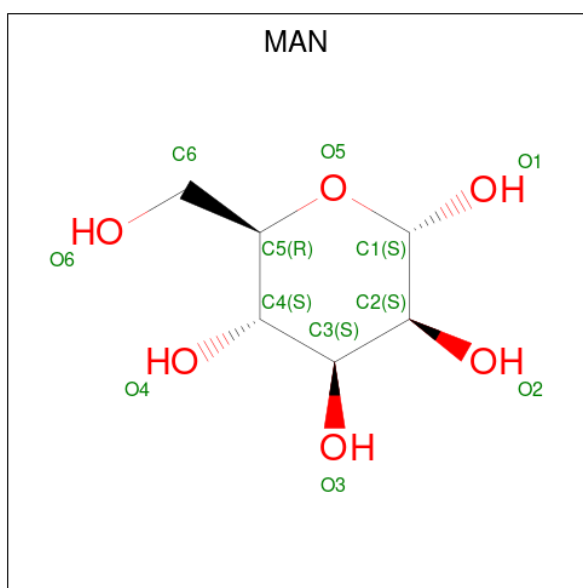
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

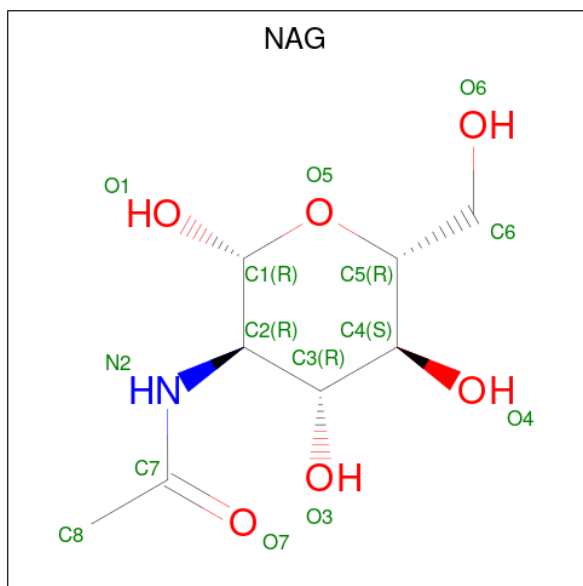
- Molecule 9 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			11	6	5		

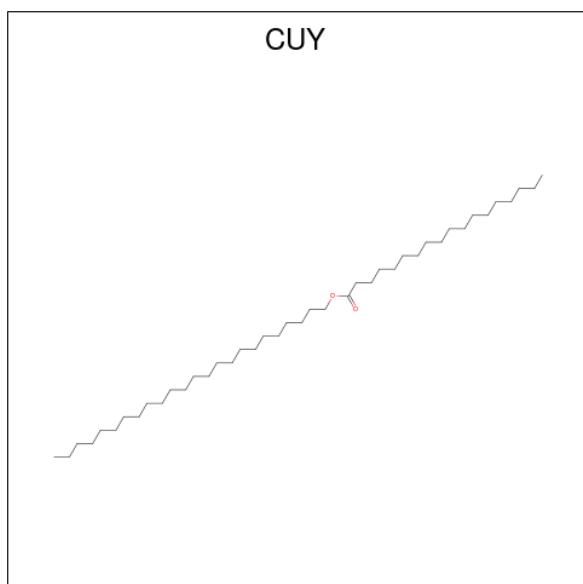
- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG)

(formula: $C_8H_{15}NO_6$).



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

- Molecule 11 is tetracosyl octadecanoate (three-letter code: CUY) (formula: $C_{42}H_{84}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	A	1	38	36	2	0	0

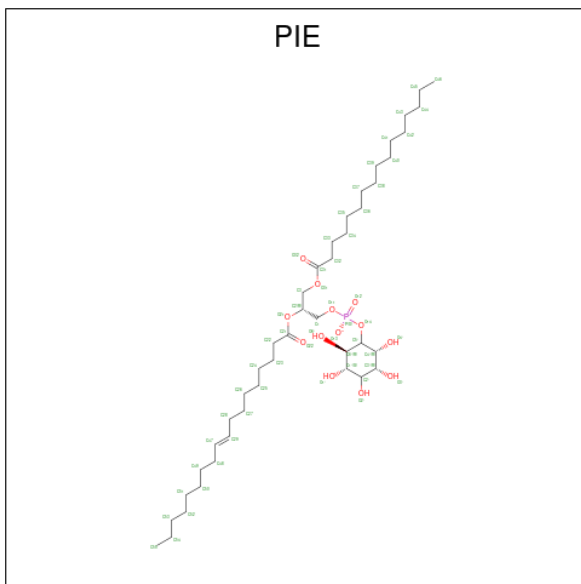
- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total Cl 1 1	0	0
12	E	2	Total Cl 2 2	0	0

- Molecule 13 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	2	Total Na 2 2	0	0
13	B	1	Total Na 1 1	0	0

- Molecule 14 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOINOSITOL (three-letter code: PIE) (formula: C₄₃H₈₀O₁₃P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	D	1	Total C O P 57 43 13 1	4	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	82	Total O 82 82	0	0

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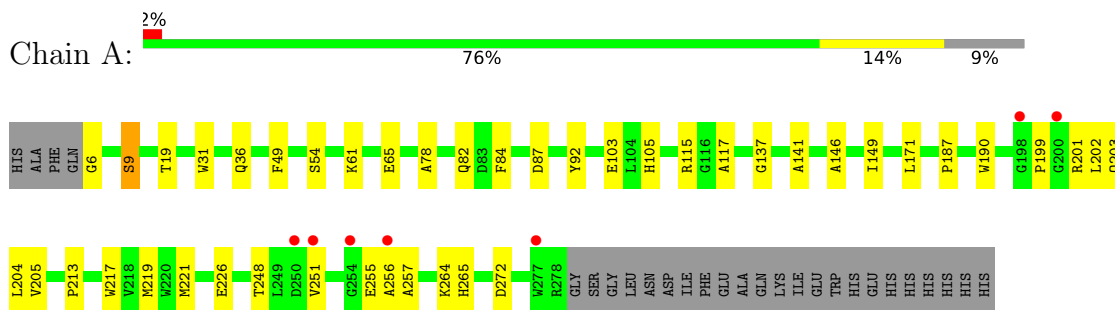
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	B	41	Total 41	O 41	0	0
15	D	43	Total 43	O 43	0	0
15	E	81	Total 81	O 81	0	0

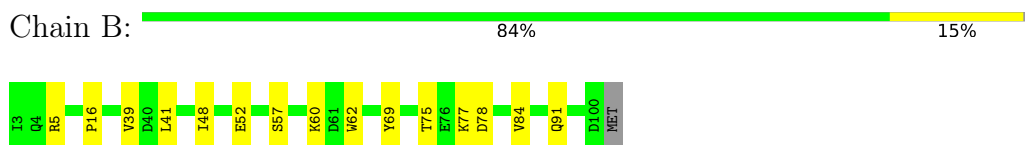
3 Residue-property plots [i](#)

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.

