



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 04:35 AM EDT

PDB ID : 6PW0
Title : Cytochrome C oxidase delta 6 mutant
Authors : Liu, J.; Ferguson-Miller, S.
Deposited on : 2019-07-21
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

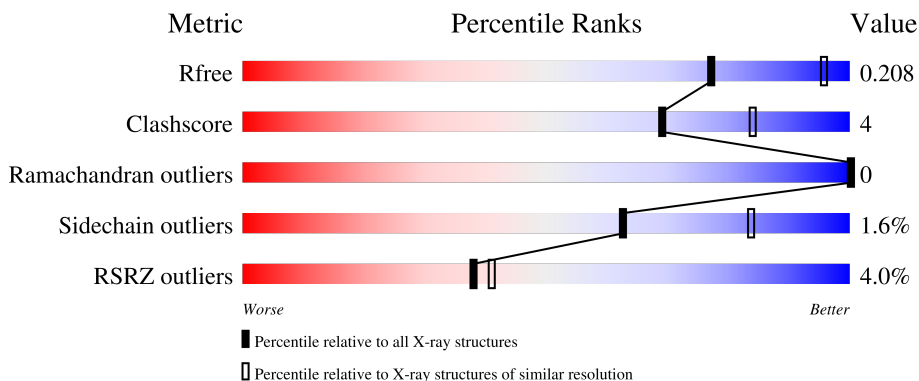
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



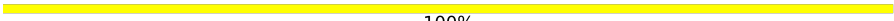
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	560	
1	C	560	
2	B	262	
2	D	262	
3	E	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	2	 100%

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
5	HEA	A	602	X	-	-	-
5	HEA	A	603	X	-	-	-
5	HEA	C	602	X	-	-	-
5	HEA	C	603	X	-	-	-
7	TRD	A	610	-	-	-	X
7	TRD	A	613	-	-	-	X

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 13540 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	535	4160	2785	655	689	31	0	0	0
1	C	531	4118	2761	645	682	30	0	0	0

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	256	2018	1316	333	363	6	0	0	0
2	D	256	1999	1305	326	362	6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

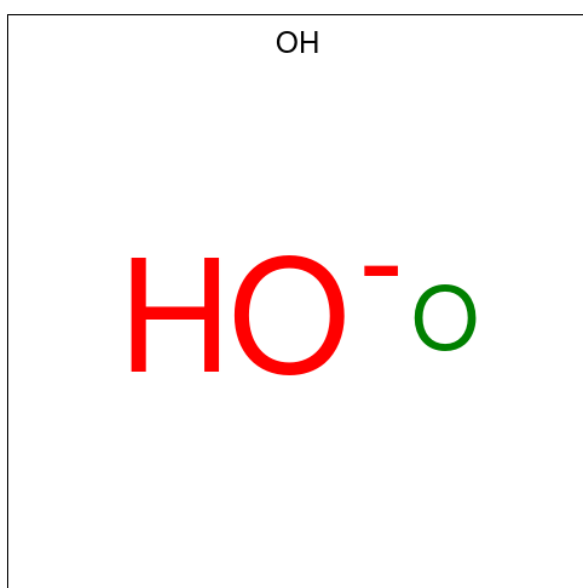
Chain	Residue	Modelled	Actual	Comment	Reference
B	282	HIS	-	expression tag	UNP Q3J5G0
B	283	HIS	-	expression tag	UNP Q3J5G0
B	284	HIS	-	expression tag	UNP Q3J5G0
B	285	HIS	-	expression tag	UNP Q3J5G0
B	286	HIS	-	expression tag	UNP Q3J5G0
B	287	HIS	-	expression tag	UNP Q3J5G0
D	282	HIS	-	expression tag	UNP Q3J5G0
D	283	HIS	-	expression tag	UNP Q3J5G0
D	284	HIS	-	expression tag	UNP Q3J5G0
D	285	HIS	-	expression tag	UNP Q3J5G0
D	286	HIS	-	expression tag	UNP Q3J5G0
D	287	HIS	-	expression tag	UNP Q3J5G0

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



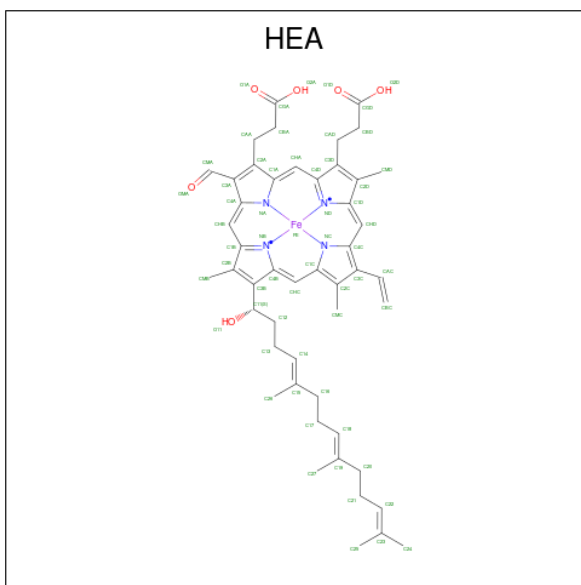
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	E	2	Total	C	O	0	0	0
			23	12	11			
3	F	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



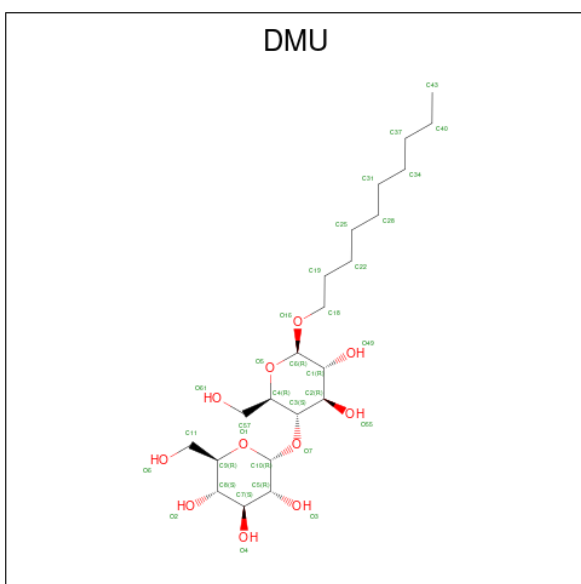
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		

- Molecule 5 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



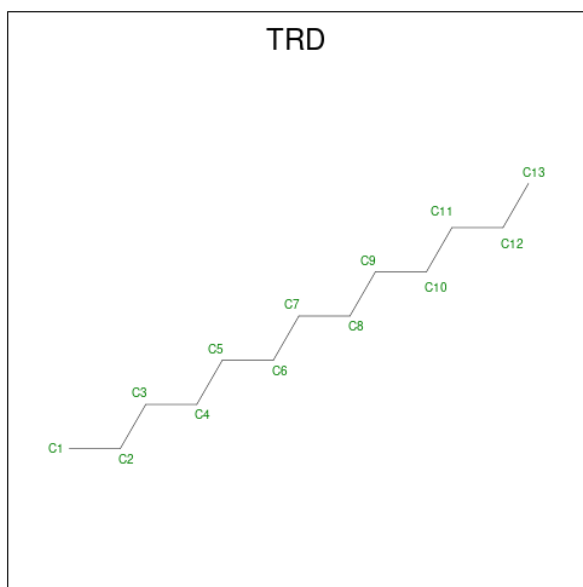
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
5	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	C	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	C	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 6 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 33 22 11	0	0
6	A	1	Total C O 33 22 11	0	0
6	A	1	Total C O 33 22 11	0	0
6	A	1	Total C O 33 22 11	0	0
6	A	1	Total C O 33 22 11	0	0
6	B	1	Total C O 30 19 11	0	0
6	C	1	Total C O 23 12 11	0	0
6	C	1	Total C O 33 22 11	0	0
6	D	1	Total C O 23 12 11	0	0

- Molecule 7 is TRIDECANE (three-letter code: TRD) (formula: C₁₃H₂₈).



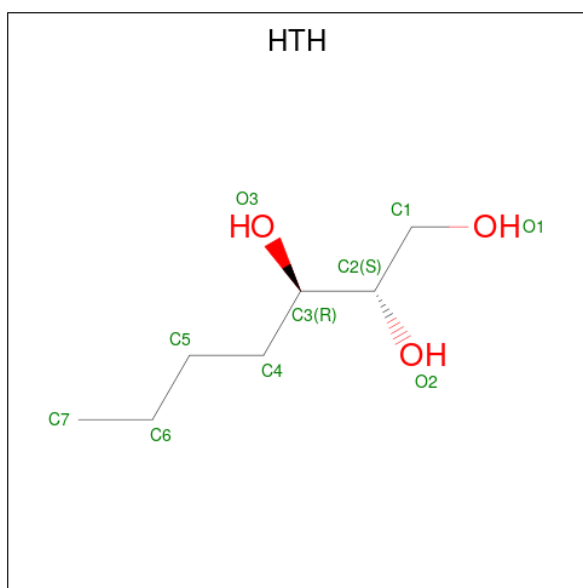
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 13 13	0	0
7	A	1	Total C 13 13	0	0
7	A	1	Total C 13 13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 13 13	0	0
7	A	1	Total C 7 7	0	0
7	A	1	Total C 13 13	0	0
7	A	1	Total C 13 13	0	0
7	B	1	Total C 13 13	0	0
7	B	1	Total C 13 13	0	0
7	B	1	Total C 13 13	0	0
7	C	1	Total C 13 13	0	0
7	C	1	Total C 13 13	0	0
7	C	1	Total C 13 13	0	0
7	D	1	Total C 13 13	0	0
7	D	1	Total C 9 9	0	0

- Molecule 8 is (2S,3R)-heptane-1,2,3-triol (three-letter code: HTH) (formula: C₇H₁₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	7	3		
8	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 9 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cu	0	0
			1	1		
9	B	2	Total	Cu	0	0
			2	2		
9	C	1	Total	Cu	0	0
			1	1		
9	D	2	Total	Cu	0	0
			2	2		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

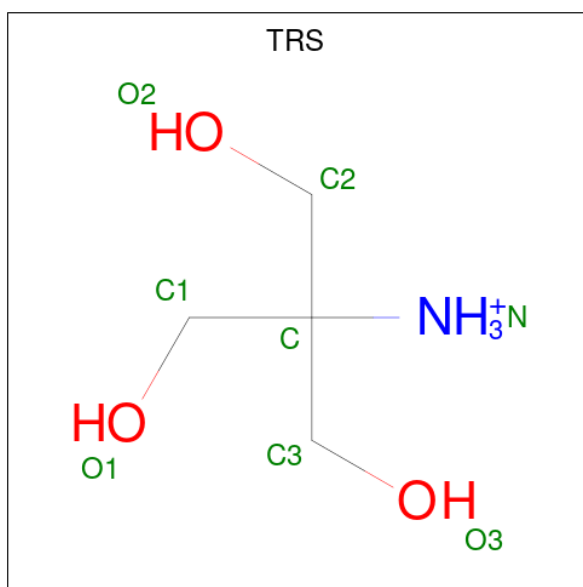
- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Ca	0	0
			1	1		
11	C	1	Total	Ca	0	0
			1	1		

- Molecule 12 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	2	Total	Cd	0	0
			2	2		
12	D	2	Total	Cd	0	0
			2	2		

- Molecule 13 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	B	1	8	4	1	3	0	0

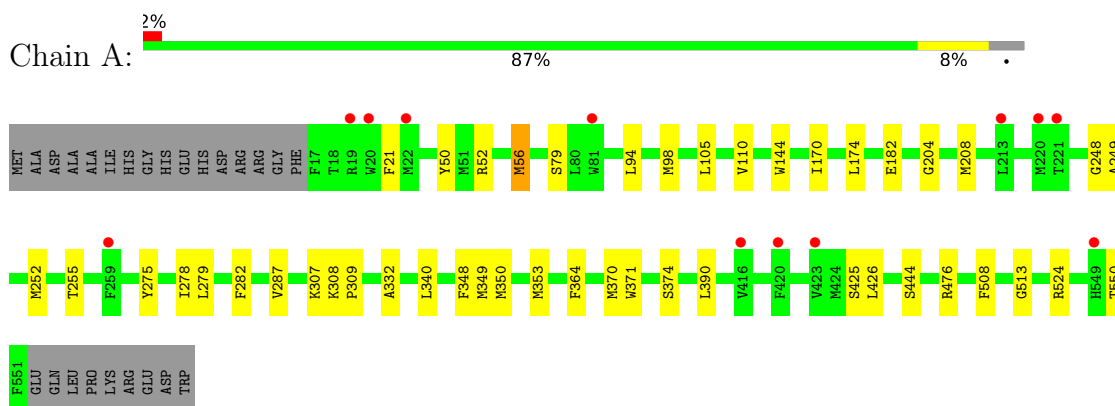
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	139	Total	O	0	0
			139	139		
14	B	129	Total	O	0	0
			129	129		
14	C	86	Total	O	0	0
			86	86		
14	D	102	Total	O	0	0
			102	102		

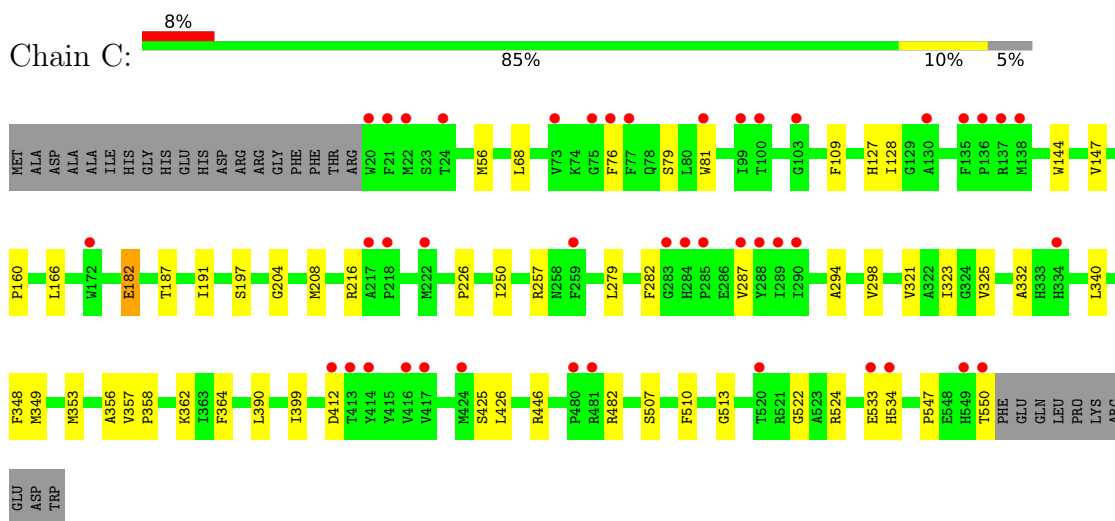
3 Residue-property plots [i](#)

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.

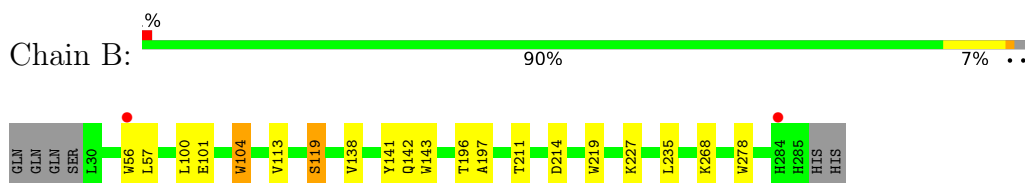
- Molecule 1: Cytochrome c oxidase subunit 1



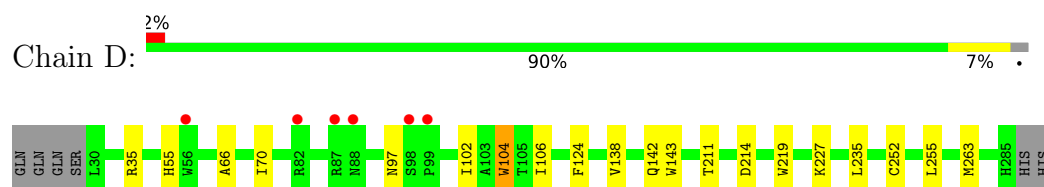
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2

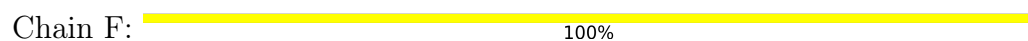


- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



GLC1
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	124.91Å 131.48Å 176.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.84 – 2.50 42.84 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.7 (42.84-2.50) 84.4 (42.84-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.14_3260, PHENIX 1.14_3260	Depositor
R, R_{free}	0.173 , 0.208 0.173 , 0.208	Depositor DCC
R_{free} test set	2984 reflections (2.54%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtrriage
Anisotropy	0.527	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.018 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13540	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: HEA, CU, CA, GLC, TRD, OH, CD, TRS, HTH, DMU, MG

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	0.38	0/4312	0.51	0/5889
1	C	0.34	0/4270	0.49	1/5836 (0.0%)
2	B	0.37	0/2080	0.54	0/2848
2	D	0.34	0/2060	0.50	0/2824
All	All	0.36	0/12722	0.51	1/17397 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	524	ARG	NE-CZ-NH2	-8.06	116.27	120.30

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	4160	0	4055	31	0
1	C	4118	0	4009	33	0
2	B	2018	0	1969	16	0
2	D	1999	0	1936	10	0
3	E	23	0	21	0	0
3	F	23	0	21	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	1	0
4	C	1	0	0	1	0
5	A	120	0	108	6	0
5	C	120	0	108	4	0
6	A	165	0	210	5	0
6	B	30	0	33	2	0
6	C	56	0	63	2	0
6	D	23	0	21	1	0
7	A	85	0	181	4	0
7	B	39	0	84	7	0
7	C	39	0	84	5	0
7	D	22	0	45	0	0
8	A	10	0	16	2	0
8	B	10	0	16	0	0
9	A	1	0	0	0	0
9	B	2	0	0	0	0
9	C	1	0	0	0	0
9	D	2	0	0	0	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
11	A	1	0	0	0	0
11	C	1	0	0	0	0
12	B	2	0	0	0	0
12	D	2	0	0	0	0
13	B	8	0	12	0	0
14	A	139	0	0	3	0
14	B	129	0	0	0	0
14	C	86	0	0	3	0
14	D	102	0	0	0	0
All	All	13540	0	12992	97	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 4.

All (97) 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:601:OH:O	14:C:701:HOH:O	1.95	0.85
4:A:601:OH:O	14:A:701:HOH:O	1.98	0.82
1:A:275:TYR:OH	1:A:279:LEU:HD13	1.84	0.78
1:A:476:ARG:HH21	7:B:304:TRD:H31	1.52	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:THR:OG1	14:A:702:HOH:O	2.06	0.73
1:C:513:GLY:HA3	7:C:607:TRD:H111	1.70	0.72
1:C:182:GLU:O	1:C:257:ARG:NH1	2.23	0.71
2:B:57:LEU:HD21	2:B:119:SER:HB2	1.73	0.70
2:B:196:THR:HB	7:B:303:TRD:H31	1.74	0.68
5:A:602:HEA:HMC1	5:A:602:HEA:HBC1	1.79	0.65
1:A:21:PHE:HB3	1:A:144:TRP:HZ2	1.61	0.63
1:A:332:ALA:HB1	1:A:340:LEU:HD11	1.80	0.62
1:C:547:PRO:HD2	1:C:550:THR:HG22	1.82	0.60
1:C:321:VAL:O	1:C:325:VAL:HG23	2.00	0.60
6:C:605:DMU:O55	14:C:702:HOH:O	2.16	0.59
1:A:390:LEU:HD13	1:A:426:LEU:HD23	1.84	0.59
1:C:446:ARG:NH1	1:C:522:GLY:O	2.36	0.58
2:B:211:THR:HB	2:B:235:LEU:HD12	1.86	0.57
1:A:204:GLY:O	1:A:208:MET:HG2	2.05	0.56
1:A:287:VAL:HB	5:A:603:HEA:CAC	2.35	0.56
5:C:602:HEA:HBC1	5:C:602:HEA:HMC1	1.87	0.56
2:B:268:LYS:HD2	7:B:303:TRD:H71	1.89	0.55
1:A:350:MET:SD	8:A:616:HTH:O2	2.63	0.55
2:B:278:TRP:HE1	7:B:303:TRD:H42	1.71	0.55
1:C:287:VAL:HB	5:C:603:HEA:CAC	2.36	0.55
2:B:196:THR:HA	7:B:303:TRD:H52	1.88	0.54
1:C:534:HIS:HD2	14:C:781:HOH:O	1.90	0.54
1:A:364:PHE:HB3	2:B:104:TRP:CE3	2.41	0.54
1:C:204:GLY:O	1:C:208:MET:HG2	2.07	0.54
1:C:533:GLU:H	1:C:533:GLU:CD	2.10	0.54
2:D:124:PHE:HB3	6:D:301:DMU:H5	1.90	0.53
1:C:349:MET:O	1:C:353:MET:HG3	2.08	0.53
6:A:605:DMU:H2	7:A:610:TRD:H121	1.92	0.52
1:C:390:LEU:HD13	1:C:426:LEU:HD23	1.92	0.52
1:C:287:VAL:HB	5:C:603:HEA:HAC	1.90	0.52
1:C:128:ILE:HB	1:C:216:ARG:HG2	1.91	0.51
1:C:187:THR:O	1:C:191:ILE:HG13	2.09	0.51
1:C:81:TRP:CZ2	7:C:608:TRD:H92	2.46	0.51
1:A:56:MET:HE1	6:A:605:DMU:H7	1.93	0.51
1:A:508:PHE:HB2	5:A:602:HEA:H261	1.93	0.50
6:A:605:DMU:H10	7:A:609:TRD:H52	1.94	0.50
2:B:138:VAL:HG11	2:B:219:TRP:CD1	2.46	0.50
1:A:287:VAL:HB	5:A:603:HEA:HAC	1.94	0.50
2:D:66:ALA:O	2:D:70:ILE:HG12	2.12	0.50
2:B:104:TRP:HZ3	6:B:301:DMU:H16	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:SER:HB3	6:A:604:DMU:H8	1.94	0.49
2:B:101:GLU:HA	2:B:104:TRP:CD1	2.48	0.49
1:A:513:GLY:HA3	6:A:608:DMU:H20	1.95	0.49
8:A:616:HTH:H3	2:B:113:VAL:HA	1.95	0.49
1:C:364:PHE:HB3	2:D:104:TRP:CE3	2.48	0.49
1:A:249:ALA:HA	1:A:252:MET:HE3	1.95	0.48
1:C:68:LEU:HD12	7:C:606:TRD:H31	1.95	0.48
1:A:105:LEU:O	1:A:110:VAL:HG23	2.14	0.48
1:A:307:LYS:HE2	1:A:374:SER:HB3	1.96	0.48
1:A:249:ALA:HB2	1:A:278:ILE:HG22	1.96	0.47
2:D:138:VAL:HG11	2:D:219:TRP:CD1	2.48	0.47
1:A:94:LEU:O	1:A:98:MET:HG2	2.15	0.47
1:C:144:TRP:CE3	1:C:147:VAL:HG11	2.50	0.46
2:D:142:GLN:HB3	2:D:143:TRP:CE2	2.50	0.46
1:C:482:ARG:HD3	2:D:255:LEU:HB2	1.98	0.46
1:C:323:ILE:HG13	1:C:358:PRO:HB2	1.97	0.45
1:C:191:ILE:HG23	1:C:250:ILE:HB	1.99	0.45
1:A:349:MET:O	1:A:353:MET:HG3	2.17	0.44
2:B:56:TRP:CE2	7:B:302:TRD:H101	2.52	0.44
2:D:252:CYS:HB2	2:D:263:MET:HG3	1.98	0.44
2:B:197:ALA:H	7:B:303:TRD:H52	1.83	0.44
1:A:50:TYR:OH	1:A:79:SER:HB3	2.18	0.44
6:C:605:DMU:H10	7:C:608:TRD:H62	1.99	0.44
1:A:371:TRP:CD1	6:B:301:DMU:H9	2.53	0.44
1:C:357:VAL:HB	1:C:358:PRO:HD3	2.00	0.43
1:C:332:ALA:HB3	1:C:348:PHE:CG	2.53	0.43
1:C:109:PHE:CE1	1:C:197:SER:HB2	2.54	0.43
1:A:425:SER:HB2	5:A:602:HEA:HMC2	2.00	0.43
1:A:332:ALA:HB3	1:A:348:PHE:CD2	2.54	0.42
2:B:141:TYR:O	2:B:143:TRP:HA	2.20	0.42
2:D:211:THR:HB	2:D:235:LEU:HD12	2.01	0.42
1:A:308:LYS:HG3	1:A:309:PRO:HD2	2.02	0.42
2:B:100:LEU:HD12	2:B:100:LEU:HA	1.81	0.42
1:A:248:GLY:HA3	14:A:833:HOH:O	2.19	0.42
1:A:287:VAL:HB	5:A:603:HEA:C3C	2.50	0.42
1:C:127:HIS:HB3	1:C:226:PRO:HG2	2.02	0.42
1:C:425:SER:HB2	5:C:602:HEA:HMC2	2.02	0.42
1:A:255:THR:HG21	7:A:614:TRD:H22	2.02	0.42
1:C:510:PHE:HA	7:C:607:TRD:H122	2.02	0.41
1:C:356:ALA:HB2	1:C:399:ILE:HD11	2.01	0.41
1:C:332:ALA:HB1	1:C:340:LEU:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1:GLC:H62	3:F:1:GLC:H1	1.82	0.41
7:A:614:TRD:H71	7:A:614:TRD:H42	1.83	0.41
2:D:102:ILE:O	2:D:106:ILE:HG12	2.21	0.41
1:C:294:ALA:O	1:C:298:VAL:HG23	2.21	0.41
1:A:370:MET:HB2	1:A:370:MET:HE2	1.89	0.41
2:B:142:GLN:HB3	2:B:143:TRP:CE2	2.56	0.41
1:C:160:PRO:HA	1:C:166:LEU:HD23	2.02	0.41
1:C:362:LYS:HB3	1:C:362:LYS:HE3	1.87	0.40
1:A:170:ILE:HD11	1:A:174:LEU:HD22	2.02	0.40
1:C:76:PHE:O	1:C:79:SER:HB2	2.22	0.40
2:D:97:ASN:ND2	3:F:1:GLC:H62	2.37	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	533/560 (95%)	519 (97%)	14 (3%)	0	100	100
1	C	529/560 (94%)	517 (98%)	12 (2%)	0	100	100
2	B	254/262 (97%)	242 (95%)	12 (5%)	0	100	100
2	D	254/262 (97%)	242 (95%)	12 (5%)	0	100	100
All	All	1570/1644 (96%)	1520 (97%)	50 (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	424/455 (93%)	419 (99%)	5 (1%)	71	88
1	C	419/455 (92%)	413 (99%)	6 (1%)	67	86
2	B	213/221 (96%)	209 (98%)	4 (2%)	57	80
2	D	209/221 (95%)	204 (98%)	5 (2%)	49	74
All	All	1265/1352 (94%)	1245 (98%)	20 (2%)	62	84

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	56	MET
1	A	182	GLU
1	A	282	PHE
1	A	524	ARG
2	B	104	TRP
2	B	119	SER
2	B	214	ASP
2	B	227	LYS
1	C	56	MET
1	C	182	GLU
1	C	279	LEU
1	C	282	PHE
1	C	412	ASP
1	C	507	SER
2	D	35	ARG
2	D	55	HIS
2	D	104	TRP
2	D	214	ASP
2	D	227	LYS

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

Mol	Chain	Res	Type
1	C	214	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	E	1	3	12,12,12	0.54	0	17,17,17	0.47	0
3	GLC	E	2	3	11,11,12	0.62	0	15,15,17	0.88	1 (6%)
3	GLC	F	1	3	12,12,12	0.56	0	17,17,17	0.72	0
3	GLC	F	2	3	11,11,12	0.57	0	15,15,17	1.01	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	E	1	3	-	1/2/22/22	0/1/1/1
3	GLC	E	2	3	-	1/2/19/22	0/1/1/1
3	GLC	F	1	3	-	1/2/22/22	0/1/1/1
3	GLC	F	2	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	GLC	C1-O5-C5	2.78	115.95	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	GLC	O5-C5-C6	2.40	110.96	107.20
3	E	2	GLC	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

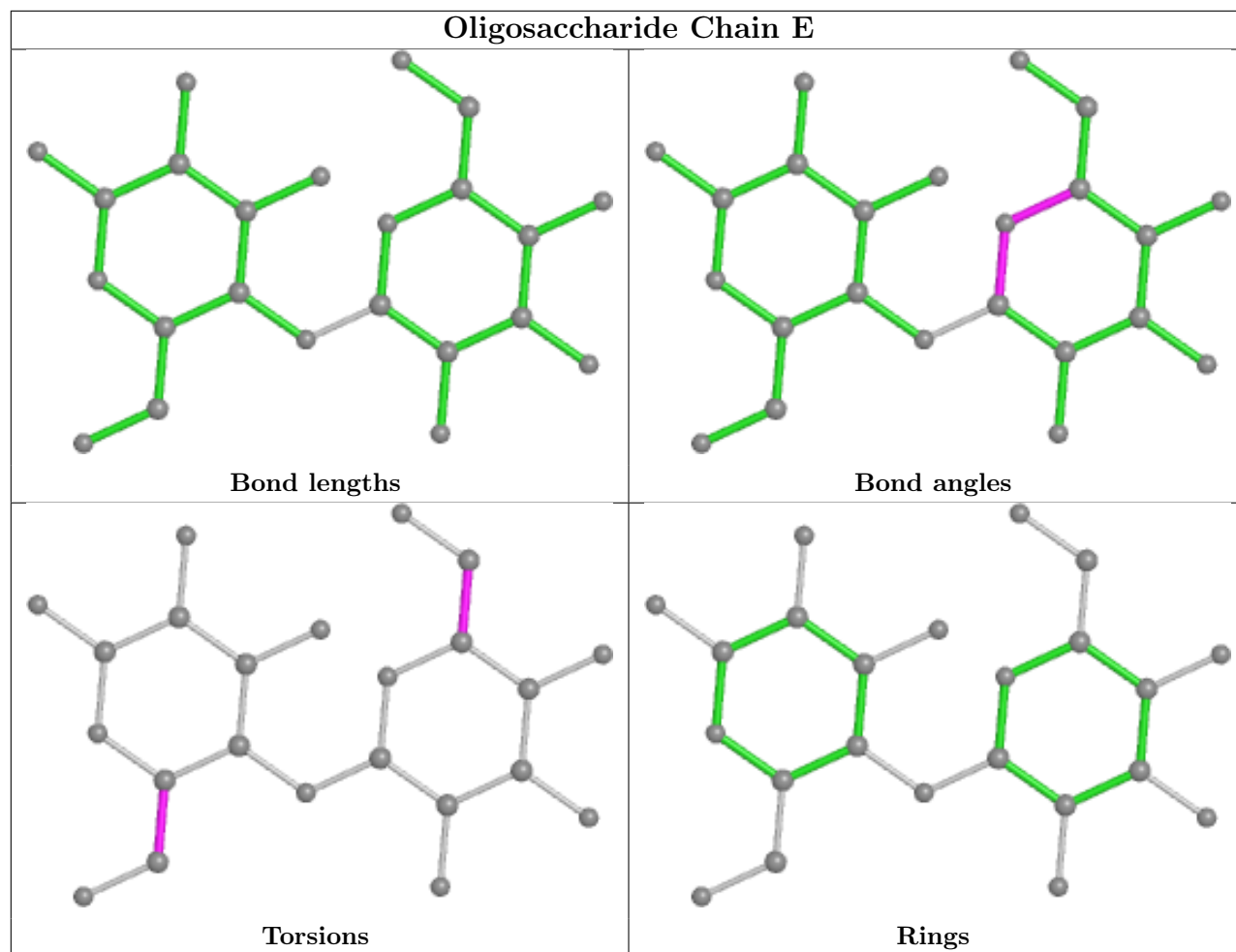
Mol	Chain	Res	Type	Atoms
3	E	1	GLC	O5-C5-C6-O6
3	F	1	GLC	O5-C5-C6-O6
3	F	2	GLC	O5-C5-C6-O6
3	E	2	GLC	O5-C5-C6-O6