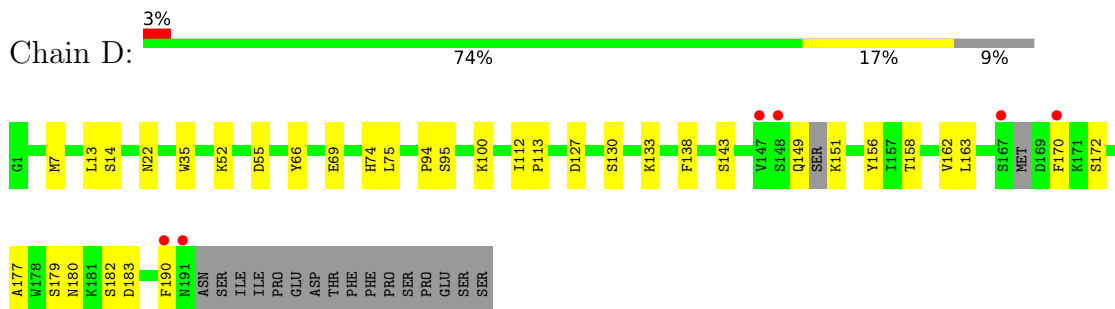
- Molecule 1: T-cell surface glycoprotein CD1b



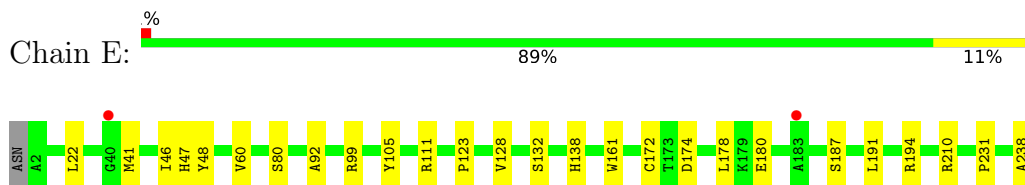
- Molecule 2: Beta-2-microglobulin



- Molecule 3: T-cell receptor alpha variable TRAV9-2



- Molecule 4: T-cell receptor beta variable TRBV6-2




- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  67% 33%

MAG1
MAG2
BMA3

- Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  25% 75%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.09Å 65.43Å 101.58Å 90.00° 102.26° 90.00°	Depositor
Resolution (Å)	46.07 – 2.40 46.07 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.07-2.40) 99.9 (46.07-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.192 , 0.255 0.191 , 0.252	Depositor DCC
R_{free} test set	1861 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtrriage
Anisotropy	0.872	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6742	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: EDO, GOL, CUY, BMA, NAG, MAN, PIE, NA, CL

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	0.41	0/2166	0.58	0/2945
2	B	0.40	0/833	0.61	0/1133
3	D	0.41	0/1437	0.62	0/1955
4	E	0.44	0/1977	0.67	0/2693
All	All	0.42	0/6413	0.62	0/8726

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2107	0	2007	33	0
2	B	807	0	749	9	0
3	D	1409	0	1297	22	0
4	E	1921	0	1829	16	0
5	C	39	0	34	0	0
6	F	50	0	43	1	0
7	A	8	0	12	1	0
7	D	8	0	12	0	0
7	E	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	12	0	16	0	0
9	A	11	0	10	0	0
10	A	14	0	13	1	0
11	A	38	0	0	0	0
12	A	1	0	0	0	0
12	E	2	0	0	0	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
14	D	57	0	80	2	0
15	A	82	0	0	7	0
15	B	41	0	0	0	0
15	D	43	0	0	1	0
15	E	81	0	0	2	0
All	All	6742	0	6114	73	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 6.