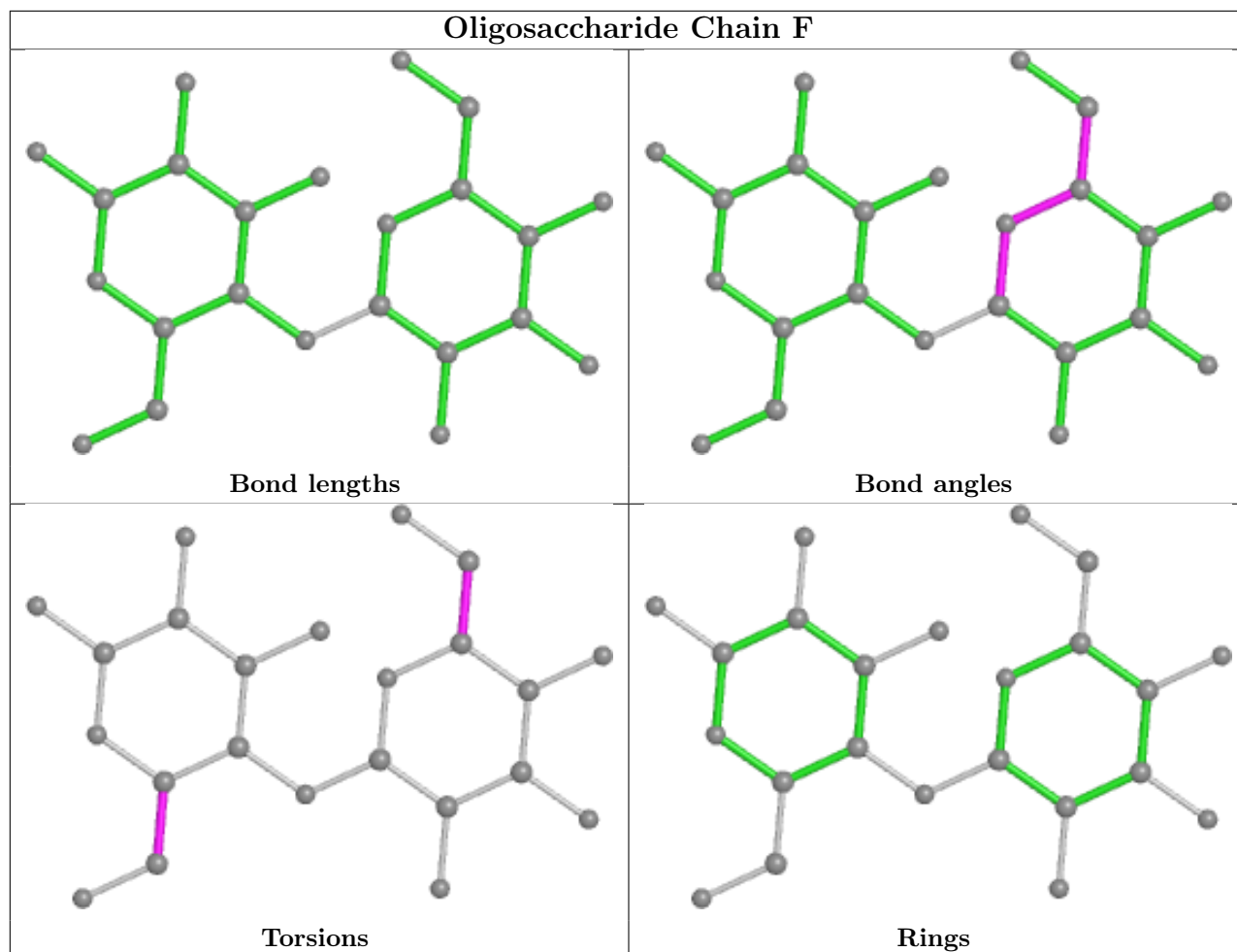
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	GLC	2	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 47 ligands modelled in this entry, 2 are modelled with single atom and 14 are monoatomic - leaving 31 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	DMU	C	604	-	24,24,34	2.09	14 (58%)	35,35,45	0.99	2 (5%)
6	DMU	B	301	-	31,31,34	2.01	13 (41%)	42,42,45	1.04	2 (4%)
6	DMU	A	604	-	34,34,34	1.96	12 (35%)	45,45,45	1.19	4 (8%)
6	DMU	A	607	-	34,34,34	1.93	12 (35%)	45,45,45	1.21	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TRD	C	608	-	12,12,12	0.13	0	11,11,11	0.78	0
7	TRD	B	304	-	12,12,12	0.16	0	11,11,11	0.73	0
5	HEA	A	603	14,1	57,67,67	2.11	17 (29%)	61,103,103	2.36	22 (36%)
7	TRD	C	606	-	12,12,12	0.14	0	11,11,11	0.79	0
8	HTH	B	306	-	9,9,9	0.33	0	10,10,10	1.23	2 (20%)
6	DMU	D	301	-	24,24,34	2.08	12 (50%)	35,35,45	1.39	6 (17%)
7	TRD	A	611	-	12,12,12	0.18	0	11,11,11	0.72	0
5	HEA	A	602	1	57,67,67	2.09	15 (26%)	61,103,103	2.44	24 (39%)
8	HTH	A	616	-	9,9,9	0.52	0	10,10,10	1.38	1 (10%)
5	HEA	C	602	1	57,67,67	2.16	17 (29%)	61,103,103	2.35	23 (37%)
5	HEA	C	603	14,1	57,67,67	2.11	17 (29%)	61,103,103	2.40	23 (37%)
7	TRD	A	614	-	12,12,12	0.13	0	11,11,11	0.78	0
13	TRS	B	311	-	7,7,7	0.36	0	9,9,9	1.10	0
7	TRD	D	302	-	12,12,12	0.12	0	11,11,11	0.90	0
7	TRD	A	615	-	12,12,12	0.17	0	11,11,11	0.71	0
6	DMU	A	605	-	34,34,34	1.94	12 (35%)	45,45,45	1.18	5 (11%)
6	DMU	A	606	-	34,34,34	1.93	12 (35%)	45,45,45	1.46	9 (20%)
7	TRD	C	607	-	12,12,12	0.14	0	11,11,11	0.74	0
7	TRD	A	613	-	6,6,12	0.18	0	5,5,11	0.48	0
7	TRD	A	612	-	12,12,12	0.17	0	11,11,11	0.75	0
7	TRD	B	302	-	12,12,12	0.16	0	11,11,11	0.66	0
7	TRD	A	609	-	12,12,12	0.12	0	11,11,11	0.78	0
7	TRD	A	610	-	12,12,12	0.14	0	11,11,11	0.82	0
7	TRD	D	303	-	8,8,12	0.12	0	7,7,11	0.84	0
6	DMU	A	608	-	34,34,34	1.89	9 (26%)	45,45,45	1.24	4 (8%)
6	DMU	C	605	-	34,34,34	2.00	14 (41%)	45,45,45	1.43	6 (13%)
7	TRD	B	303	-	12,12,12	0.20	0	11,11,11	0.46	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
6	DMU	C	604	-	-	4/8/48/59	0/2/2/2
6	DMU	B	301	-	-	10/16/56/59	0/2/2/2
6	DMU	A	604	-	-	11/19/59/59	0/2/2/2
6	DMU	A	607	-	-	8/19/59/59	0/2/2/2
7	TRD	C	608	-	-	0/10/10/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TRD	B	304	-	-	6/10/10/10	-
5	HEA	A	603	14,1	2/2/7/16	4/32/76/76	-
7	TRD	C	606	-	-	4/10/10/10	-
8	HTH	B	306	-	-	6/10/10/10	-
6	DMU	D	301	-	-	4/8/48/59	0/2/2/2
7	TRD	A	611	-	-	2/10/10/10	-
5	HEA	A	602	1	2/2/7/16	5/32/76/76	-
8	HTH	A	616	-	-	5/10/10/10	-
5	HEA	C	602	1	2/2/7/16	5/32/76/76	-
5	HEA	C	603	14,1	2/2/7/16	6/32/76/76	-
7	TRD	A	614	-	-	6/10/10/10	-
13	TRS	B	311	-	-	6/9/9/9	-
7	TRD	D	302	-	-	5/10/10/10	-
7	TRD	A	615	-	-	6/10/10/10	-
6	DMU	A	605	-	-	11/19/59/59	0/2/2/2
6	DMU	A	606	-	-	5/19/59/59	0/2/2/2
7	TRD	C	607	-	-	1/10/10/10	-
7	TRD	A	613	-	-	2/4/4/10	-
7	TRD	A	612	-	-	3/10/10/10	-
7	TRD	B	302	-	-	7/10/10/10	-
7	TRD	A	609	-	-	0/10/10/10	-
7	TRD	A	610	-	-	1/10/10/10	-
7	TRD	D	303	-	-	4/6/6/10	-
6	DMU	A	608	-	-	7/19/59/59	0/2/2/2
6	DMU	C	605	-	-	10/19/59/59	0/2/2/2
7	TRD	B	303	-	-	6/10/10/10	-

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEA	C3B-C2B	5.83	1.47	1.34
5	C	602	HEA	C3B-C2B	5.79	1.47	1.34
5	C	602	HEA	C3C-C2C	5.68	1.48	1.40
5	C	603	HEA	C3B-C2B	5.58	1.47	1.34
5	C	602	HEA	C3D-C2D	5.34	1.48	1.36
5	A	603	HEA	C3A-C2A	5.25	1.47	1.40
5	A	603	HEA	CHD-C1D	5.20	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	603	HEA	CHD-C1D	5.18	1.48	1.35
5	C	602	HEA	C3A-C2A	5.14	1.47	1.40
5	A	603	HEA	C3B-C2B	5.12	1.46	1.34
5	A	602	HEA	C3D-C2D	5.12	1.47	1.36
5	C	603	HEA	C3D-C2D	5.06	1.47	1.36
5	A	602	HEA	C3C-C2C	4.99	1.47	1.40
5	C	603	HEA	C3A-C2A	4.98	1.47	1.40
6	A	608	DMU	O16-C6	-4.95	1.31	1.40
5	A	603	HEA	C3D-C2D	4.93	1.47	1.36
5	C	602	HEA	CHD-C1D	4.93	1.47	1.35
5	A	603	HEA	CHC-C4B	4.91	1.47	1.35
5	C	602	HEA	CHC-C4B	4.87	1.47	1.35
5	C	603	HEA	CHC-C4B	4.85	1.47	1.35
5	A	602	HEA	C3A-C2A	4.79	1.47	1.40
5	C	603	HEA	C3C-C2C	4.64	1.46	1.40
5	A	602	HEA	CHC-C4B	4.61	1.46	1.35
5	A	602	HEA	CHD-C1D	4.59	1.46	1.35
5	A	603	HEA	C3C-C2C	4.50	1.46	1.40
6	A	607	DMU	O16-C6	-4.31	1.32	1.40
6	A	605	DMU	O16-C6	-4.21	1.33	1.40
6	A	606	DMU	O16-C6	-4.14	1.33	1.40
6	C	605	DMU	O16-C6	-3.98	1.33	1.40
6	A	604	DMU	O16-C6	-3.97	1.33	1.40
6	B	301	DMU	O16-C6	-3.90	1.33	1.40
6	C	605	DMU	O5-C6	3.90	1.51	1.41
6	B	301	DMU	O1-C9	3.82	1.53	1.44
6	A	606	DMU	C11-C9	-3.73	1.39	1.51
6	A	605	DMU	O1-C9	3.72	1.53	1.44
6	A	608	DMU	C11-C9	-3.69	1.39	1.51
6	C	604	DMU	O1-C9	3.68	1.53	1.44
6	A	604	DMU	O1-C9	3.66	1.53	1.44
6	C	605	DMU	C11-C9	-3.65	1.39	1.51
6	B	301	DMU	C11-C9	-3.63	1.39	1.51
6	C	604	DMU	C11-C9	-3.63	1.39	1.51
6	A	608	DMU	O1-C9	3.62	1.53	1.44
6	A	604	DMU	C11-C9	-3.61	1.39	1.51
6	D	301	DMU	C11-C9	-3.61	1.39	1.51
6	A	605	DMU	C11-C9	-3.59	1.39	1.51
6	D	301	DMU	O1-C9	3.53	1.52	1.44
6	A	607	DMU	C11-C9	-3.52	1.40	1.51
6	A	606	DMU	O5-C6	3.45	1.50	1.41
6	A	607	DMU	O1-C9	3.43	1.52	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	605	DMU	O1-C9	3.40	1.52	1.44
6	A	607	DMU	O5-C6	3.36	1.50	1.41
6	A	604	DMU	O5-C6	3.34	1.50	1.41
6	A	606	DMU	O1-C9	3.33	1.52	1.44
5	C	602	HEA	C2A-C1A	3.31	1.50	1.42
5	A	602	HEA	C4B-NB	-3.25	1.34	1.40
6	B	301	DMU	O5-C6	3.22	1.50	1.41
5	A	603	HEA	C4B-C3B	3.22	1.50	1.44
5	A	603	HEA	FE-NB	3.19	2.12	1.96
6	A	605	DMU	O5-C6	3.08	1.49	1.41
5	C	603	HEA	FE-NB	3.07	2.12	1.96
5	A	602	HEA	C2A-C1A	3.06	1.49	1.42
5	A	602	HEA	FE-ND	3.04	2.11	1.96
6	C	604	DMU	O5-C6	2.98	1.50	1.42
5	A	603	HEA	C4B-NB	-2.97	1.35	1.40
5	C	603	HEA	FE-ND	2.96	2.11	1.96
6	A	607	DMU	C7-C5	-2.94	1.44	1.52
6	A	608	DMU	C2-C3	-2.92	1.44	1.52
5	A	603	HEA	C2A-C1A	2.92	1.49	1.42
6	C	605	DMU	C7-C5	-2.92	1.44	1.52
5	C	602	HEA	C1D-ND	-2.86	1.35	1.40
6	A	608	DMU	O4-C7	2.85	1.49	1.43
6	A	605	DMU	C7-C5	-2.85	1.45	1.52
6	A	605	DMU	O7-C3	2.84	1.51	1.43
6	C	605	DMU	O7-C3	2.83	1.51	1.43
6	B	301	DMU	O7-C3	2.83	1.51	1.43
6	D	301	DMU	C7-C5	-2.83	1.45	1.52
5	C	603	HEA	C1D-C2D	2.83	1.50	1.44
5	C	602	HEA	C4B-NB	-2.83	1.35	1.40
5	A	603	HEA	FE-ND	2.83	2.10	1.96
5	C	603	HEA	C2A-C1A	2.82	1.48	1.42
5	A	603	HEA	C1D-ND	-2.81	1.35	1.40
6	A	607	DMU	C2-C3	-2.80	1.44	1.52
5	C	602	HEA	FE-NB	2.80	2.10	1.96
5	C	602	HEA	FE-ND	2.80	2.10	1.96
5	A	602	HEA	C1D-ND	-2.79	1.35	1.40
6	A	604	DMU	C2-C3	-2.78	1.44	1.52
6	A	604	DMU	O7-C3	2.78	1.51	1.43
6	D	301	DMU	O5-C6	2.75	1.49	1.42
6	B	301	DMU	O4-C7	2.75	1.49	1.43
6	A	604	DMU	O4-C7	2.70	1.49	1.43
5	C	603	HEA	C4B-NB	-2.69	1.35	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	604	DMU	O7-C3	2.68	1.50	1.43
6	C	605	DMU	O4-C7	2.68	1.49	1.43
6	D	301	DMU	O7-C3	2.68	1.50	1.43
6	C	604	DMU	C2-C3	-2.63	1.45	1.52
6	C	605	DMU	C2-C3	-2.63	1.45	1.52
6	A	608	DMU	O7-C3	2.62	1.50	1.43
5	C	603	HEA	C4B-C3B	2.62	1.49	1.44
6	A	608	DMU	O5-C6	2.62	1.48	1.41
6	A	604	DMU	C7-C5	-2.61	1.45	1.52
5	A	602	HEA	FE-NB	2.61	2.09	1.96
6	A	605	DMU	O4-C7	2.61	1.49	1.43
6	A	606	DMU	O5-C4	2.60	1.50	1.44
6	A	606	DMU	C7-C5	-2.60	1.45	1.52
5	A	603	HEA	C1D-C2D	2.59	1.49	1.44
6	C	604	DMU	C7-C5	-2.59	1.45	1.52
6	A	606	DMU	C2-C3	-2.58	1.45	1.52
6	C	604	DMU	O4-C7	2.57	1.49	1.43
5	C	603	HEA	C4C-CHD	2.54	1.48	1.41
5	C	603	HEA	C1D-ND	-2.54	1.35	1.40
6	D	301	DMU	O4-C7	2.53	1.48	1.43
6	B	301	DMU	C2-C3	-2.52	1.45	1.52
6	A	606	DMU	O7-C3	2.50	1.50	1.43
6	A	608	DMU	C7-C5	-2.49	1.46	1.52
6	A	604	DMU	O5-C4	2.48	1.50	1.44
5	A	602	HEA	C1D-C2D	2.48	1.49	1.44
6	B	301	DMU	C7-C5	-2.48	1.46	1.52
6	A	607	DMU	O4-C7	2.46	1.48	1.43
6	A	604	DMU	C8-C9	2.44	1.58	1.53
6	A	605	DMU	C8-C9	2.43	1.58	1.53
6	D	301	DMU	C8-C9	2.43	1.58	1.53
6	C	605	DMU	O1-C10	2.40	1.48	1.41
6	D	301	DMU	C2-C3	-2.40	1.45	1.52
6	C	605	DMU	O55-C2	2.40	1.48	1.43
5	C	602	HEA	C4B-C3B	2.37	1.48	1.44
5	A	603	HEA	C4C-CHD	2.37	1.47	1.41
5	C	602	HEA	C1D-C2D	2.35	1.49	1.44
6	A	605	DMU	O55-C2	2.35	1.48	1.43
6	A	606	DMU	O4-C7	2.33	1.48	1.43
6	B	301	DMU	C8-C9	2.32	1.57	1.53
6	C	605	DMU	O5-C4	2.30	1.49	1.44
6	A	607	DMU	O55-C2	2.29	1.48	1.43
6	A	606	DMU	O55-C2	2.28	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	605	DMU	O3-C5	2.28	1.48	1.43
6	A	606	DMU	O3-C5	2.27	1.48	1.43
6	D	301	DMU	O16-C6	-2.26	1.32	1.39
5	C	603	HEA	C1C-CHC	2.26	1.47	1.41
6	A	605	DMU	C2-C3	-2.26	1.46	1.52
6	D	301	DMU	O3-C5	2.24	1.48	1.43
6	A	605	DMU	O1-C10	2.24	1.47	1.41
6	B	301	DMU	O1-C10	2.23	1.47	1.41
5	A	603	HEA	C1C-CHC	2.23	1.47	1.41
6	A	607	DMU	C8-C9	2.23	1.57	1.53
5	C	602	HEA	CHB-C1B	2.22	1.47	1.41
6	C	604	DMU	O16-C6	-2.21	1.32	1.39
6	A	604	DMU	O55-C2	2.21	1.48	1.43
6	A	604	DMU	O3-C5	2.21	1.48	1.43
5	C	602	HEA	C1C-CHC	2.21	1.47	1.41
6	D	301	DMU	O55-C2	2.21	1.48	1.43
6	A	607	DMU	C3-C4	-2.20	1.47	1.52
6	A	608	DMU	C8-C9	2.19	1.57	1.53
5	C	602	HEA	C4C-CHD	2.19	1.47	1.41
6	C	605	DMU	C8-C9	2.19	1.57	1.53
6	A	606	DMU	C8-C9	2.17	1.57	1.53
6	D	301	DMU	O5-C4	2.16	1.49	1.44
5	A	602	HEA	C4C-CHD	2.16	1.47	1.41
6	B	301	DMU	O55-C2	2.16	1.48	1.43
6	A	605	DMU	O3-C5	2.16	1.48	1.43
6	C	604	DMU	O55-C2	2.16	1.48	1.43
5	A	603	HEA	C1B-C2B	2.15	1.48	1.44
6	A	607	DMU	O3-C5	2.14	1.48	1.43
6	C	604	DMU	O3-C5	2.13	1.48	1.43
5	C	603	HEA	CHB-C1B	2.12	1.47	1.41
6	C	604	DMU	C8-C9	2.11	1.57	1.53
5	A	602	HEA	C1C-CHC	2.10	1.46	1.41
6	A	607	DMU	O7-C3	2.10	1.49	1.43
6	B	301	DMU	O3-C5	2.10	1.47	1.43
6	B	301	DMU	O5-C4	2.09	1.49	1.44
5	C	602	HEA	CHA-C4D	2.09	1.47	1.41
5	C	603	HEA	C1B-C2B	2.09	1.48	1.44
6	C	604	DMU	O5-C4	2.07	1.49	1.44
6	C	604	DMU	O1-C10	2.05	1.47	1.41
5	A	603	HEA	CHA-C4D	2.05	1.47	1.41
5	A	602	HEA	CHB-C1B	2.01	1.46	1.41
6	C	605	DMU	C2-C1	-2.01	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	604	DMU	C8-C7	-2.00	1.47	1.52

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	603	HEA	C3D-C4D-ND	6.60	116.75	110.36
5	A	602	HEA	C3D-C4D-ND	6.32	116.48	110.36
5	A	603	HEA	C3D-C4D-ND	6.19	116.35	110.36
5	C	602	HEA	C3D-C4D-ND	6.04	116.20	110.36
5	A	603	HEA	C2B-C1B-NB	6.01	117.08	109.88
5	C	603	HEA	C2B-C1B-NB	5.62	116.61	109.88
5	C	602	HEA	C2B-C1B-NB	5.41	116.37	109.88
5	A	602	HEA	C2B-C1B-NB	5.30	116.23	109.88
5	C	603	HEA	C3B-C4B-NB	5.21	116.02	109.84
5	C	602	HEA	C3B-C4B-NB	5.21	116.01	109.84
5	A	602	HEA	C2D-C1D-ND	5.14	115.93	109.84
5	C	603	HEA	CBA-CAA-C2A	-5.13	103.95	112.60
5	A	603	HEA	C3B-C4B-NB	5.12	115.90	109.84
5	A	602	HEA	C3B-C4B-NB	5.08	115.86	109.84
5	A	603	HEA	CBA-CAA-C2A	-4.62	104.82	112.60
5	C	602	HEA	C2D-C1D-ND	4.61	115.30	109.84
5	C	603	HEA	C2D-C1D-ND	4.43	115.09	109.84
6	C	605	DMU	O1-C10-C5	4.35	119.56	110.35
5	A	602	HEA	C1D-C2D-C3D	-4.33	102.40	106.96
5	C	603	HEA	C1D-C2D-C3D	-4.23	102.51	106.96
5	C	602	HEA	C3C-C4C-NC	4.14	114.56	109.21
5	A	603	HEA	C1B-C2B-C3B	-4.13	101.86	106.80
5	A	602	HEA	C1B-C2B-C3B	-4.08	101.92	106.80
5	C	602	HEA	CBA-CAA-C2A	-4.05	105.78	112.60
5	A	602	HEA	C3C-C4C-NC	4.04	114.43	109.21
5	A	603	HEA	C2D-C1D-ND	4.02	114.61	109.84
8	A	616	HTH	C5-C4-C3	-4.00	107.59	114.18
6	A	607	DMU	C10-O7-C3	-4.00	108.06	117.96
5	C	603	HEA	CAD-CBD-CGD	-4.00	105.00	113.60
5	C	602	HEA	CMC-C2C-C3C	3.90	131.97	124.68
6	D	301	DMU	O5-C6-C1	-3.89	103.35	110.28
5	A	602	HEA	CMC-C2C-C3C	3.88	131.93	124.68
5	C	603	HEA	C1B-C2B-C3B	-3.87	102.17	106.80
5	C	602	HEA	C1B-C2B-C3B	-3.80	102.25	106.80
6	C	605	DMU	C10-O7-C3	-3.71	108.79	117.96
5	A	603	HEA	CAD-CBD-CGD	-3.69	105.67	113.60
5	A	602	HEA	CAD-CBD-CGD	-3.63	105.80	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	602	HEA	C1D-C2D-C3D	-3.62	103.15	106.96
5	C	603	HEA	C3C-C4C-NC	3.49	113.72	109.21
6	D	301	DMU	O5-C4-C3	3.45	117.02	109.75
5	C	603	HEA	CHA-C4D-C3D	-3.41	119.83	124.84
5	A	603	HEA	CMB-C2B-C1B	3.41	130.23	125.04
5	A	603	HEA	C1D-C2D-C3D	-3.38	103.41	106.96
5	A	602	HEA	CBA-CAA-C2A	-3.34	106.97	112.60
5	A	602	HEA	C27-C19-C20	3.32	120.86	115.27
5	C	602	HEA	C4D-C3D-C2D	-3.32	102.06	106.90
5	C	602	HEA	C27-C19-C20	3.31	120.83	115.27
5	A	603	HEA	CMC-C2C-C3C	3.29	130.83	124.68
6	A	606	DMU	O5-C4-C3	3.28	116.66	109.75
6	C	605	DMU	C10-C5-C7	3.27	116.80	110.00
5	A	603	HEA	C4D-C3D-C2D	-3.21	102.22	106.90
5	A	603	HEA	C3C-C4C-NC	3.21	113.36	109.21
5	A	602	HEA	C13-C14-C15	-3.18	120.00	127.66
5	C	603	HEA	C13-C12-C11	-3.13	109.65	114.35
5	A	603	HEA	CHA-C4D-C3D	-3.12	120.25	124.84
6	A	608	DMU	C10-O7-C3	-3.10	110.28	117.96
6	A	606	DMU	O16-C6-C1	3.10	113.14	108.30
5	C	602	HEA	CAD-CBD-CGD	-3.09	106.96	113.60
5	C	603	HEA	CMD-C2D-C1D	3.06	129.70	125.04
6	A	604	DMU	C18-O16-C6	3.04	118.88	113.84
5	A	602	HEA	C4D-C3D-C2D	-3.03	102.48	106.90
5	C	602	HEA	CMD-C2D-C1D	3.02	129.64	125.04
5	A	602	HEA	C25-C23-C22	-3.02	113.93	122.65
5	A	603	HEA	C4B-NB-C1B	-3.00	101.97	105.07
6	A	604	DMU	C10-O7-C3	-2.98	110.58	117.96
6	A	606	DMU	C10-O7-C3	-2.97	110.60	117.96
6	A	607	DMU	O16-C6-C1	2.97	112.94	108.30
5	A	603	HEA	CHB-C1B-C2B	-2.94	120.38	124.98
5	A	602	HEA	CMD-C2D-C1D	2.92	129.49	125.04
5	C	603	HEA	CMC-C2C-C3C	2.91	130.13	124.68
5	C	603	HEA	C4D-C3D-C2D	-2.90	102.67	106.90
5	C	602	HEA	CHB-C1B-C2B	-2.90	120.44	124.98
6	B	301	DMU	O5-C4-C3	2.81	115.69	109.75
5	A	603	HEA	C27-C19-C20	2.80	119.99	115.27
5	C	602	HEA	C4B-C3B-C2B	-2.80	102.63	107.41
5	C	602	HEA	C13-C14-C15	-2.72	121.11	127.66
5	C	603	HEA	C4B-C3B-C2B	-2.72	102.77	107.41
5	A	602	HEA	C4B-C3B-C2B	-2.71	102.79	107.41
6	C	604	DMU	C10-O7-C3	-2.67	111.35	117.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	606	DMU	O5-C6-C1	-2.65	104.74	110.35
5	C	602	HEA	CAD-C3D-C4D	2.62	129.23	124.66
5	A	602	HEA	CHA-C4D-C3D	-2.58	121.04	124.84
5	C	603	HEA	C4B-NB-C1B	-2.57	102.42	105.07
5	A	603	HEA	CMD-C2D-C1D	2.57	128.95	125.04
5	A	602	HEA	C20-C21-C22	-2.57	103.44	111.88
6	A	606	DMU	C2-C3-C4	2.53	116.73	110.93
5	A	603	HEA	C13-C14-C15	-2.53	121.57	127.66
5	C	603	HEA	C26-C15-C16	2.52	119.52	115.27
5	C	603	HEA	C13-C14-C15	-2.51	121.61	127.66
5	A	602	HEA	OMA-CMA-C3A	-2.50	119.46	124.91
5	C	603	HEA	CHB-C1B-C2B	-2.49	121.10	124.98
5	A	603	HEA	C4B-C3B-C2B	-2.48	103.17	107.41
5	C	602	HEA	C13-C12-C11	-2.47	110.64	114.35
6	C	604	DMU	O5-C6-C1	-2.44	105.92	110.28
5	A	602	HEA	CHB-C1B-C2B	-2.44	121.16	124.98
5	C	603	HEA	C27-C19-C20	2.43	119.36	115.27
6	D	301	DMU	C2-C3-C4	2.41	116.45	110.93
6	A	604	DMU	O5-C6-C1	-2.40	105.28	110.35
6	A	606	DMU	C8-C7-C5	2.38	114.98	110.82
6	D	301	DMU	C10-O7-C3	-2.33	112.20	117.96
5	C	602	HEA	CHA-C4D-C3D	-2.32	121.43	124.84
5	A	602	HEA	C25-C23-C24	2.32	119.73	114.60
5	A	602	HEA	C1D-ND-C4D	-2.29	102.70	105.07
6	A	606	DMU	O4-C7-C8	-2.28	105.08	110.35
5	C	602	HEA	C4B-NB-C1B	-2.27	102.73	105.07
6	A	606	DMU	C7-C8-C9	2.25	114.26	110.24
6	A	606	DMU	O1-C9-C8	-2.25	105.60	109.69
6	C	605	DMU	O7-C3-C2	2.25	113.27	107.28
6	A	605	DMU	O5-C6-C1	-2.24	105.62	110.35
6	C	605	DMU	C2-C3-C4	-2.22	105.83	110.93
5	C	603	HEA	CMB-C2B-C1B	2.22	128.42	125.04
6	A	605	DMU	C1-C2-C3	2.22	114.75	109.68
6	D	301	DMU	O7-C3-C4	-2.22	103.37	109.45
8	B	306	HTH	C1-C2-C3	-2.20	108.34	113.11
6	A	608	DMU	O5-C6-C1	-2.18	105.73	110.35
6	C	605	DMU	O55-C2-C3	2.18	115.71	109.94
6	A	608	DMU	O1-C10-C5	2.17	114.94	110.35
5	A	603	HEA	C13-C12-C11	-2.16	111.11	114.35
5	A	603	HEA	C26-C15-C16	2.12	118.84	115.27
6	A	605	DMU	O5-C4-C3	2.12	114.23	109.75
6	A	604	DMU	C8-C7-C5	2.10	114.49	110.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	605	DMU	C6-C1-C2	2.10	114.37	110.00
5	C	602	HEA	C17-C18-C19	-2.10	122.61	127.66
6	A	608	DMU	C11-C9-C8	-2.10	108.09	113.00
5	A	603	HEA	C25-C23-C24	2.08	119.20	114.60
5	A	602	HEA	CHC-C4B-C3B	-2.08	120.44	125.80
5	C	603	HEA	C25-C23-C24	2.06	119.16	114.60
5	A	602	HEA	CAD-C3D-C4D	2.05	128.25	124.66
6	B	301	DMU	O5-C6-C1	-2.05	106.00	110.35
6	A	605	DMU	O7-C3-C4	-2.05	103.82	109.45
6	A	607	DMU	C6-O5-C4	-2.05	109.67	113.69
6	D	301	DMU	C1-C2-C3	2.04	114.34	109.68
8	B	306	HTH	C5-C4-C3	-2.04	110.83	114.18
5	C	602	HEA	CHC-C4B-C3B	-2.04	120.56	125.80
5	C	603	HEA	C1D-ND-C4D	-2.03	102.98	105.07
5	C	602	HEA	C25-C23-C24	2.02	119.08	114.60

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	602	HEA	ND
5	A	602	HEA	NB
5	A	603	HEA	ND
5	A	603	HEA	NB
5	C	602	HEA	ND
5	C	602	HEA	NB
5	C	603	HEA	ND
5	C	603	HEA	NB

All (160) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	HEA	C19-C20-C21-C22
5	C	602	HEA	C19-C20-C21-C22
6	A	605	DMU	C19-C18-O16-C6
6	A	607	DMU	C1-C6-O16-C18
6	A	607	DMU	O5-C6-O16-C18
6	A	608	DMU	C1-C6-O16-C18
6	A	608	DMU	O5-C6-O16-C18
6	B	301	DMU	C19-C18-O16-C6
6	C	605	DMU	C1-C6-O16-C18
6	C	605	DMU	O5-C6-O16-C18
8	A	616	HTH	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	616	HTH	C1-C2-C3-C4
8	A	616	HTH	O2-C2-C3-O3
8	A	616	HTH	O2-C2-C3-C4
13	B	311	TRS	C1-C-C2-O2
13	B	311	TRS	C3-C-C2-O2
13	B	311	TRS	C1-C-C3-O3
13	B	311	TRS	C2-C-C3-O3
13	B	311	TRS	N-C-C3-O3
6	C	605	DMU	O5-C4-C57-O61
6	B	301	DMU	C3-C4-C57-O61
7	B	303	TRD	C4-C5-C6-C7
6	A	604	DMU	O5-C4-C57-O61
6	C	604	DMU	O5-C4-C57-O61
6	A	605	DMU	O5-C6-O16-C18
6	C	605	DMU	C3-C4-C57-O61
7	B	303	TRD	C9-C10-C11-C12
6	C	604	DMU	O6-C11-C9-O1
6	A	605	DMU	C3-C4-C57-O61
6	B	301	DMU	O6-C11-C9-C8
6	C	604	DMU	C3-C4-C57-O61
6	B	301	DMU	O5-C4-C57-O61
6	A	605	DMU	O1-C10-O7-C3
6	D	301	DMU	O5-C4-C57-O61
6	A	604	DMU	O6-C11-C9-O1
6	A	604	DMU	C3-C4-C57-O61
6	A	605	DMU	O6-C11-C9-C8
6	A	607	DMU	O6-C11-C9-C8
6	A	605	DMU	O16-C18-C19-C22
6	B	301	DMU	O6-C11-C9-O1
6	A	604	DMU	O16-C18-C19-C22
6	B	301	DMU	O16-C18-C19-C22
6	A	604	DMU	C22-C25-C28-C31
7	C	606	TRD	C3-C4-C5-C6
7	C	607	TRD	C5-C6-C7-C8
7	A	611	TRD	C3-C4-C5-C6
7	B	302	TRD	C7-C8-C9-C10
7	A	615	TRD	C7-C8-C9-C10
7	D	302	TRD	C3-C4-C5-C6
7	A	612	TRD	C9-C10-C11-C12
6	A	608	DMU	C22-C25-C28-C31
6	A	607	DMU	O6-C11-C9-O1
6	A	605	DMU	C4-C3-O7-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	303	TRD	C5-C6-C7-C8
7	D	303	TRD	C3-C4-C5-C6
6	A	604	DMU	C31-C34-C37-C40
7	A	614	TRD	C6-C7-C8-C9
7	A	615	TRD	C6-C7-C8-C9
7	A	614	TRD	C9-C10-C11-C12
7	B	304	TRD	C11-C10-C9-C8
6	C	605	DMU	C31-C34-C37-C40
6	A	607	DMU	C19-C18-O16-C6
8	B	306	HTH	O3-C3-C4-C5
7	B	302	TRD	C6-C7-C8-C9
8	B	306	HTH	O1-C1-C2-C3
7	B	302	TRD	C2-C3-C4-C5
6	A	605	DMU	C2-C3-O7-C10
6	A	604	DMU	C19-C22-C25-C28
6	A	605	DMU	O6-C11-C9-O1
6	B	301	DMU	C22-C25-C28-C31
7	D	303	TRD	C5-C6-C7-C8
7	C	606	TRD	C6-C7-C8-C9
5	C	602	HEA	C14-C15-C16-C17
6	A	606	DMU	C25-C28-C31-C34
7	C	606	TRD	C2-C3-C4-C5
7	A	615	TRD	C9-C10-C11-C12
7	B	302	TRD	C4-C5-C6-C7
6	A	608	DMU	C19-C22-C25-C28
7	B	303	TRD	C7-C8-C9-C10
6	D	301	DMU	C2-C3-O7-C10
6	A	606	DMU	C19-C22-C25-C28
6	A	607	DMU	C28-C31-C34-C37
5	C	602	HEA	C26-C15-C16-C17
6	D	301	DMU	O6-C11-C9-O1
7	D	302	TRD	C9-C10-C11-C12
7	A	614	TRD	C10-C11-C12-C13
6	A	607	DMU	C18-C19-C22-C25
6	D	301	DMU	C4-C3-O7-C10
6	C	604	DMU	O6-C11-C9-C8
7	A	614	TRD	C4-C5-C6-C7
7	A	615	TRD	C1-C2-C3-C4
6	C	605	DMU	C19-C22-C25-C28
7	B	302	TRD	C11-C10-C9-C8
6	B	301	DMU	O5-C6-O16-C18
7	A	615	TRD	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	612	TRD	C10-C11-C12-C13
7	B	303	TRD	C6-C7-C8-C9
6	A	606	DMU	O16-C18-C19-C22
8	B	306	HTH	O1-C1-C2-O2
7	B	302	TRD	C3-C4-C5-C6
6	A	605	DMU	O5-C4-C57-O61
6	A	604	DMU	O6-C11-C9-C8
6	A	604	DMU	C19-C18-O16-C6
6	A	604	DMU	C34-C37-C40-C43
6	B	301	DMU	C18-C19-C22-C25
7	D	303	TRD	C6-C7-C8-C9
6	A	605	DMU	C31-C34-C37-C40
6	A	608	DMU	C25-C28-C31-C34
8	B	306	HTH	C2-C3-C4-C5
13	B	311	TRS	N-C-C2-O2
7	D	302	TRD	C5-C6-C7-C8
7	A	614	TRD	C7-C8-C9-C10
7	D	303	TRD	C4-C5-C6-C7
6	B	301	DMU	C25-C28-C31-C34
6	C	605	DMU	O16-C18-C19-C22
6	A	604	DMU	C25-C28-C31-C34
7	D	302	TRD	C1-C2-C3-C4
8	B	306	HTH	O2-C2-C3-O3
6	C	605	DMU	C4-C3-O7-C10
7	B	304	TRD	C10-C11-C12-C13
7	B	304	TRD	C3-C4-C5-C6
7	B	304	TRD	C4-C5-C6-C7
6	A	608	DMU	C3-C4-C57-O61
8	B	306	HTH	C1-C2-C3-O3
5	C	603	HEA	CAA-CBA-CGA-O1A
5	A	603	HEA	CAD-CBD-CGD-O1D
5	A	603	HEA	CAD-CBD-CGD-O2D
6	A	606	DMU	C28-C31-C34-C37
6	C	605	DMU	C2-C3-O7-C10
5	C	603	HEA	CAA-CBA-CGA-O2A
5	C	602	HEA	CAD-CBD-CGD-O2D
7	A	610	TRD	C2-C3-C4-C5
5	C	602	HEA	CAD-CBD-CGD-O1D
5	C	603	HEA	CAD-CBD-CGD-O2D
7	A	613	TRD	C1-C2-C3-C4
5	A	603	HEA	CAA-CBA-CGA-O1A
5	A	602	HEA	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	614	TRD	C1-C2-C3-C4
5	C	603	HEA	CAD-CBD-CGD-O1D
6	A	608	DMU	C31-C34-C37-C40
7	A	613	TRD	C3-C4-C5-C6
7	A	615	TRD	C11-C10-C9-C8
7	B	304	TRD	C7-C8-C9-C10
6	A	607	DMU	O16-C18-C19-C22
5	A	602	HEA	CAD-CBD-CGD-O2D
5	A	602	HEA	CAD-CBD-CGD-O1D
7	A	611	TRD	C1-C2-C3-C4
7	B	303	TRD	C11-C10-C9-C8
7	D	302	TRD	C11-C10-C9-C8
7	B	302	TRD	C9-C10-C11-C12
7	A	612	TRD	C6-C7-C8-C9
5	A	603	HEA	CAA-CBA-CGA-O2A
5	C	603	HEA	O11-C11-C12-C13
7	C	606	TRD	C11-C10-C9-C8
8	A	616	HTH	C3-C4-C5-C6
5	C	603	HEA	C3B-C11-C12-C13
6	A	606	DMU	C31-C34-C37-C40
7	B	304	TRD	C5-C6-C7-C8
5	A	602	HEA	C26-C15-C16-C17
6	C	605	DMU	C34-C37-C40-C43

There are no ring outliers.