All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:MET:HE1	1:A:226:GLU:HA	1.59	0.84
3:D:163:LEU:HB3	4:E:172:CYS:HB2	1.64	0.77
2:B:75:THR:HG22	2:B:77:LYS:H	1.54	0.71
1:A:6:GLY:N	15:A:702:HOH:O	2.23	0.70
1:A:187:PRO:HD3	15:A:709:HOH:O	1.93	0.68
1:A:257:ALA:O	15:A:701:HOH:O	2.11	0.67
1:A:264:LYS:HB3	7:A:601:EDO:H21	1.77	0.67
4:E:161:TRP:HB2	4:E:210:ARG:HB3	1.80	0.64
10:A:604:NAG:H3	10:A:604:NAG:H83	1.81	0.62
3:D:7:MET:HE3	3:D:22:ASN:H	1.65	0.62
3:D:158:THR:HA	4:E:178[A]:LEU:HD21	1.82	0.62
3:D:170:PHE:CE1	3:D:172:SER:HB3	2.36	0.61
1:A:251:VAL:HG11	1:A:256:ALA:HB2	1.82	0.60
3:D:170:PHE:HE1	3:D:172:SER:HB3	1.66	0.60
4:E:111:ARG:HG3	7:E:302:EDO:H12	1.84	0.59
4:E:174:ASP:HB2	4:E:191:LEU:HD12	1.86	0.57
3:D:94:PRO:HG3	14:D:501:PIE:H4'1	1.87	0.56
3:D:95:SER:O	15:D:601:HOH:O	2.18	0.56
3:D:149:GLN:O	3:D:151:LYS:N	2.38	0.56
3:D:35:TRP:CE2	3:D:75:LEU:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:NH1	15:A:706:HOH:O	2.34	0.54
1:A:205:VAL:HG22	1:A:248:THR:HG22	1.90	0.53
1:A:251:VAL:HG22	1:A:255:GLU:HB3	1.89	0.53
3:D:127:ASP:HB3	3:D:130:SER:O	2.08	0.53
1:A:9:SER:HB2	1:A:103:GLU:HB3	1.91	0.52
2:B:75:THR:HB	2:B:78:ASP:OD2	2.11	0.51
4:E:210:ARG:HD3	15:E:460:HOH:O	2.11	0.51
4:E:46:ILE:HG22	4:E:47:HIS:CD2	2.47	0.50
1:A:49:PHE:HB3	1:A:54:SER:HB2	1.93	0.49
1:A:202:LEU:HD12	1:A:203:GLN:H	1.76	0.49
1:A:19:THR:O	1:A:92:TYR:HB3	2.13	0.49
1:A:84:PHE:CZ	4:E:99:ARG:HD2	2.47	0.49
4:E:123:PRO:HD3	4:E:231:PRO:HB3	1.95	0.48
3:D:69:GLU:H	3:D:69:GLU:CD	2.17	0.47
4:E:41:MET:HB3	15:E:411:HOH:O	2.15	0.46
1:A:190:TRP:CD2	2:B:16:PRO:HG3	2.50	0.46
3:D:113:PRO:HG3	3:D:162:VAL:HG11	1.97	0.46
4:E:128:VAL:HG23	4:E:238:ALA:HB3	1.97	0.45
1:A:213:PRO:HG2	15:A:761:HOH:O	2.17	0.45
1:A:265:HIS:CG	15:A:709:HOH:O	2.69	0.45
2:B:39:VAL:HG22	2:B:84:VAL:HG22	1.99	0.44
3:D:100:LYS:HD3	4:E:48:TYR:CE1	2.53	0.44
14:D:501:PIE:H6'1	14:D:501:PIE:H12	1.99	0.44
1:A:87:ASP:CG	4:E:99:ARG:HH22	2.21	0.44
3:D:138:PHE:HB2	3:D:190:PHE:CE2	2.53	0.43
2:B:41:LEU:O	2:B:48:ILE:HG13	2.19	0.43
4:E:60:VAL:O	4:E:60:VAL:HG13	2.18	0.43
1:A:204:LEU:HD11	1:A:256:ALA:HB1	2.00	0.43
3:D:133:LYS:HB2	3:D:133:LYS:HE2	1.62	0.43
1:A:137:GLY:HA3	1:A:141:ALA:HB2	2.01	0.43
1:A:171:LEU:HD12	6:F:2:NAG:H82	2.00	0.43
1:A:199:PRO:C	1:A:201:ARG:H	2.22	0.43
2:B:52:GLU:HB2	2:B:69:TYR:CZ	2.54	0.43
1:A:264:LYS:NZ	1:A:272:ASP:OD2	2.49	0.42
1:A:204:LEU:O	1:A:248:THR:HA	2.19	0.42
3:D:52:LYS:O	3:D:55:ASP:HB2	2.19	0.42
1:A:78:ALA:O	1:A:82:GLN:HG2	2.20	0.42
1:A:31:TRP:CZ2	2:B:57:SER:HB2	2.54	0.42
2:B:5[B]:ARG:HE	2:B:5[B]:ARG:HB3	1.43	0.42
1:A:117:ALA:HB2	2:B:62:TRP:CE2	2.55	0.42
1:A:103:GLU:OE2	1:A:105:HIS:NE2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:NZ	1:A:65:GLU:OE2	2.53	0.41
3:D:156:TYR:O	3:D:177:ALA:HA	2.20	0.41
3:D:179:SER:HB2	3:D:182:SER:HB3	2.03	0.41
1:A:146:ALA:O	1:A:149:ILE:HG22	2.21	0.41
1:A:217:TRP:CZ2	1:A:219:MET:HG3	2.56	0.41
3:D:156:TYR:HE1	4:E:180:GLU:O	2.03	0.41
3:D:22:ASN:HA	3:D:74:HIS:ND1	2.36	0.40
1:A:31:TRP:CZ3	1:A:36:GLN:HB2	2.55	0.40
1:A:265:HIS:ND1	15:A:709:HOH:O	2.37	0.40
3:D:156:TYR:HE2	3:D:180:ASN:HD21	1.69	0.40
3:D:112:ILE:HG22	3:D:143:SER:HB3	2.04	0.40
4:E:92:ALA:HA	4:E:105:TYR:O	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	271/300 (90%)	263 (97%)	8 (3%)	0	100	100
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
3	D	183/207 (88%)	176 (96%)	7 (4%)	0	100	100
4	E	244/245 (100%)	239 (98%)	5 (2%)	0	100	100
All	All	795/851 (93%)	773 (97%)	22 (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	216/247 (87%)	215 (100%)	1 (0%)	88	95
2	B	88/94 (94%)	86 (98%)	2 (2%)	50	70
3	D	151/182 (83%)	147 (97%)	4 (3%)	46	66
4	E	205/211 (97%)	199 (97%)	6 (3%)	42	62
All	All	660/734 (90%)	647 (98%)	13 (2%)	55	74

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
2	B	60	LYS
2	B	91	GLN
3	D	13	LEU
3	D	14	SER
3	D	66	TYR
3	D	183	ASP
4	E	22	LEU
4	E	80	SER
4	E	132	SER
4	E	138	HIS
4	E	187	SER
4	E	194	ARG

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

7 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
5	NAG	C	1	5,1	14,14,15	0.54	0	17,19,21	0.60	0
5	NAG	C	2	5	14,14,15	0.31	0	17,19,21	0.64	0
5	BMA	C	3	5	11,11,12	1.04	1 (9%)	15,15,17	1.11	2 (13%)
6	NAG	F	1	6,1	14,14,15	0.55	0	17,19,21	0.57	0
6	NAG	F	2	6	14,14,15	0.34	0	17,19,21	0.48	0
6	BMA	F	3	6	11,11,12	1.27	1 (9%)	15,15,17	1.30	2 (13%)
6	MAN	F	4	6	11,11,12	1.00	0	15,15,17	1.37	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
5	NAG	C	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1
6	NAG	F	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	BMA	F	3	6	-	2/2/19/22	0/1/1/1
6	MAN	F	4	6	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	3	BMA	C2-C3	3.06	1.57	1.52
5	C	3	BMA	C1-C2	2.35	1.57	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	4	MAN	C1-O5-C5	4.39	118.14	112.19
6	F	3	BMA	C1-C2-C3	2.90	113.23	109.67
5	C	3	BMA	C1-O5-C5	2.51	115.59	112.19
6	F	3	BMA	O5-C1-C2	2.19	114.15	110.77
5	C	3	BMA	O2-C2-C3	-2.14	105.85	110.14

There are no chirality outliers.