20 monomers are involved in 35 short contacts:

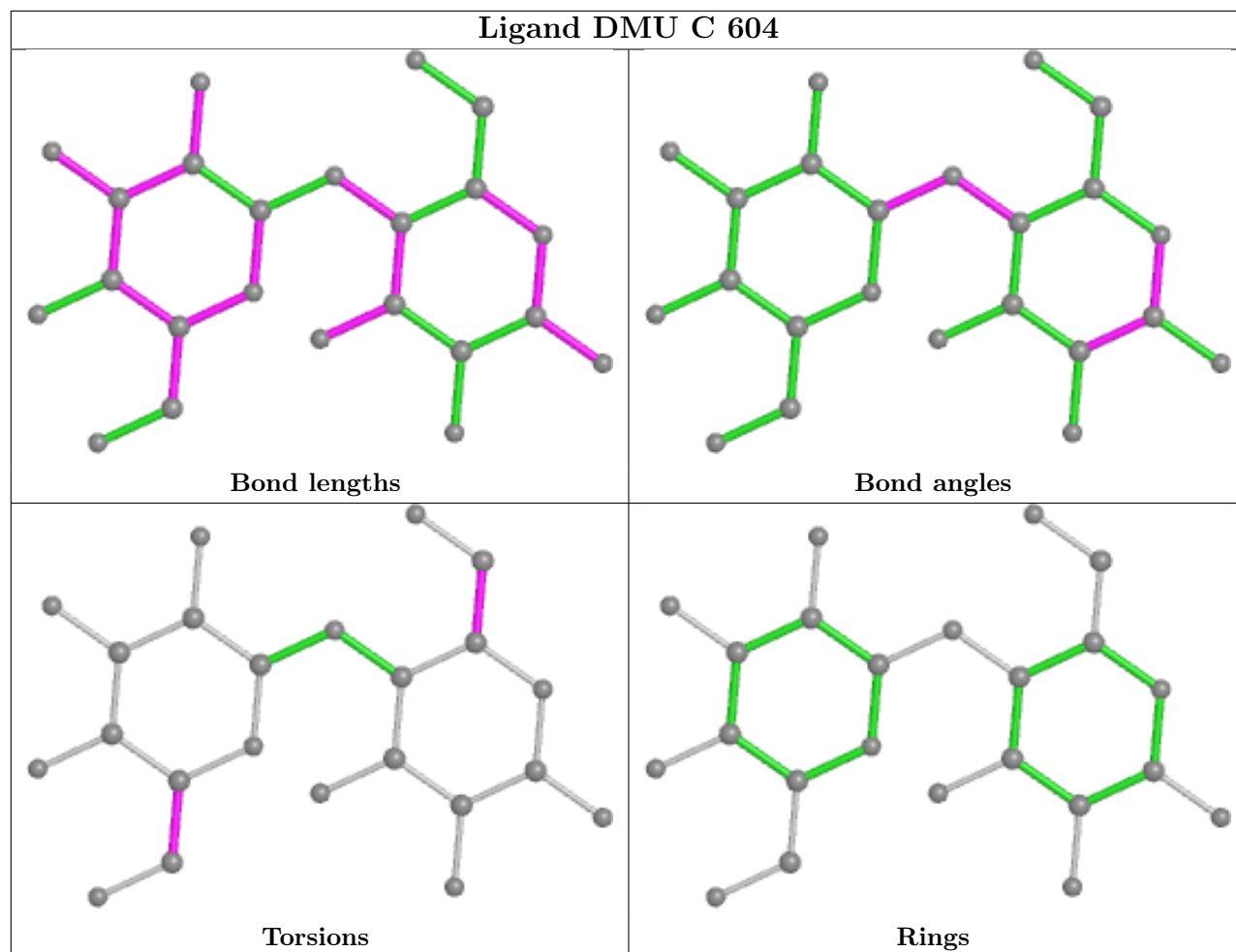
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	301	DMU	2	0
6	A	604	DMU	1	0
7	C	608	TRD	2	0
7	B	304	TRD	1	0
5	A	603	HEA	3	0
7	C	606	TRD	1	0
6	D	301	DMU	1	0
5	A	602	HEA	3	0
8	A	616	HTH	2	0
5	C	602	HEA	2	0
5	C	603	HEA	2	0
7	A	614	TRD	2	0
6	A	605	DMU	3	0
7	C	607	TRD	2	0

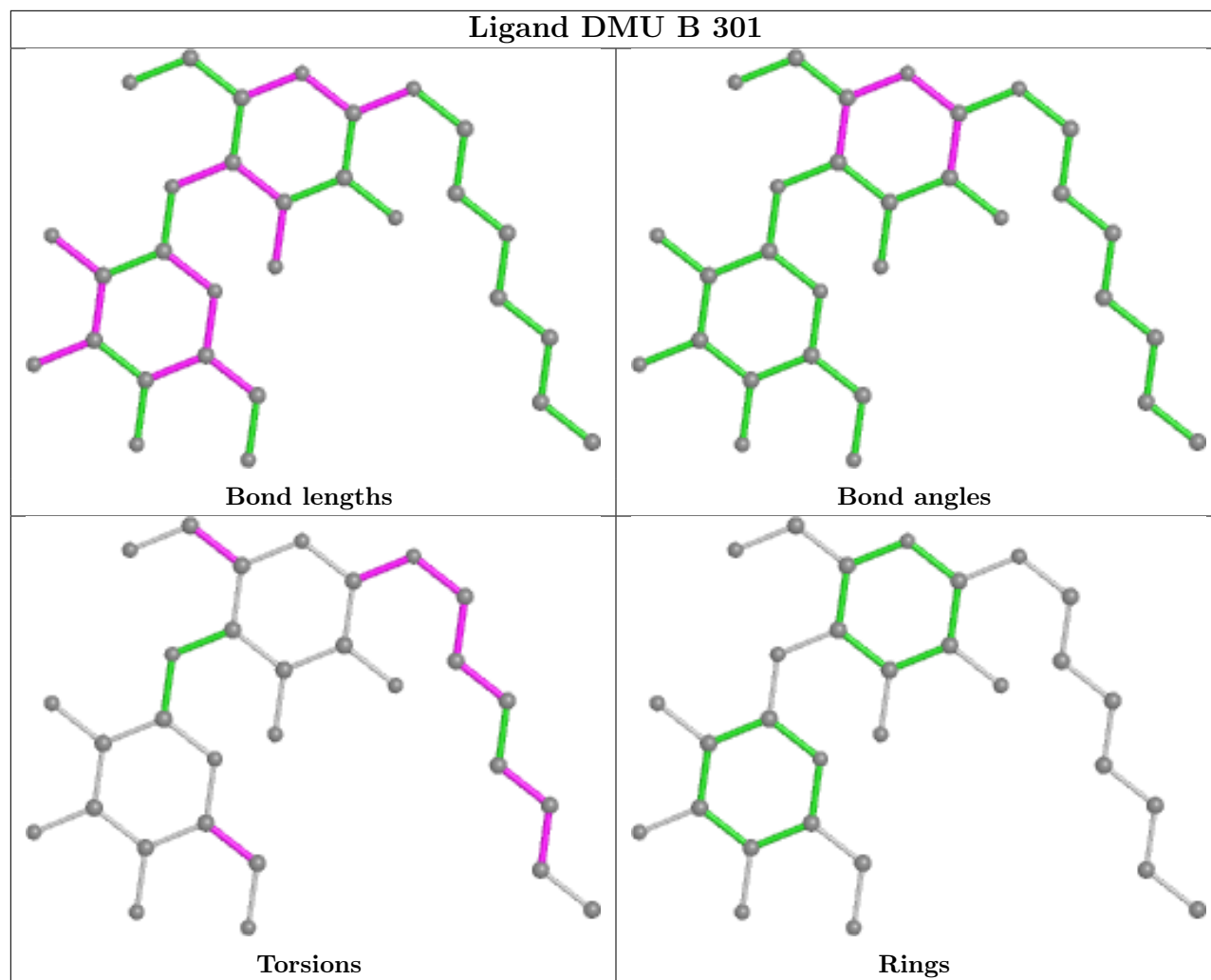
Continued on next page...

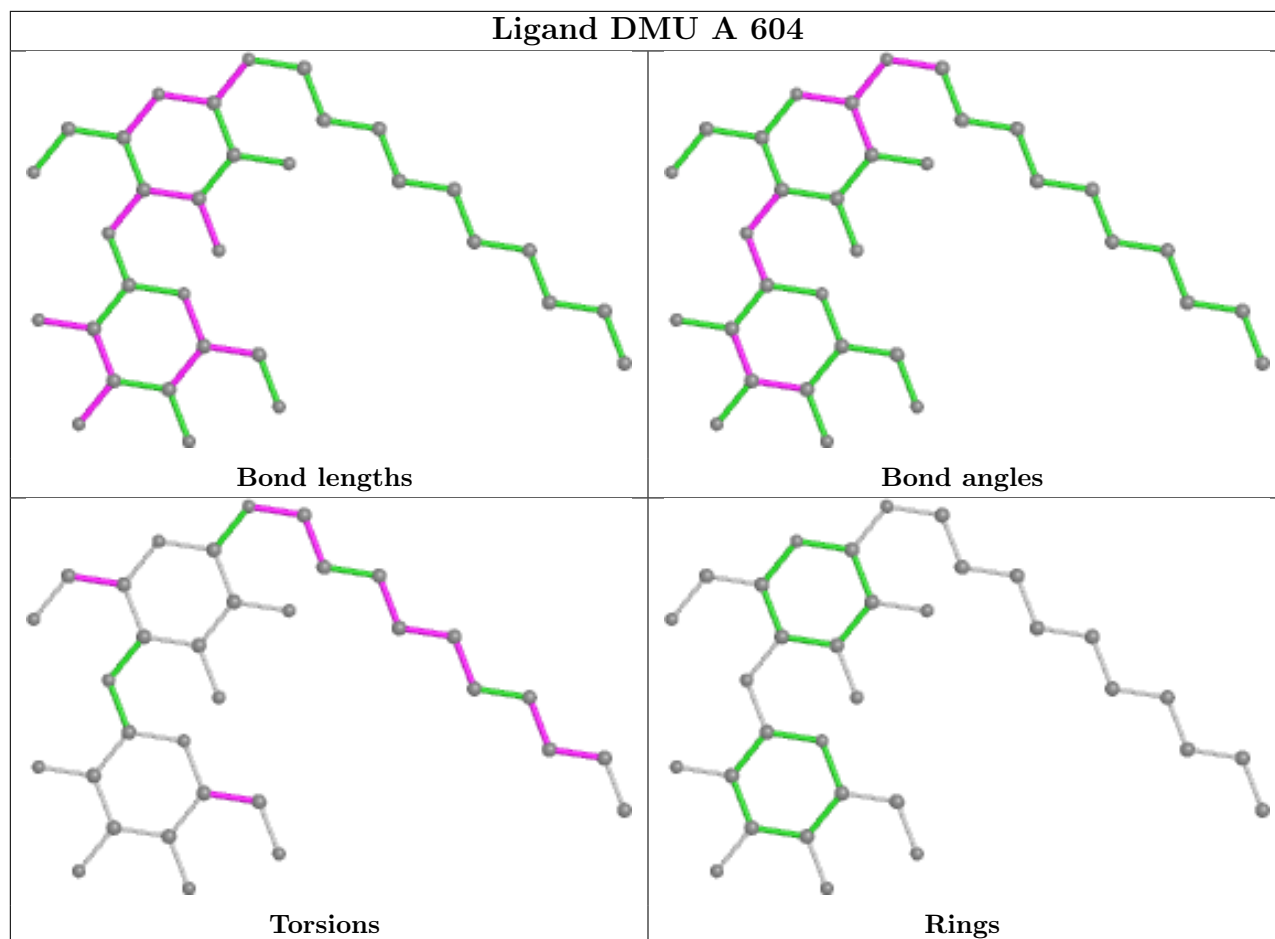
Continued from previous page...

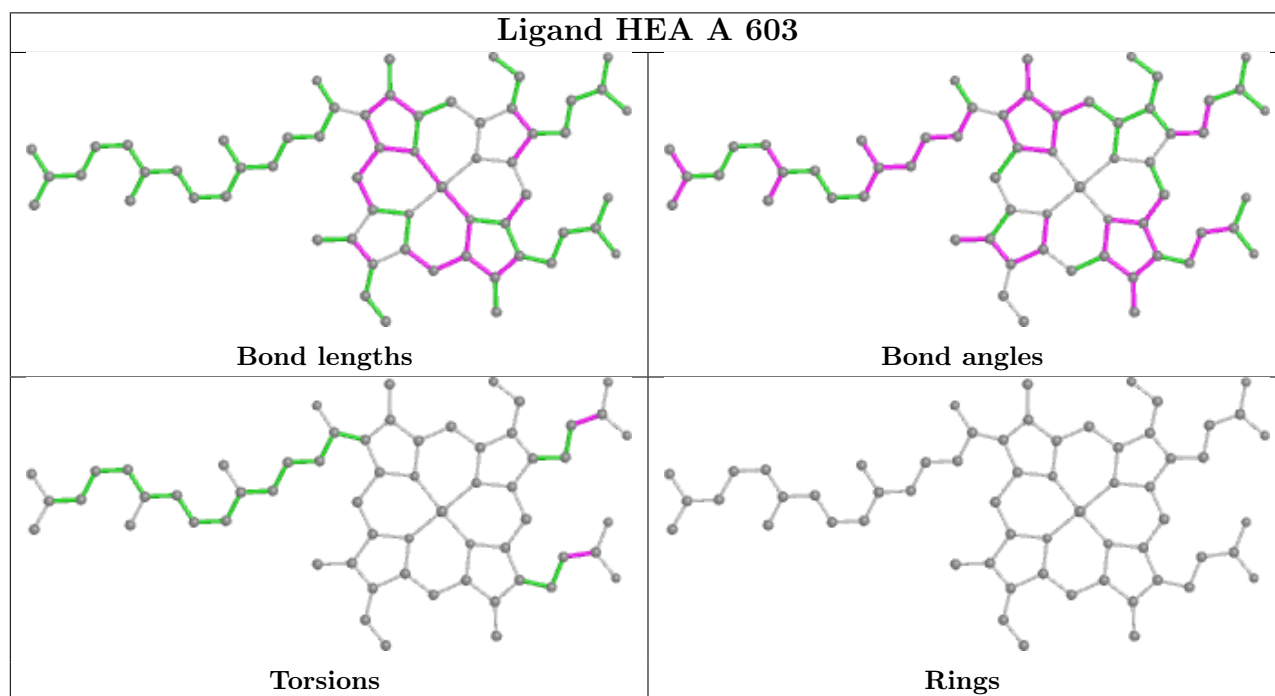
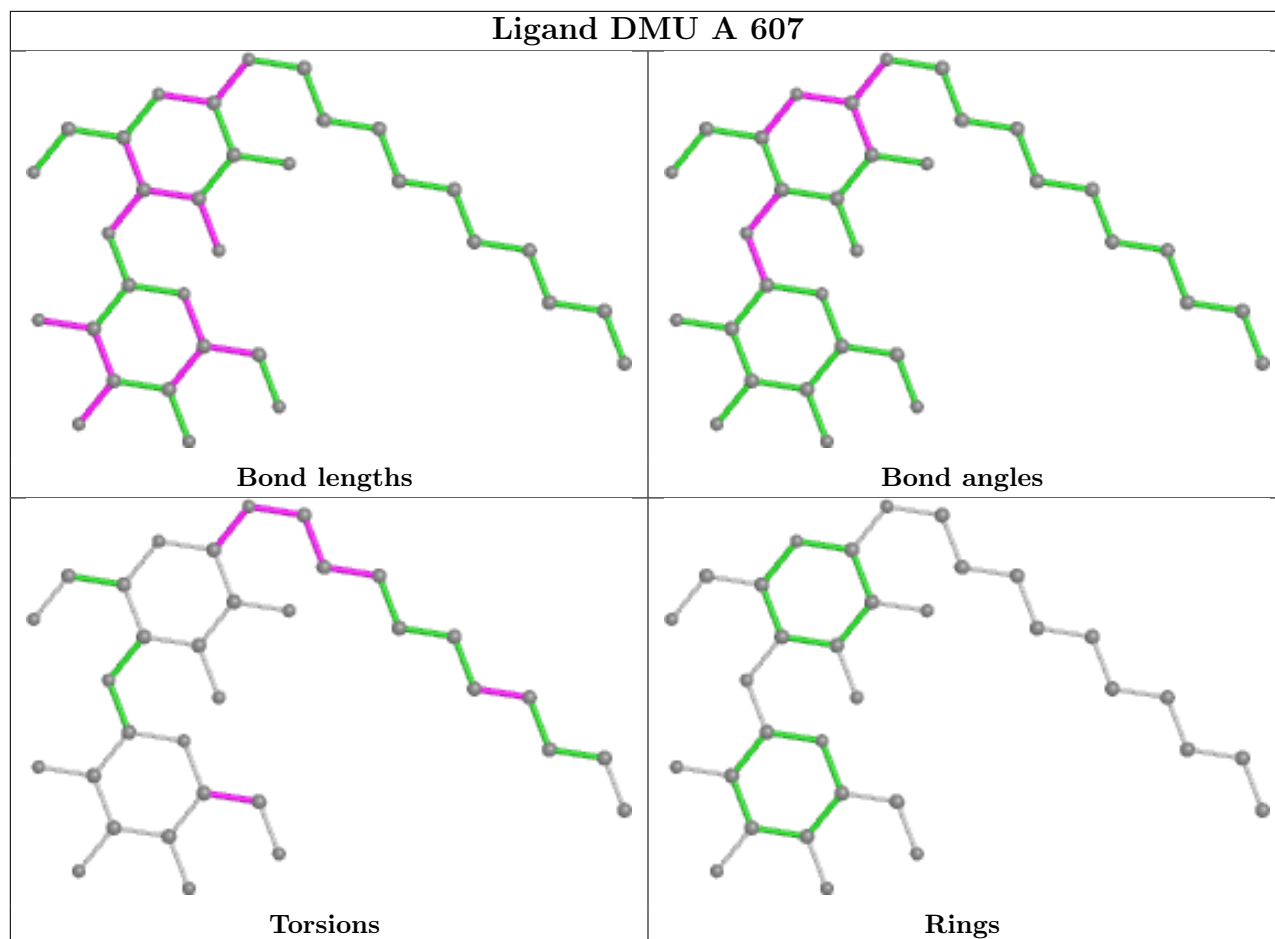
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	302	TRD	1	0
7	A	609	TRD	1	0
7	A	610	TRD	1	0
6	A	608	DMU	1	0
6	C	605	DMU	2	0
7	B	303	TRD	5	0

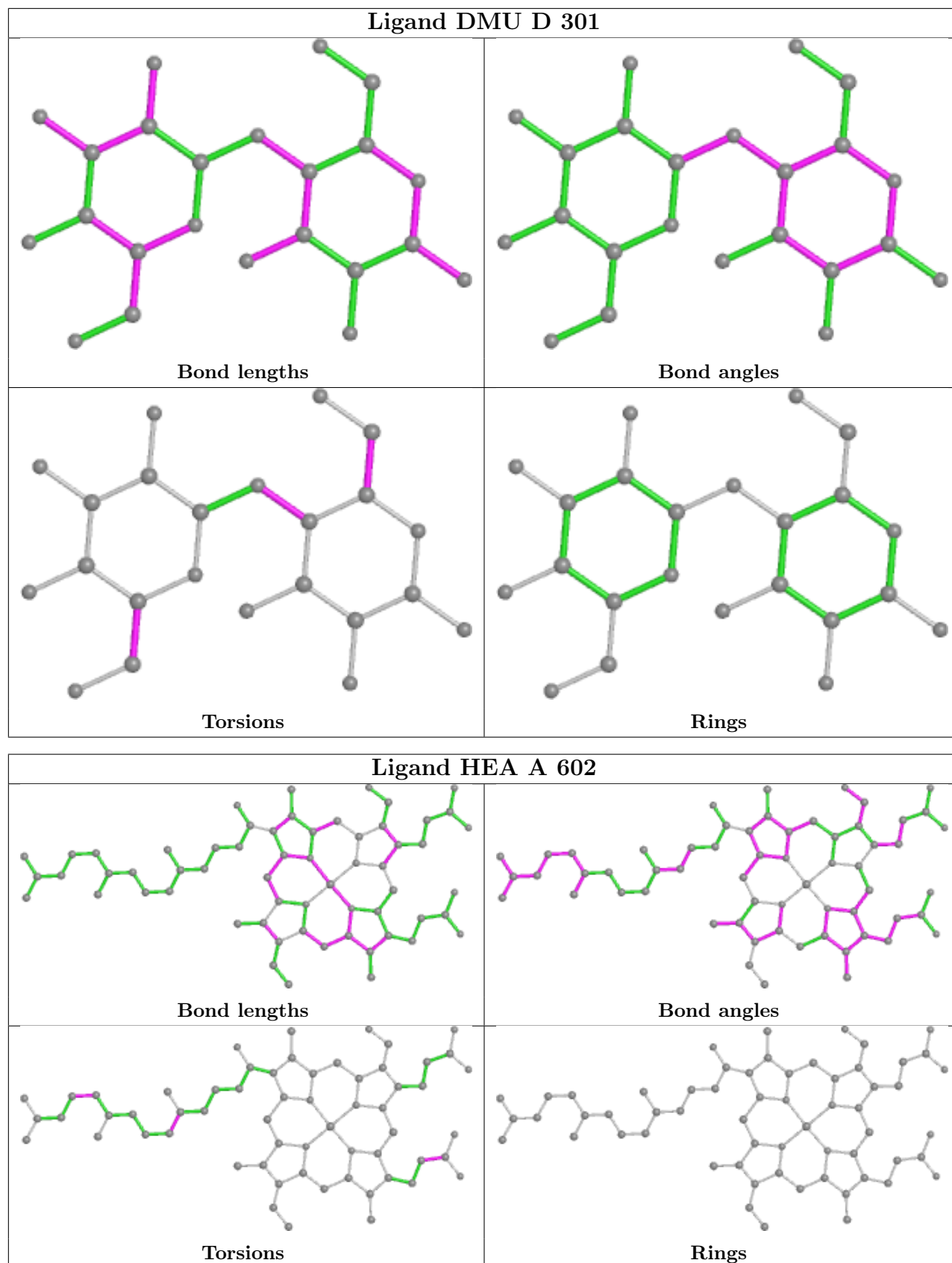
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