All (7) torsion outliers are listed below:

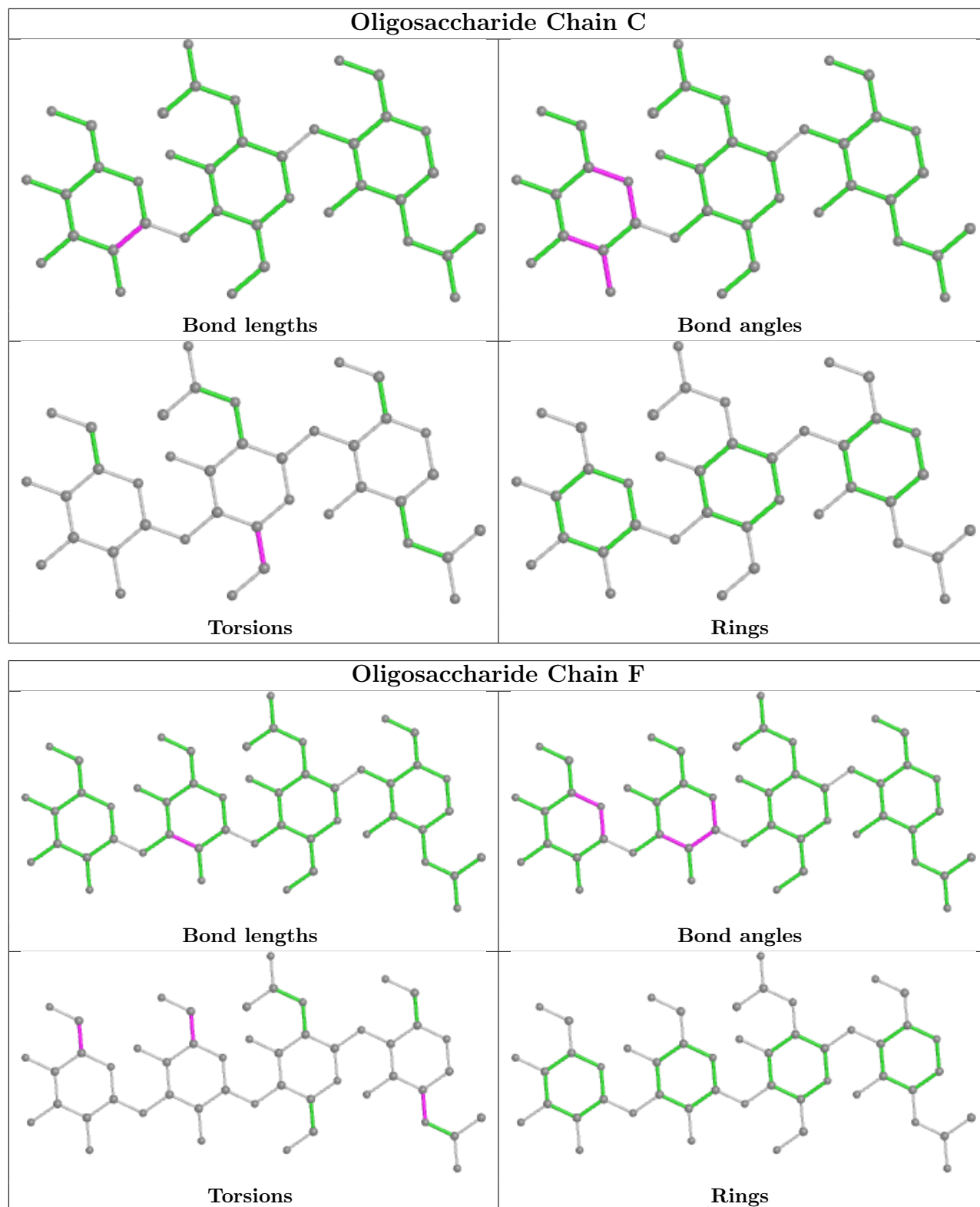
Mol	Chain	Res	Type	Atoms
6	F	3	BMA	O5-C5-C6-O6
6	F	3	BMA	C4-C5-C6-O6
5	C	2	NAG	O5-C5-C6-O6
6	F	4	MAN	C4-C5-C6-O6
6	F	4	MAN	O5-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6
6	F	1	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	2	NAG	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 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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
7	EDO	A	601	-	3,3,3	0.62	0	2,2,2	0.20	0
7	EDO	E	302	-	3,3,3	0.58	0	2,2,2	0.21	0
7	EDO	E	301	-	3,3,3	0.68	0	2,2,2	0.10	0
14	PIE	D	501	-	57,57,57	0.33	0	67,69,69	0.71	2 (2%)
11	CUY	A	605	-	37,37,43	0.26	0	37,37,43	0.58	0
9	MAN	A	603	-	11,11,12	1.79	3 (27%)	15,15,17	1.49	4 (26%)
8	GOL	A	602	-	5,5,5	1.17	0	5,5,5	0.91	0
10	NAG	A	604	1	14,14,15	0.71	1 (7%)	17,19,21	1.46	3 (17%)
7	EDO	D	503	-	3,3,3	0.51	0	2,2,2	0.25	0
7	EDO	A	607	-	3,3,3	0.48	0	2,2,2	0.32	0
8	GOL	A	609	-	5,5,5	0.92	0	5,5,5	0.96	0
7	EDO	D	502	-	3,3,3	0.42	0	2,2,2	0.21	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
7	EDO	A	601	-	-	0/1/1/1	-
7	EDO	E	302	-	-	1/1/1/1	-
7	EDO	E	301	-	-	0/1/1/1	-
14	PIE	D	501	-	-	17/52/76/76	0/1/1/1
11	CUY	A	605	-	-	9/36/36/42	-
9	MAN	A	603	-	-	2/2/19/22	0/1/1/1
8	GOL	A	602	-	-	2/4/4/4	-
10	NAG	A	604	1	-	5/6/23/26	0/1/1/1
7	EDO	D	503	-	-	0/1/1/1	-
7	EDO	A	607	-	-	0/1/1/1	-
8	GOL	A	609	-	-	0/4/4/4	-
7	EDO	D	502	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	603	MAN	C2-C3	3.91	1.58	1.52
9	A	603	MAN	O5-C5	2.74	1.49	1.43
10	A	604	NAG	C1-C2	2.34	1.55	1.52
9	A	603	MAN	O5-C1	-2.19	1.40	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	604	NAG	C2-N2-C7	4.40	129.16	122.90
14	D	501	PIE	P-O14-C5'	3.27	131.29	119.41
9	A	603	MAN	C1-O5-C5	2.92	116.16	112.19
10	A	604	NAG	C1-O5-C5	2.79	115.97	112.19
14	D	501	PIE	O21-C2-C3	-2.41	99.66	108.40
10	A	604	NAG	C1-C2-N2	2.24	114.31	110.49
9	A	603	MAN	O5-C5-C6	2.12	110.53	107.20
9	A	603	MAN	C2-C3-C4	2.09	114.51	110.89
9	A	603	MAN	C1-C2-C3	2.04	112.18	109.67