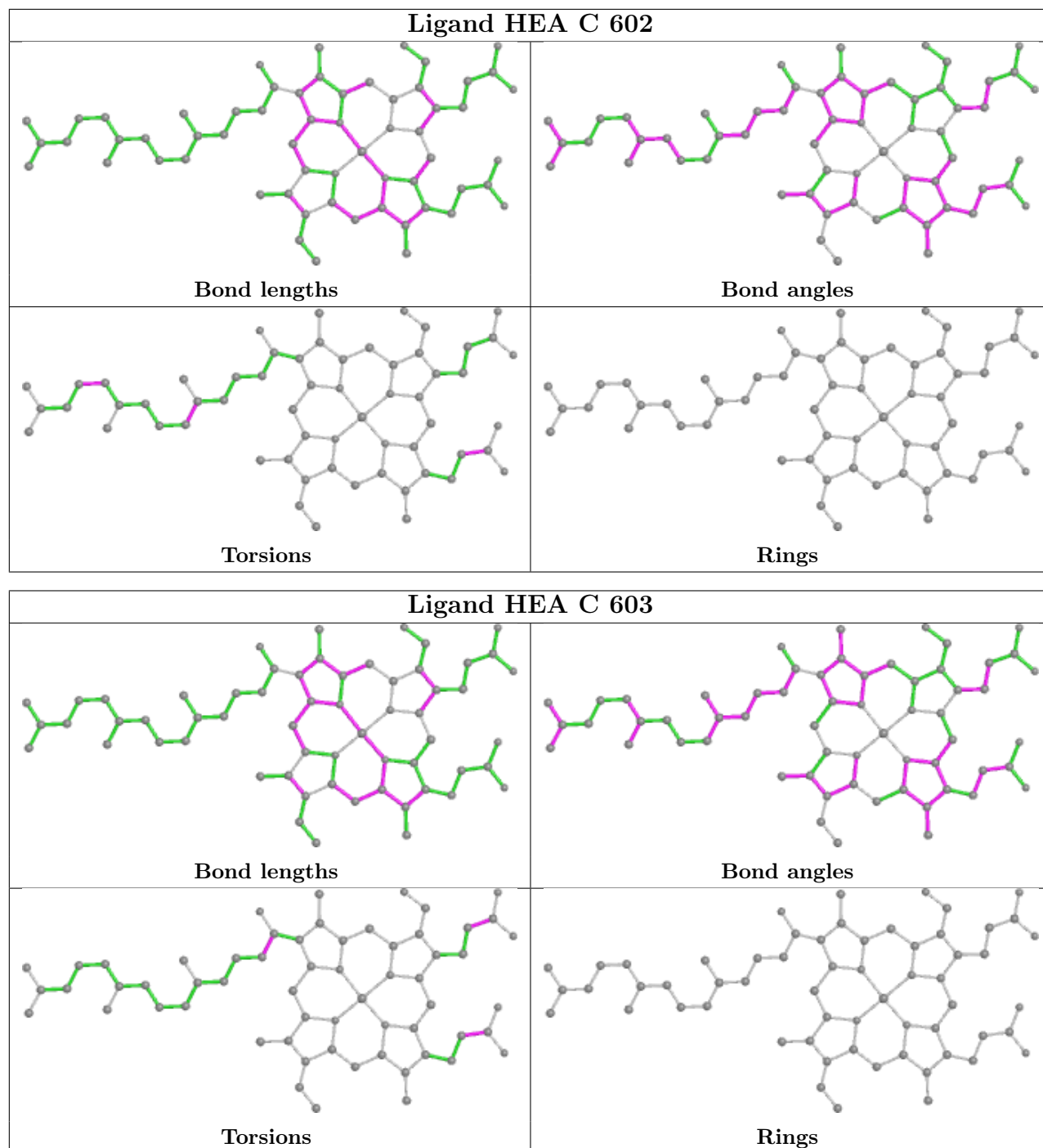


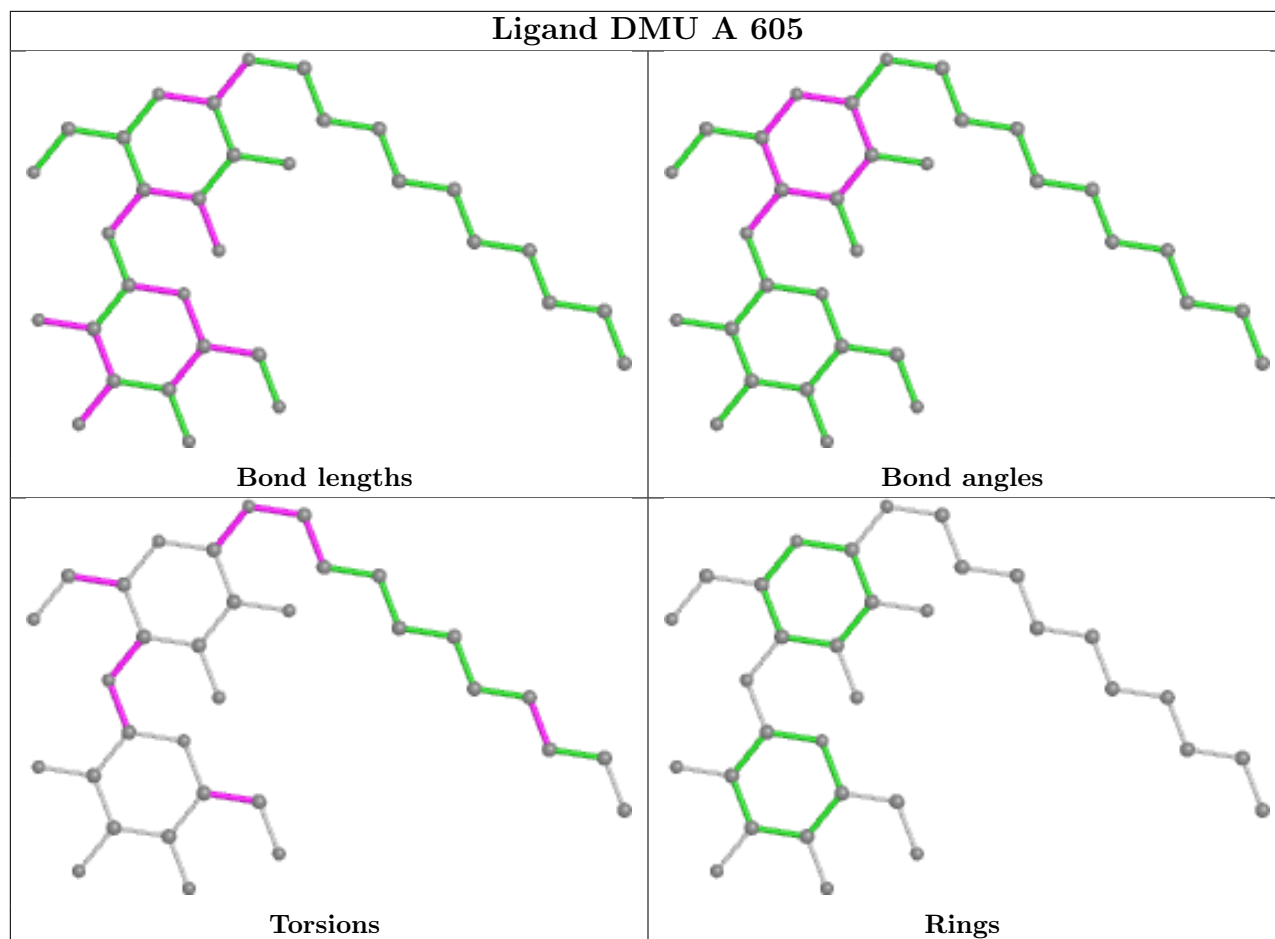


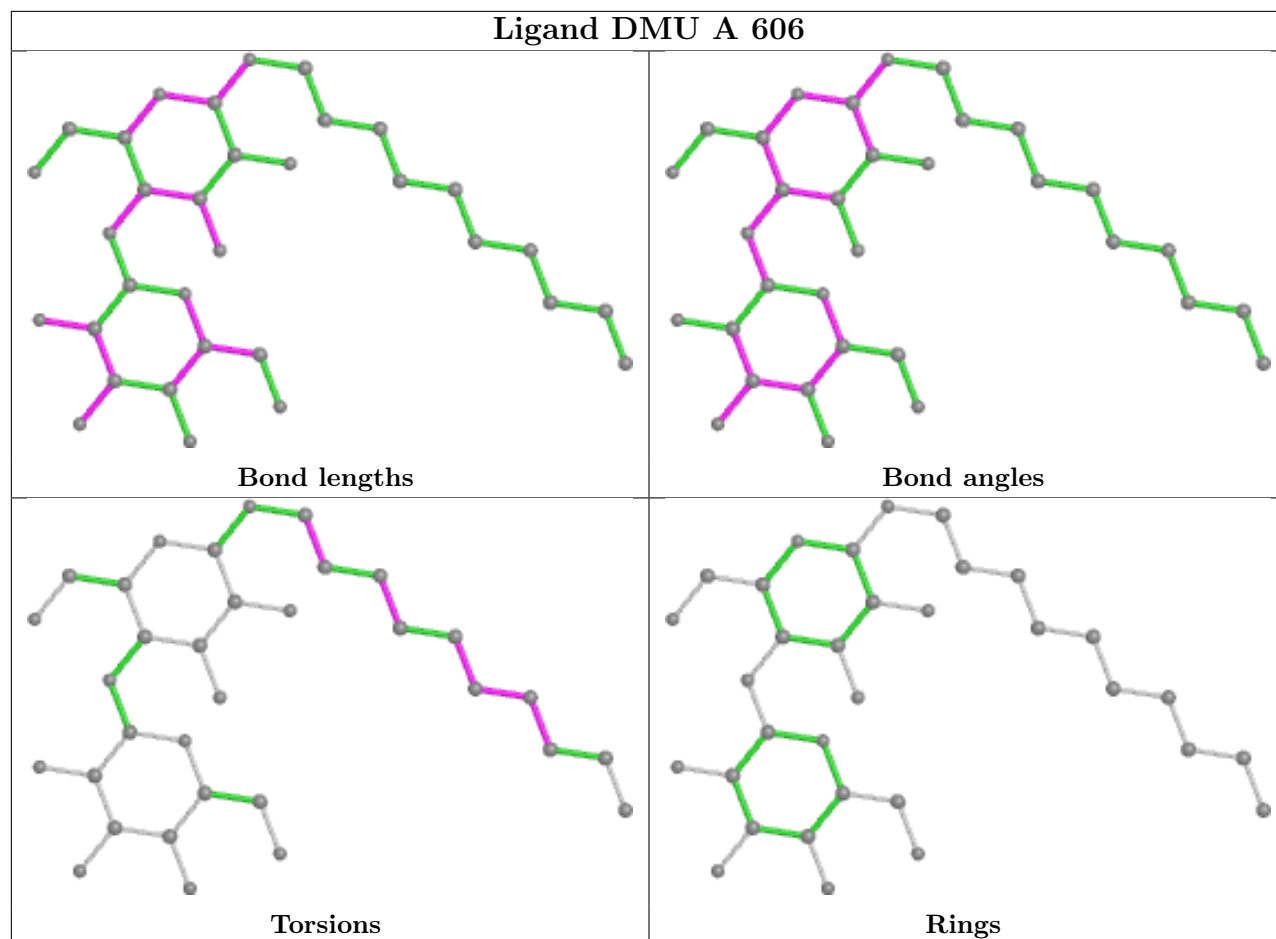


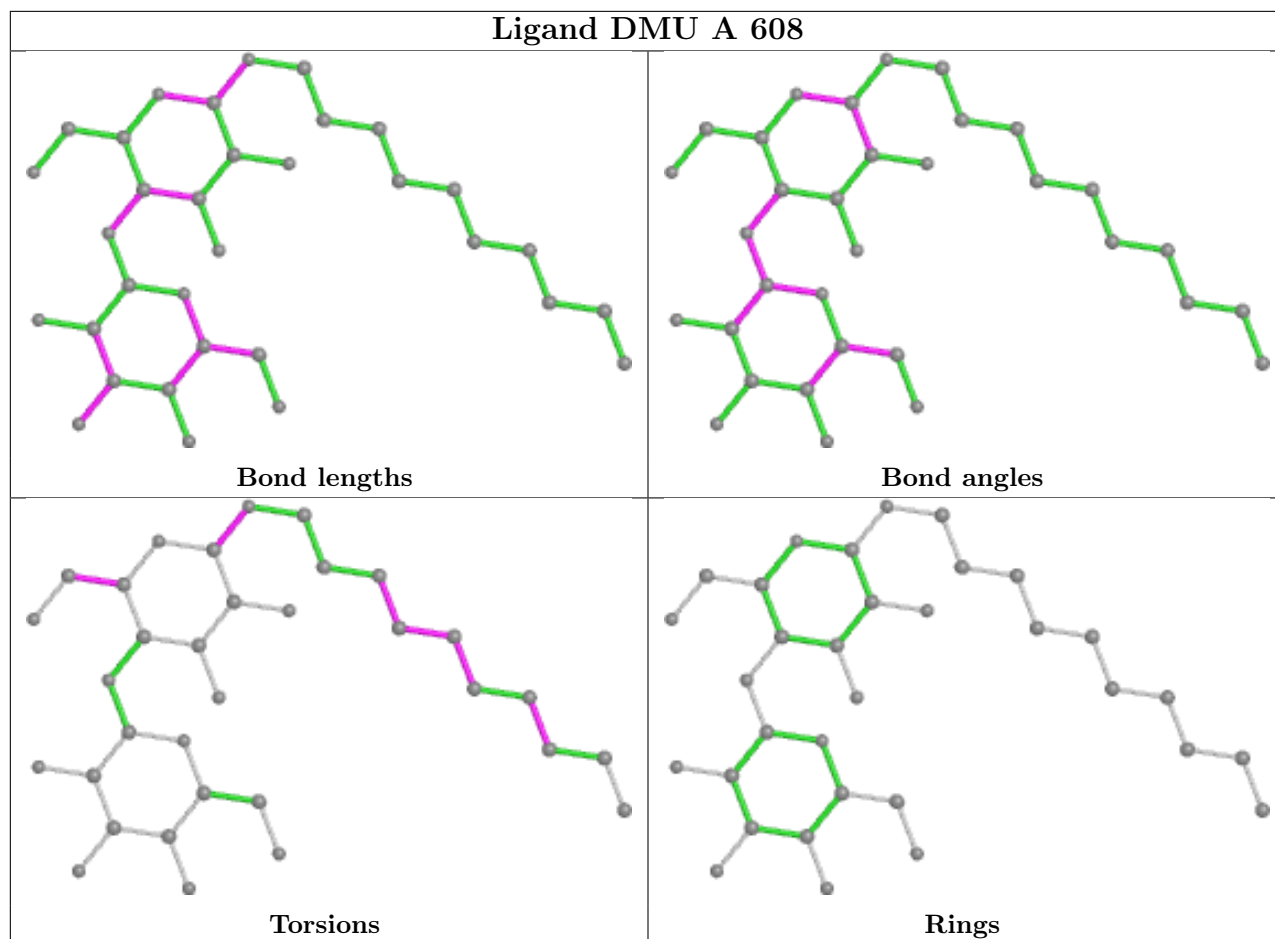


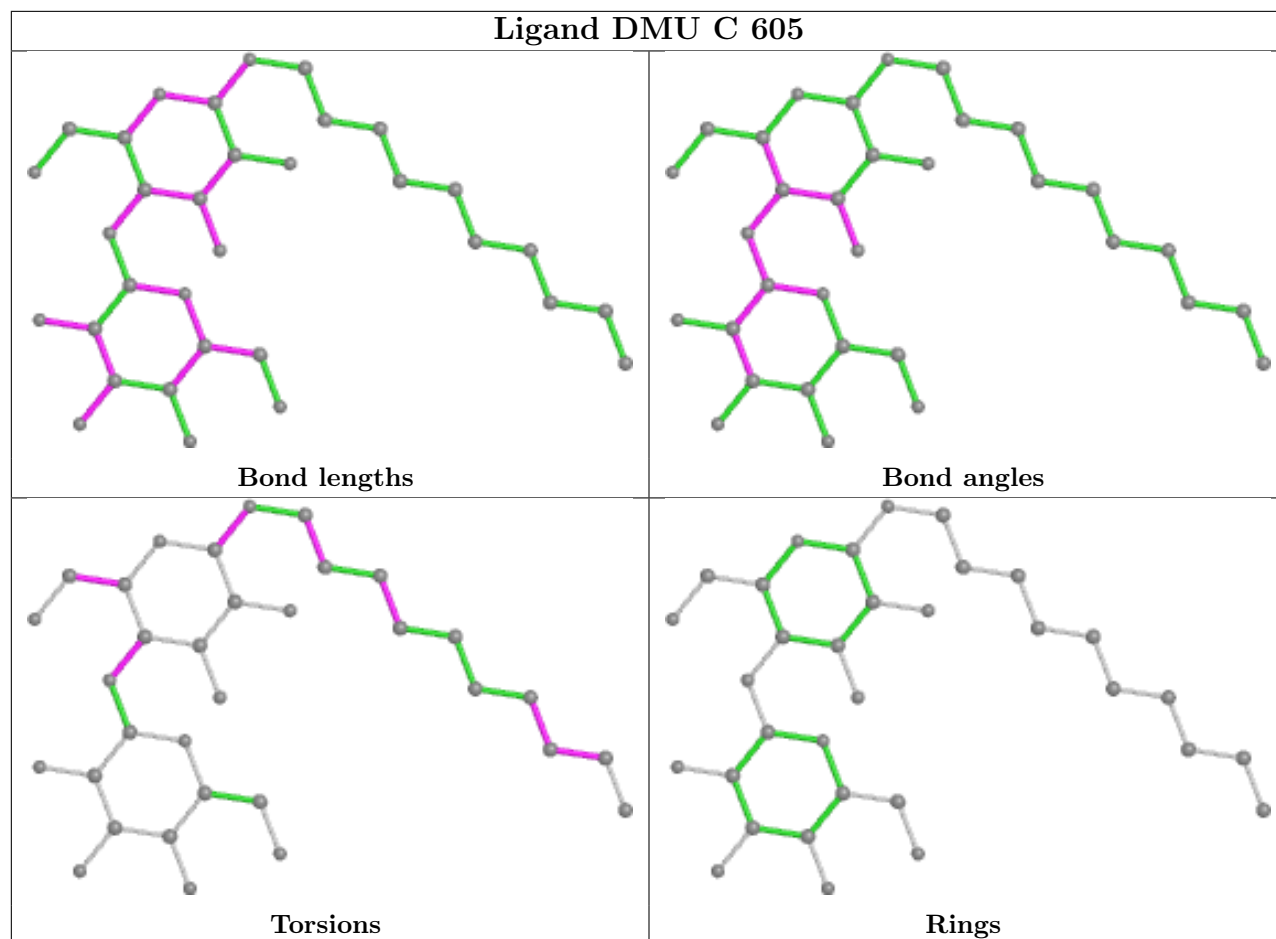












5.7 Other polymers [\(i\)](#)

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	535/560 (95%)	-0.33	12 (2%) 62 65	30, 42, 66, 99	0
1	C	531/560 (94%)	0.15	43 (8%) 12 12	39, 56, 80, 110	0
2	B	256/262 (97%)	-0.62	2 (0%) 86 87	31, 46, 63, 73	0
2	D	256/262 (97%)	-0.47	6 (2%) 60 63	37, 50, 71, 87	0
All	All	1578/1644 (95%)	-0.24	63 (3%) 38 41	30, 48, 74, 110	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	TRP	5.0
1	C	222	MET	4.7
1	C	259	PHE	4.7
1	C	218	PRO	4.2
1	C	217	ALA	3.9
1	C	81	TRP	3.9
1	C	138	MET	3.7
1	C	21	PHE	3.6
2	D	87	ARG	3.6
2	B	284	HIS	3.4
1	C	22	MET	3.3
2	D	82	ARG	3.3
2	D	56	TRP	3.3
1	C	77	PHE	3.2
1	C	413	THR	3.1
1	C	520	THR	3.1
1	C	550	THR	3.1
1	C	172	TRP	3.1
1	C	549	HIS	3.1
1	C	416	VAL	3.0
1	A	213	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	73	VAL	2.8
1	C	290	ILE	2.8
2	B	56	TRP	2.8
1	C	287	VAL	2.7
2	D	98	SER	2.7
1	A	22	MET	2.7
2	D	88	ASN	2.6
1	A	416	VAL	2.6
1	C	417	VAL	2.6
2	D	99	PRO	2.5
1	A	220	MET	2.5
1	C	136	PRO	2.5
1	C	130	ALA	2.5
1	C	103	GLY	2.5
1	A	549	HIS	2.5
1	A	259	PHE	2.5
1	C	289	ILE	2.4
1	C	414	TYR	2.4
1	A	20	TRP	2.4
1	C	135	PHE	2.4
1	A	81	TRP	2.3
1	C	288	TYR	2.3
1	C	480	PRO	2.3
1	C	76	PHE	2.3
1	C	284	HIS	2.3
1	C	283	GLY	2.2
1	C	534	HIS	2.2
1	C	481	ARG	2.2
1	C	533	GLU	2.2
1	A	19	ARG	2.2
1	C	412	ASP	2.2
1	C	334	HIS	2.1
1	A	420	PHE	2.1
1	A	423	VAL	2.1
1	C	137	ARG	2.1
1	C	424	MET	2.1
1	C	24	THR	2.1
1	C	100	THR	2.1
1	C	75	GLY	2.0
1	C	285	PRO	2.0
1	A	221	THR	2.0
1	C	99	ILE	2.0

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

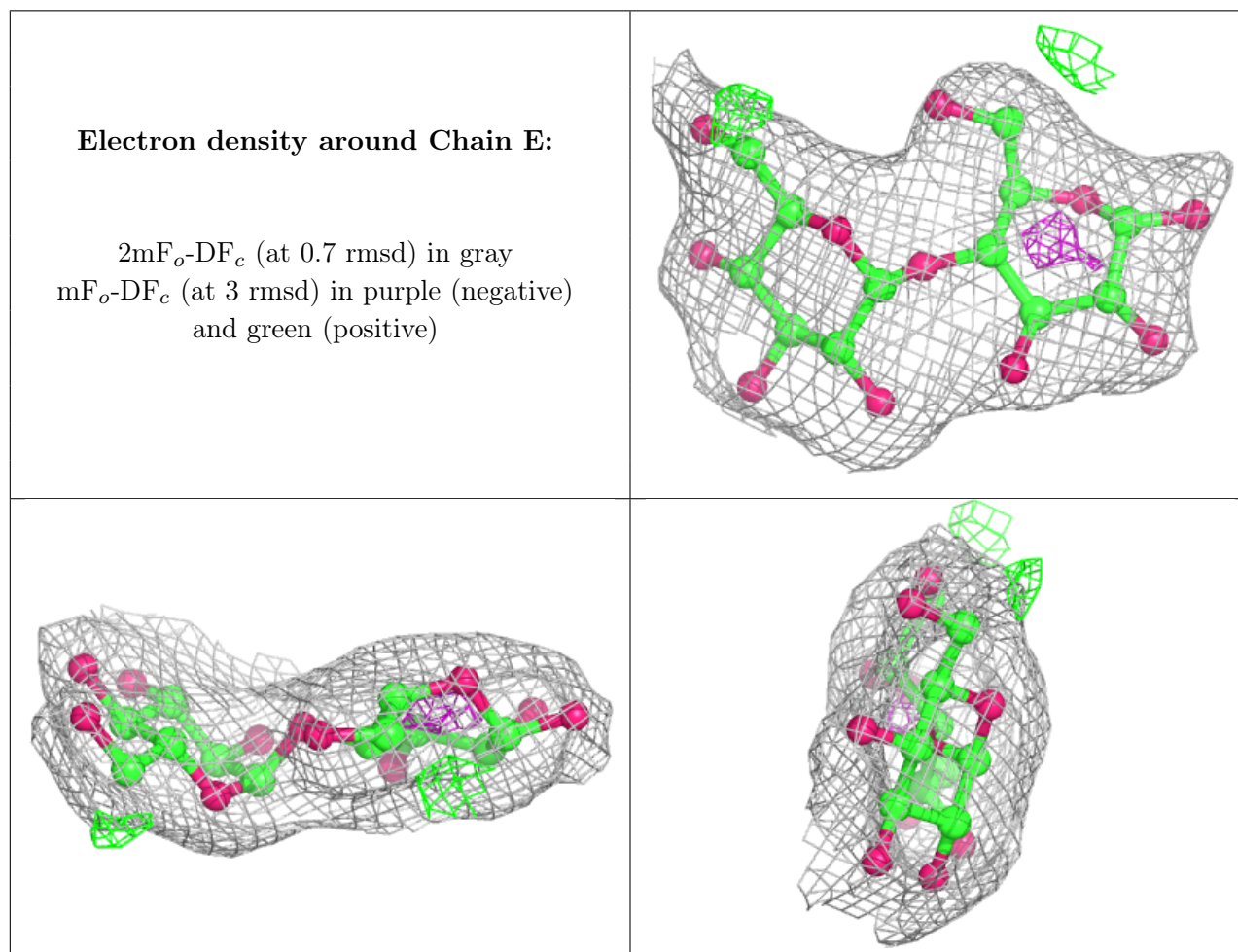
There are no non-standard protein/DNA/RNA residues in this entry.

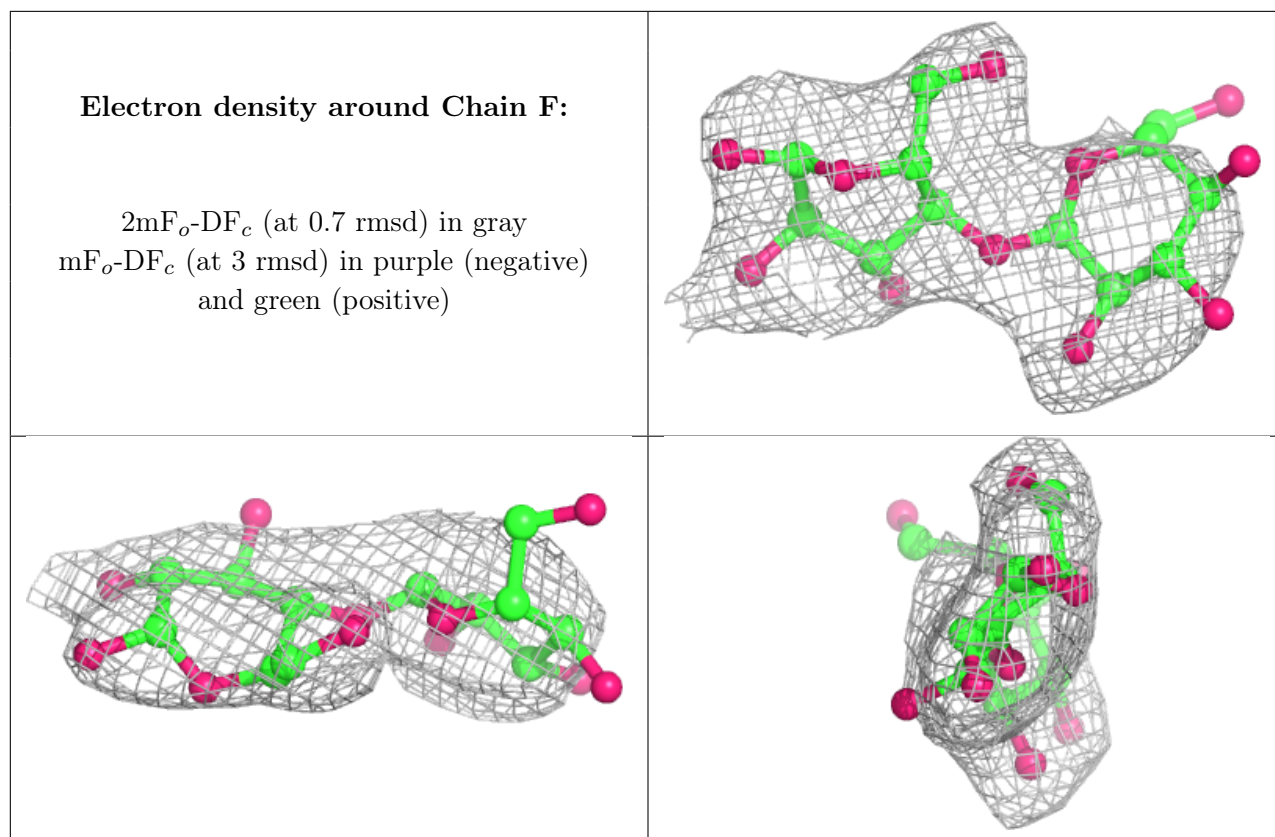
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	GLC	F	2	11/12	0.76	0.39	106,117,124,135	0
3	GLC	F	1	12/12	0.82	0.32	85,97,108,111	0
3	GLC	E	1	12/12	0.84	0.28	76,89,98,98	0
3	GLC	E	2	11/12	0.91	0.23	74,78,81,89	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.