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	602	GOL	C1-C2-C3-O3
14	D	501	PIE	C4'-C5'-O14-P
14	D	501	PIE	C6'-C5'-O14-P
14	D	501	PIE	O32-C31-O31-C3
14	D	501	PIE	C32-C31-O31-C3
9	A	603	MAN	O5-C5-C6-O6
10	A	604	NAG	C8-C7-N2-C2
10	A	604	NAG	O7-C7-N2-C2
9	A	603	MAN	C4-C5-C6-O6
10	A	604	NAG	O5-C5-C6-O6
11	A	605	CUY	CAT-CAU-CAV-CAW
11	A	605	CUY	CBH-CBI-CBJ-CBK
11	A	605	CUY	CAI-CAJ-CAK-CAL
11	A	605	CUY	CAD-CAE-CAF-CAG
11	A	605	CUY	CBF-CBG-CBH-CBI
14	D	501	PIE	C33-C34-C35-C36
14	D	501	PIE	C31-C32-C33-C34
8	A	602	GOL	O2-C2-C3-O3
11	A	605	CUY	CBG-CBH-CBI-CBJ
11	A	605	CUY	CAU-CAV-CAW-CBM

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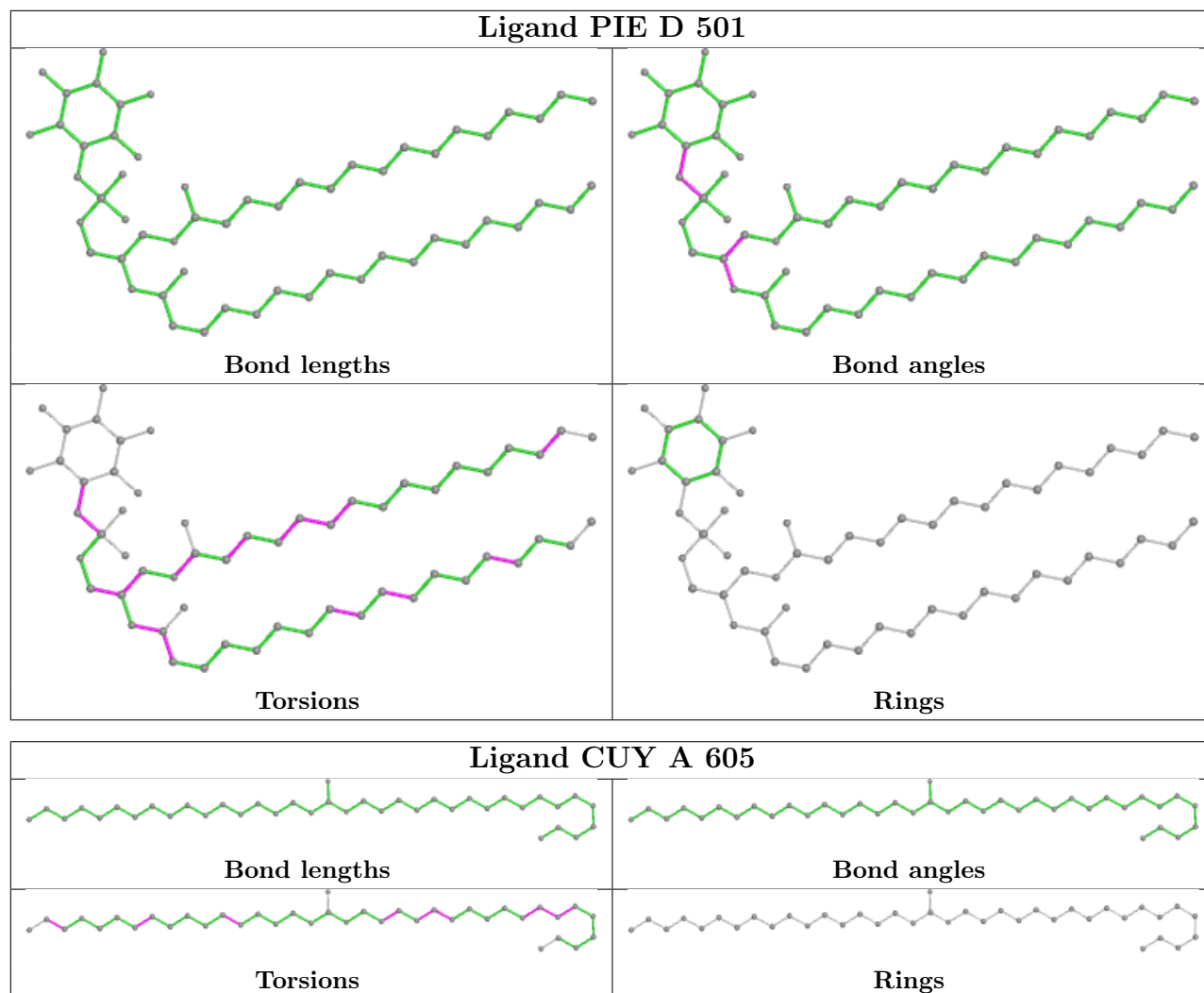
Mol	Chain	Res	Type	Atoms
7	E	302	EDO	O1-C1-C2-O2
14	D	501	PIE	C5'-O14-P-O11
11	A	605	CUY	C41-C40-CAA-CAB
14	D	501	PIE	C34-C35-C36-C37
10	A	604	NAG	C4-C5-C6-O6
14	D	501	PIE	C50-C51-C52-C53
14	D	501	PIE	C27-C28-C29-C47
14	D	501	PIE	C43-C44-C45-C46
14	D	501	PIE	O21-C21-C22-C23
10	A	604	NAG	C3-C2-N2-C7
14	D	501	PIE	O11-C1-C2-O21
14	D	501	PIE	O21-C2-C3-O31
14	D	501	PIE	C22-C21-O21-C2
11	A	605	CUY	CAR-CAS-CAT-CAU
14	D	501	PIE	C29-C47-C48-C49
14	D	501	PIE	C35-C36-C37-C38

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	601	EDO	1	0
7	E	302	EDO	1	0
14	D	501	PIE	2	0
10	A	604	NAG	1	0

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

6.1 Protein, DNA and RNA chains [i](#)

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	273/300 (91%)	0.10	7 (2%) 56 54	33, 48, 88, 111	0
2	B	98/99 (98%)	-0.07	0 100 100	32, 47, 73, 81	0
3	D	189/207 (91%)	0.14	6 (3%) 47 46	33, 56, 100, 130	0
4	E	244/245 (99%)	-0.11	2 (0%) 86 84	31, 45, 66, 84	0
All	All	804/851 (94%)	0.02	15 (1%) 66 64	31, 48, 86, 130	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	190	PHE	4.0
1	A	200	GLY	3.8
4	E	183	ALA	3.5
3	D	167	SER	3.1
1	A	254	GLY	3.0
1	A	256	ALA	2.7
3	D	147	VAL	2.7
4	E	40	GLY	2.6
3	D	170	PHE	2.5
3	D	148	SER	2.3
3	D	191	ASN	2.3
1	A	277	TRP	2.3
1	A	250	ASP	2.1
1	A	251	VAL	2.1
1	A	198	GLY	2.1

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

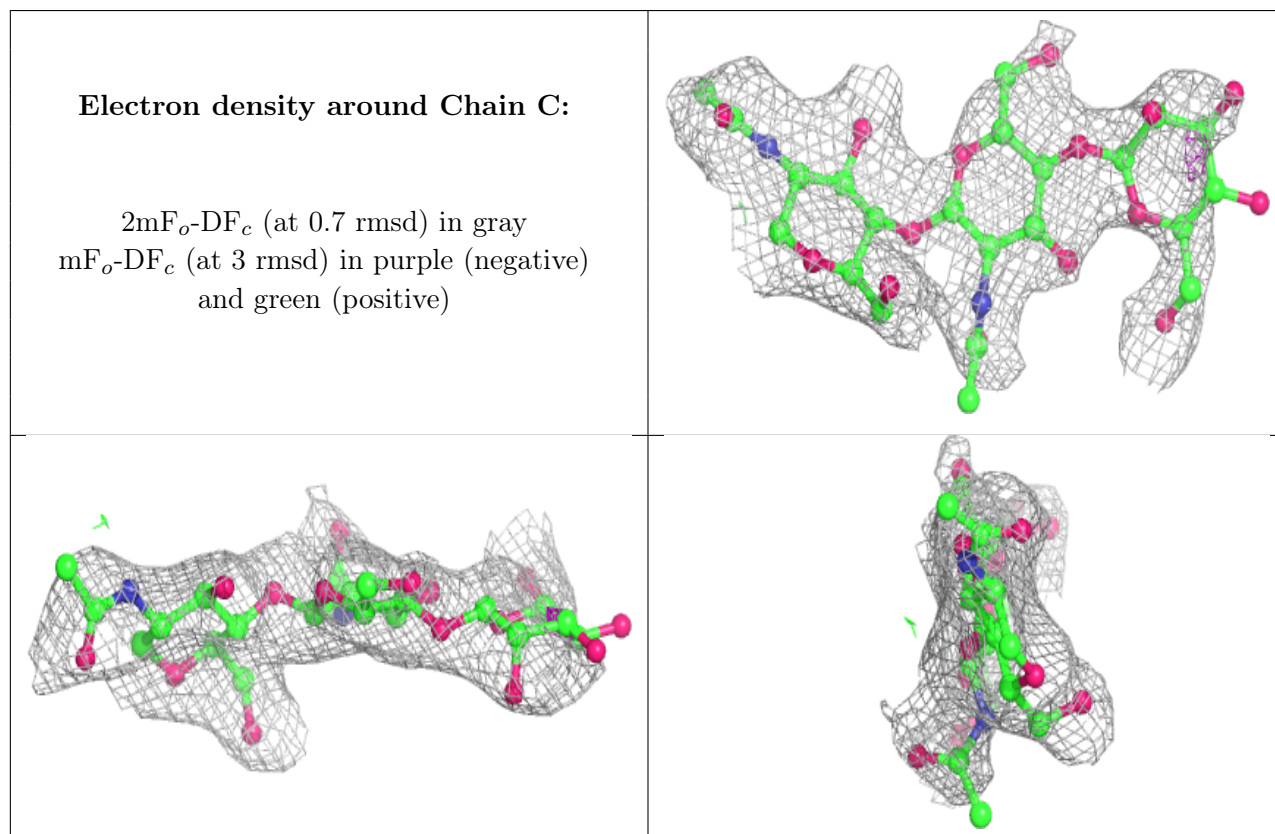
There are no non-standard protein/DNA/RNA residues in this entry.

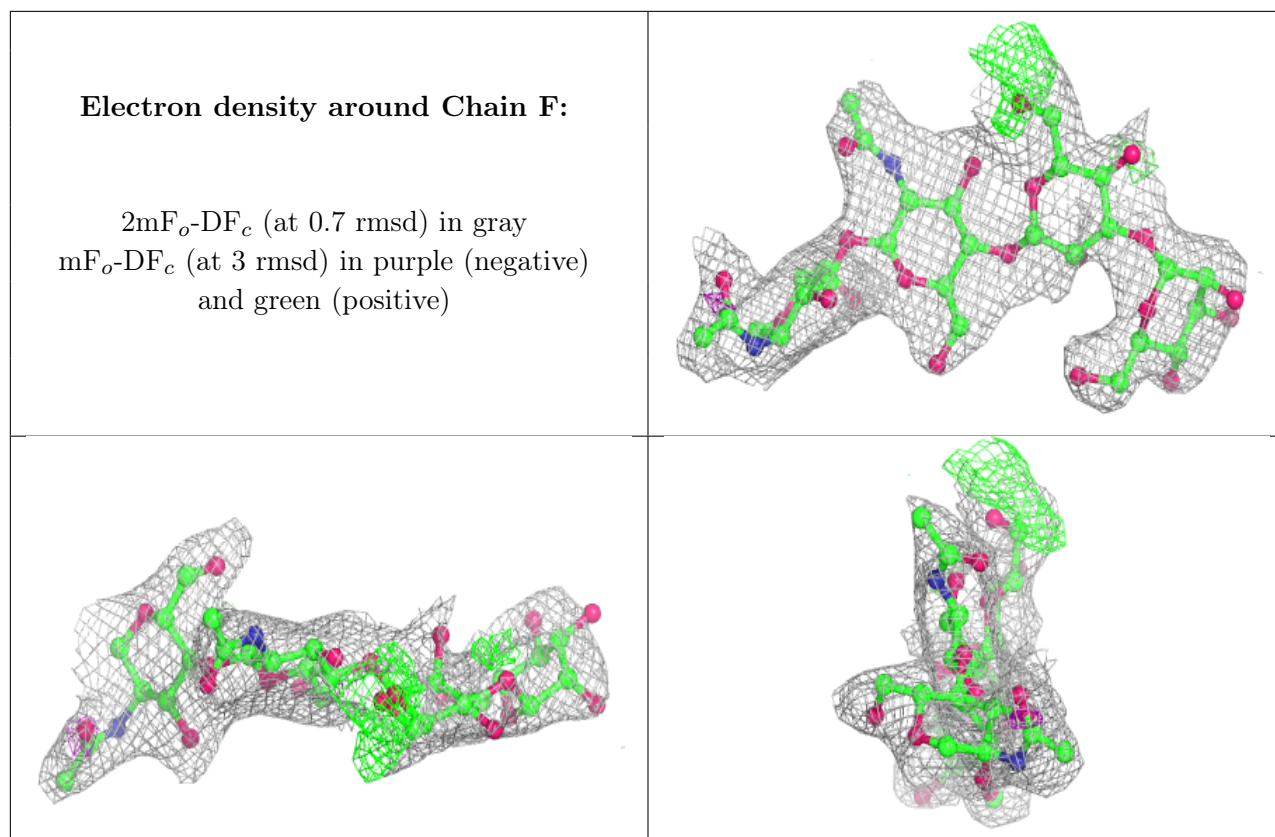
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	BMA	F	3	11/12	0.53	0.18	75,90,94,94	0
5	BMA	C	3	11/12	0.72	0.31	92,102,108,111	0
6	MAN	F	4	11/12	0.86	0.15	89,94,99,99	0
5	NAG	C	1	14/15	0.88	0.14	57,70,74,77	0
5	NAG	C	2	14/15	0.89	0.24	80,89,94,95	0
6	NAG	F	2	14/15	0.93	0.13	55,69,77,84	0
6	NAG	F	1	14/15	0.94	0.15	44,50,58,66	0

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





6.4 Ligands [i](#)

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

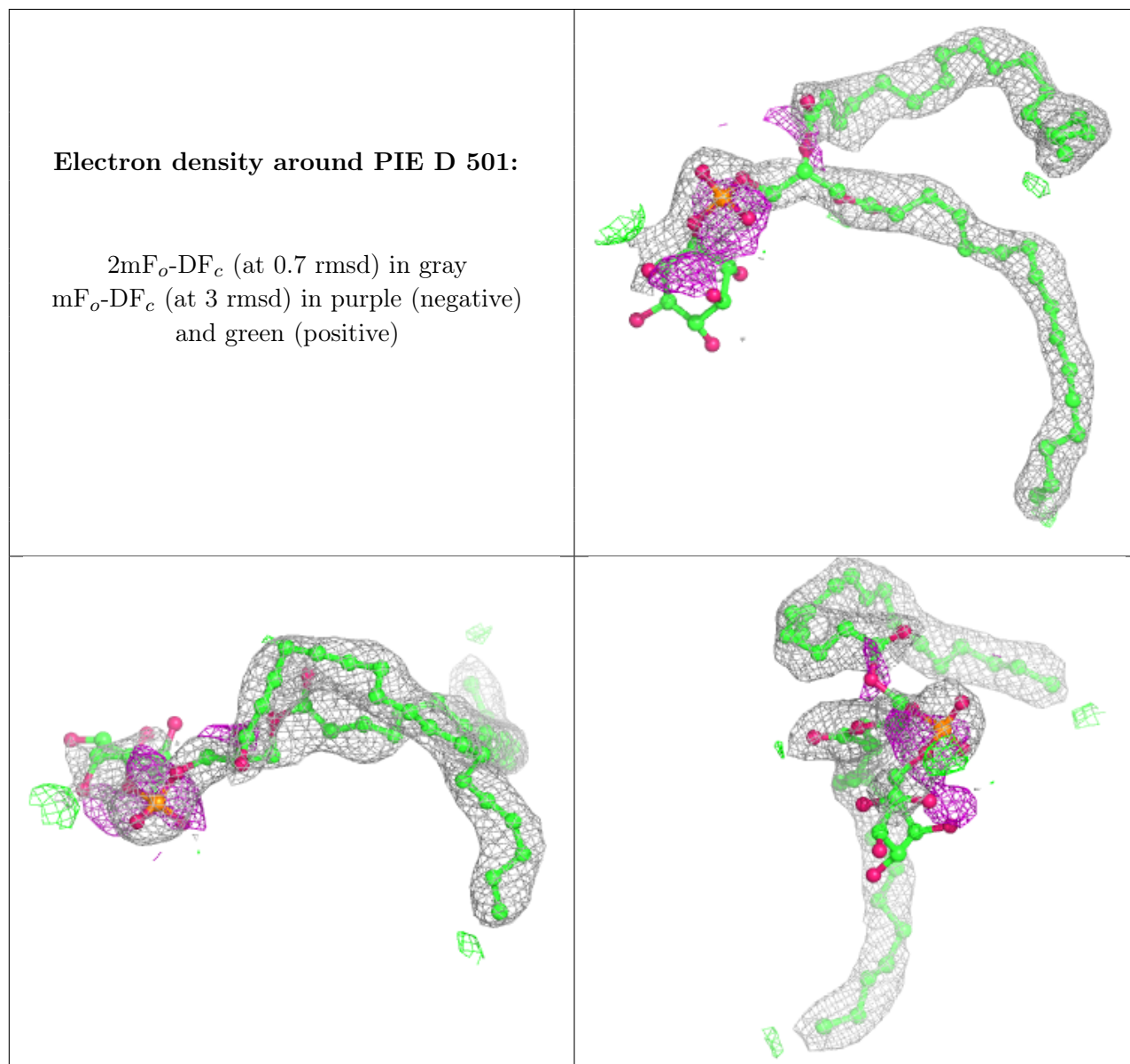
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	MAN	A	603	11/12	0.59	0.29	72,88,97,97	0
13	NA	A	610	1/1	0.66	0.22	66,66,66,66	0
8	GOL	A	602	6/6	0.67	0.23	73,84,88,89	0
7	EDO	D	503	4/4	0.69	0.26	72,80,88,90	0
12	CL	E	303	1/1	0.70	0.14	83,83,83,83	0
8	GOL	A	609	6/6	0.72	0.30	80,86,92,92	0
10	NAG	A	604	14/15	0.72	0.41	91,105,115,116	0
7	EDO	A	601	4/4	0.78	0.34	60,60,61,64	0
14	PIE	D	501	57/57	0.85	0.25	34,53,81,86	4
7	EDO	E	301	4/4	0.86	0.31	44,48,49,57	0
13	NA	A	608	1/1	0.88	0.30	68,68,68,68	0
11	CUY	A	605	38/44	0.90	0.22	37,47,54,59	0
7	EDO	D	502	4/4	0.92	0.23	47,48,57,57	0
12	CL	A	606	1/1	0.92	0.11	64,64,64,64	0

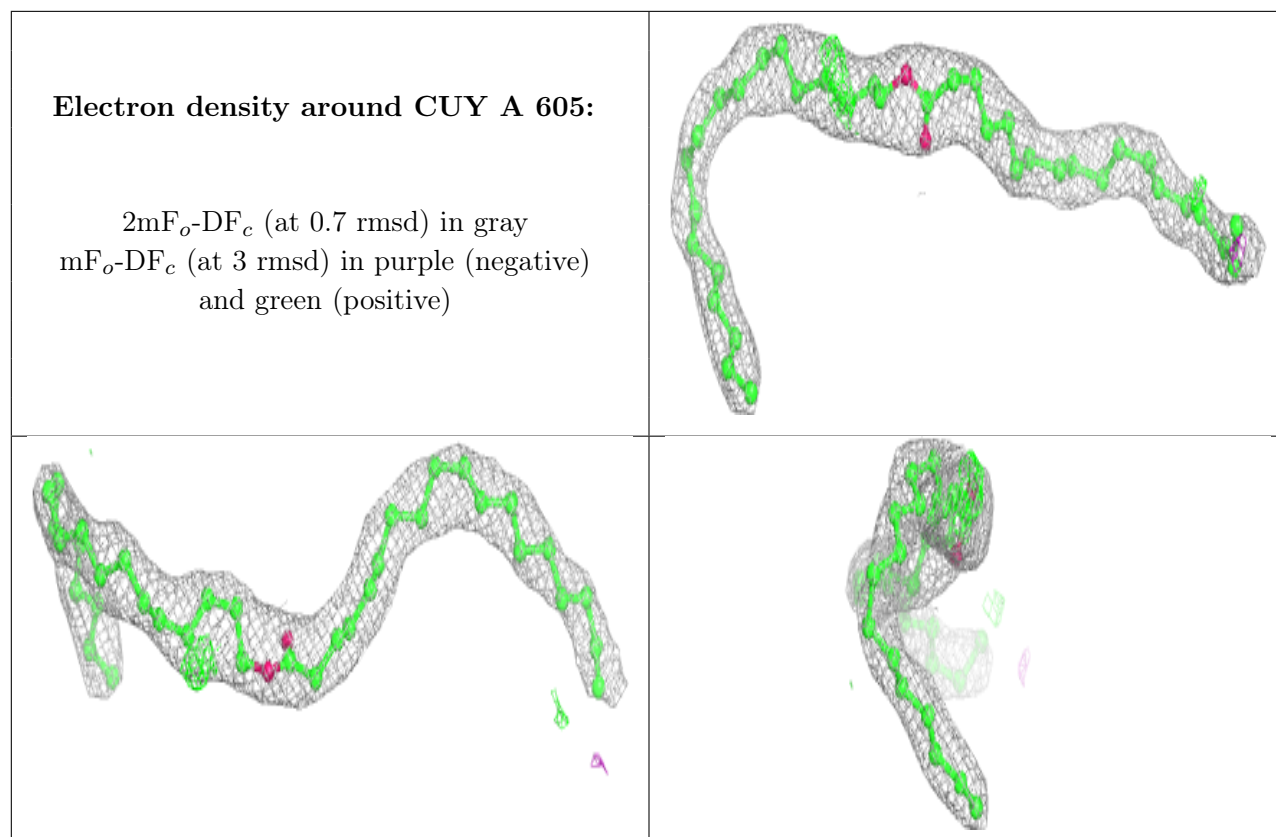
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	A	607	4/4	0.93	0.14	43,44,46,46	0
7	EDO	E	302	4/4	0.93	0.18	48,50,53,54	0
13	NA	B	201	1/1	0.94	0.19	63,63,63,63	0
12	CL	E	304	1/1	0.94	0.14	62,62,62,62	0

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.