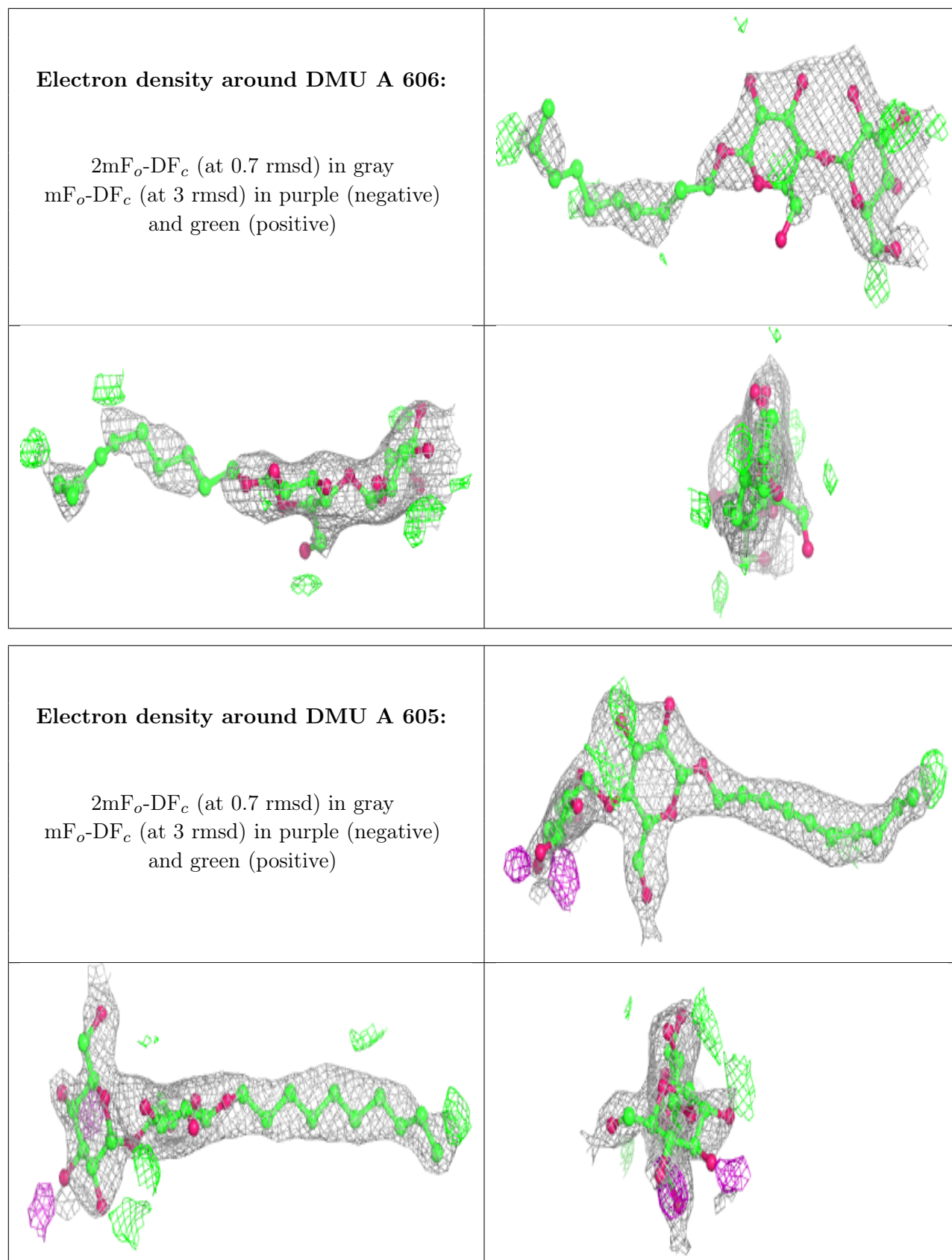
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TRD	C	607	13/13	0.55	0.36	68,74,86,87	0
7	TRD	B	302	13/13	0.68	0.36	61,73,81,81	0
7	TRD	A	610	13/13	0.70	0.41	55,67,75,80	0
7	TRD	C	608	13/13	0.75	0.37	74,77,95,97	0
7	TRD	A	613	7/13	0.77	0.40	52,60,66,69	0
6	DMU	A	606	33/33	0.77	0.30	50,63,72,79	33
7	TRD	A	609	13/13	0.78	0.36	59,67,80,81	0
13	TRS	B	311	8/8	0.78	0.13	53,71,79,80	0
6	DMU	A	605	33/33	0.79	0.34	40,61,75,75	33
6	DMU	A	604	33/33	0.79	0.28	38,84,122,125	0
7	TRD	A	612	13/13	0.79	0.20	49,60,66,66	0
8	HTH	A	616	10/10	0.79	0.37	56,69,80,87	0
6	DMU	C	604	23/33	0.79	0.36	83,89,98,101	23
7	TRD	B	303	13/13	0.80	0.36	38,58,71,72	0

Continued on next page...

Continued from previous page...

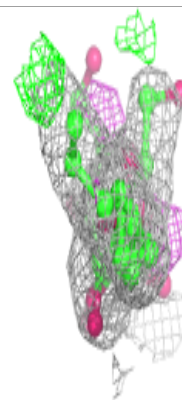
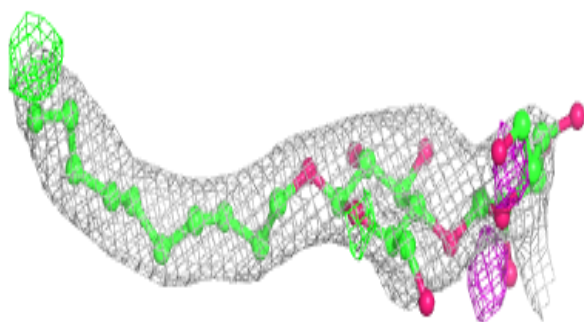
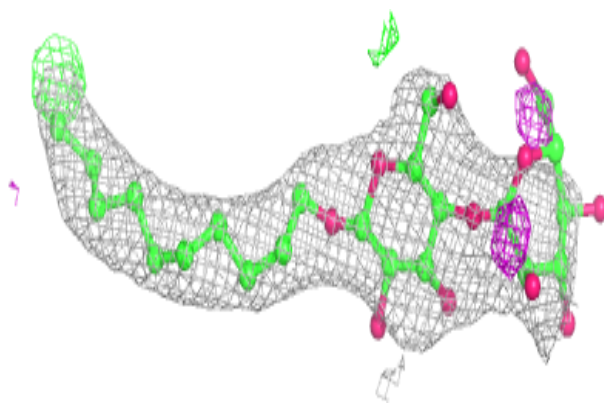
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	DMU	D	301	23/33	0.81	0.30	66,80,91,102	23
7	TRD	A	611	13/13	0.82	0.20	46,59,76,77	0
6	DMU	C	605	33/33	0.83	0.23	57,82,92,93	33
7	TRD	A	614	13/13	0.83	0.44	60,70,84,86	0
6	DMU	B	301	30/33	0.84	0.35	52,79,88,89	0
7	TRD	C	606	13/13	0.84	0.21	57,64,73,74	0
7	TRD	A	615	13/13	0.86	0.25	50,56,75,75	0
8	HTH	B	306	10/10	0.88	0.29	48,60,71,73	0
7	TRD	D	303	9/13	0.88	0.17	59,63,68,70	0
7	TRD	B	304	13/13	0.89	0.23	43,48,56,68	0
7	TRD	D	302	13/13	0.92	0.20	45,52,55,56	0
6	DMU	A	607	33/33	0.93	0.26	51,66,80,83	0
12	CD	D	308	1/1	0.95	0.06	84,84,84,84	1
4	OH	C	601	1/1	0.95	0.23	48,48,48,48	0
5	HEA	A	603	60/60	0.96	0.25	29,37,46,48	0
6	DMU	A	608	33/33	0.97	0.10	35,46,58,60	0
5	HEA	C	602	60/60	0.97	0.26	35,44,63,75	0
5	HEA	C	603	60/60	0.97	0.23	37,44,50,52	0
12	CD	B	310	1/1	0.98	0.05	69,69,69,69	1
5	HEA	A	602	60/60	0.98	0.22	27,32,40,59	0
11	CA	C	611	1/1	0.98	0.06	50,50,50,50	0
11	CA	A	619	1/1	0.99	0.09	35,35,35,35	0
9	CU	B	307	1/1	0.99	0.13	37,37,37,37	0
9	CU	C	609	1/1	0.99	0.16	44,44,44,44	0
10	MG	A	618	1/1	0.99	0.24	19,19,19,19	0
10	MG	C	610	1/1	0.99	0.23	24,24,24,24	0
9	CU	A	617	1/1	1.00	0.15	38,38,38,38	0
9	CU	D	305	1/1	1.00	0.15	40,40,40,40	0
12	CD	B	309	1/1	1.00	0.11	49,49,49,49	0
9	CU	D	306	1/1	1.00	0.11	38,38,38,38	0
12	CD	D	307	1/1	1.00	0.11	49,49,49,49	0
4	OH	A	601	1/1	1.00	0.20	40,40,40,40	0
9	CU	B	308	1/1	1.00	0.12	33,33,33,33	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.

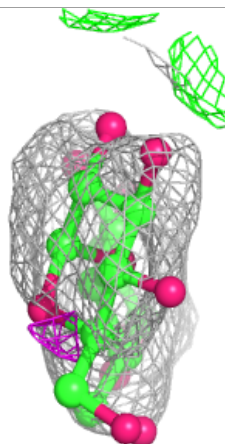
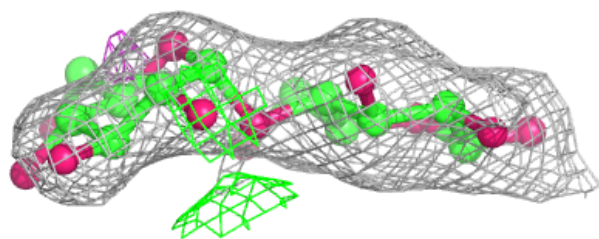
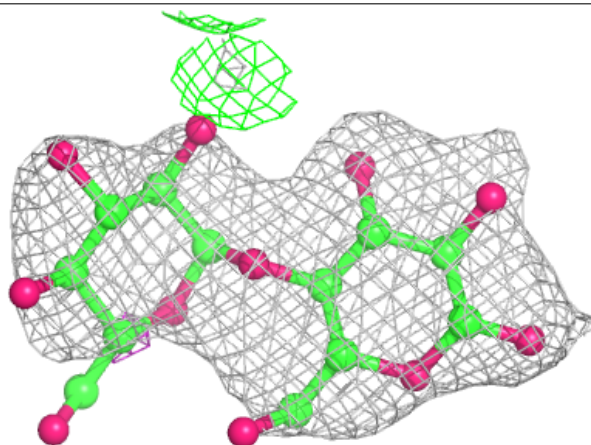


Electron density around DMU A 604:

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

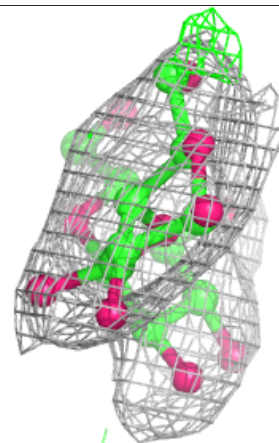
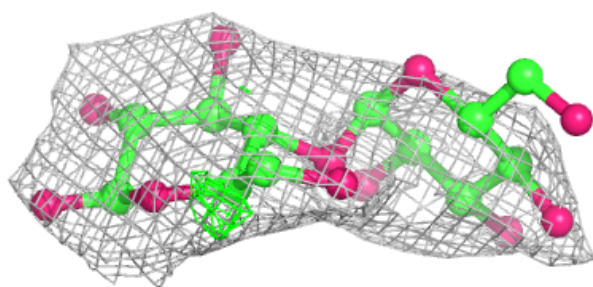
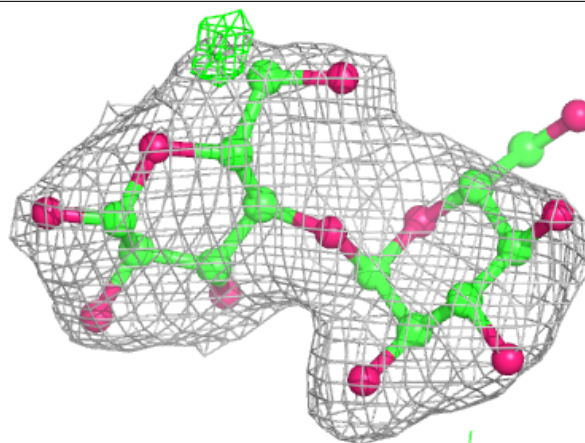
**Electron density around DMU C 604:**

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

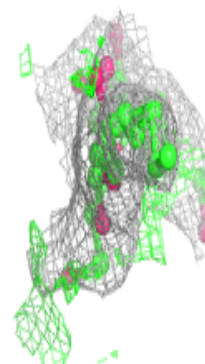
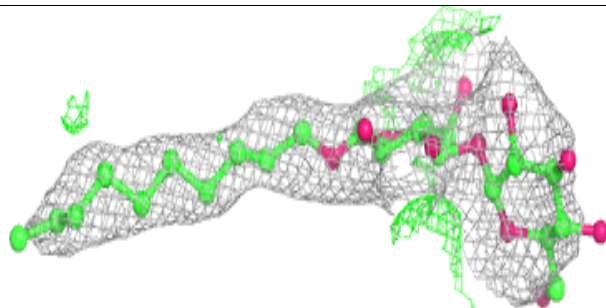
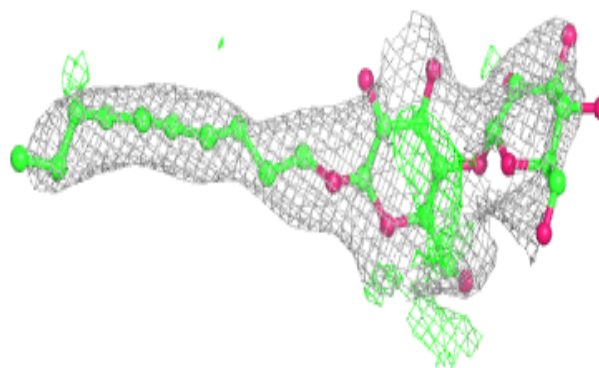


Electron density around DMU D 301:

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

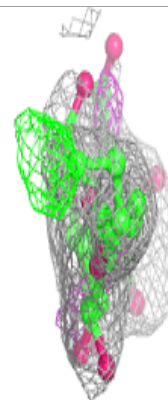
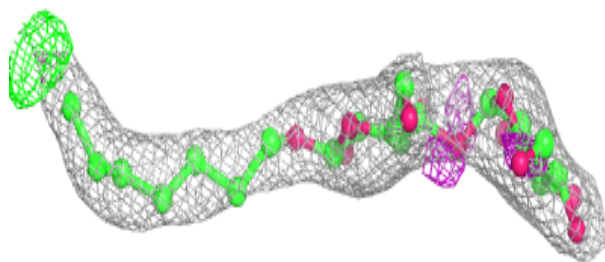
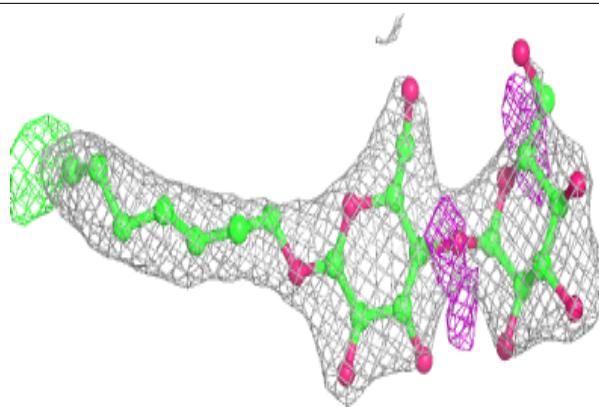
**Electron density around DMU C 605:**

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

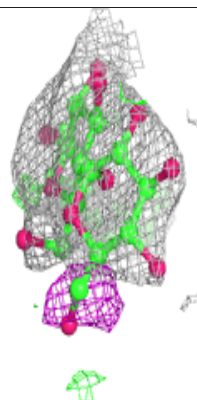
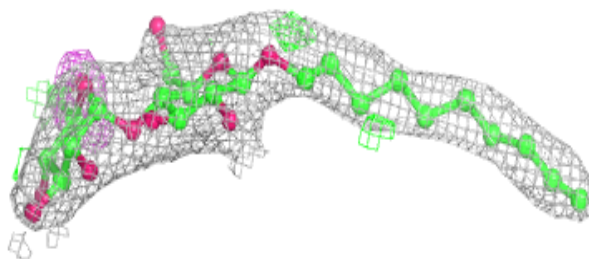
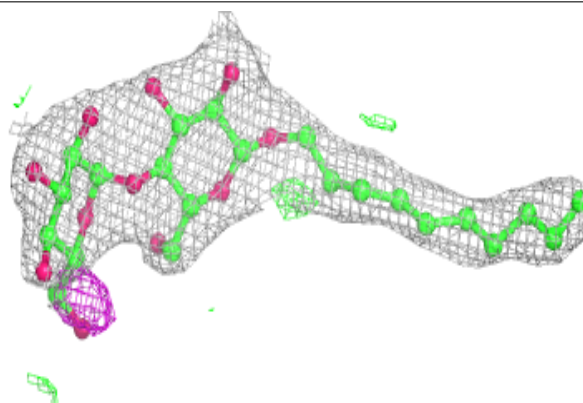


Electron density around DMU B 301:

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

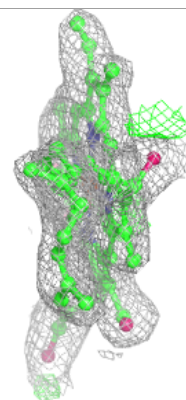
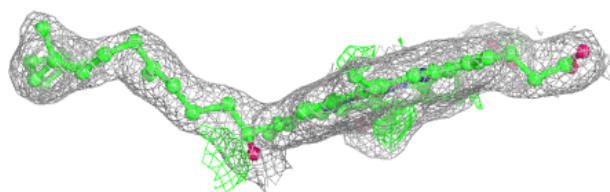
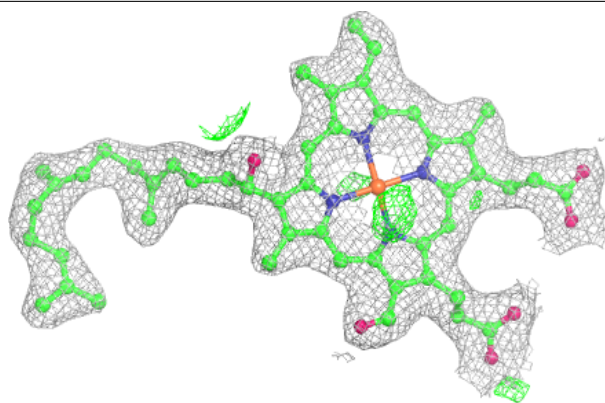
**Electron density around DMU A 607:**

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

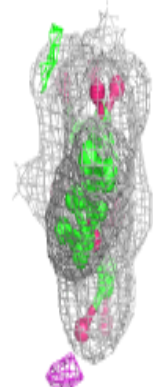
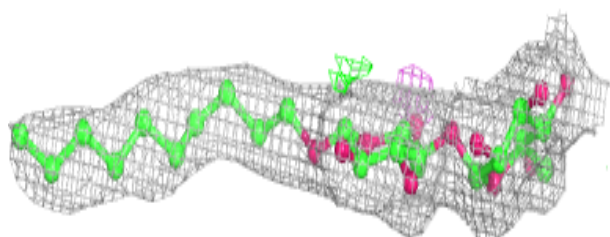
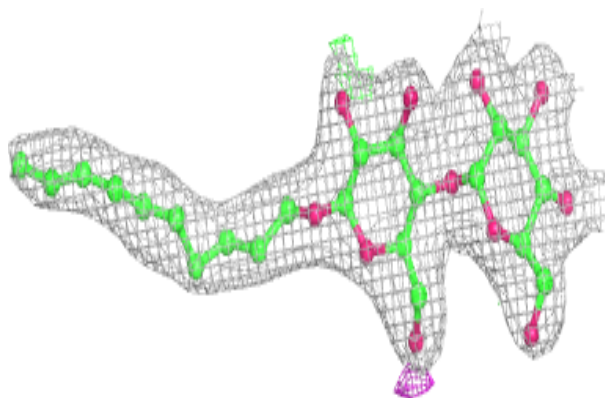


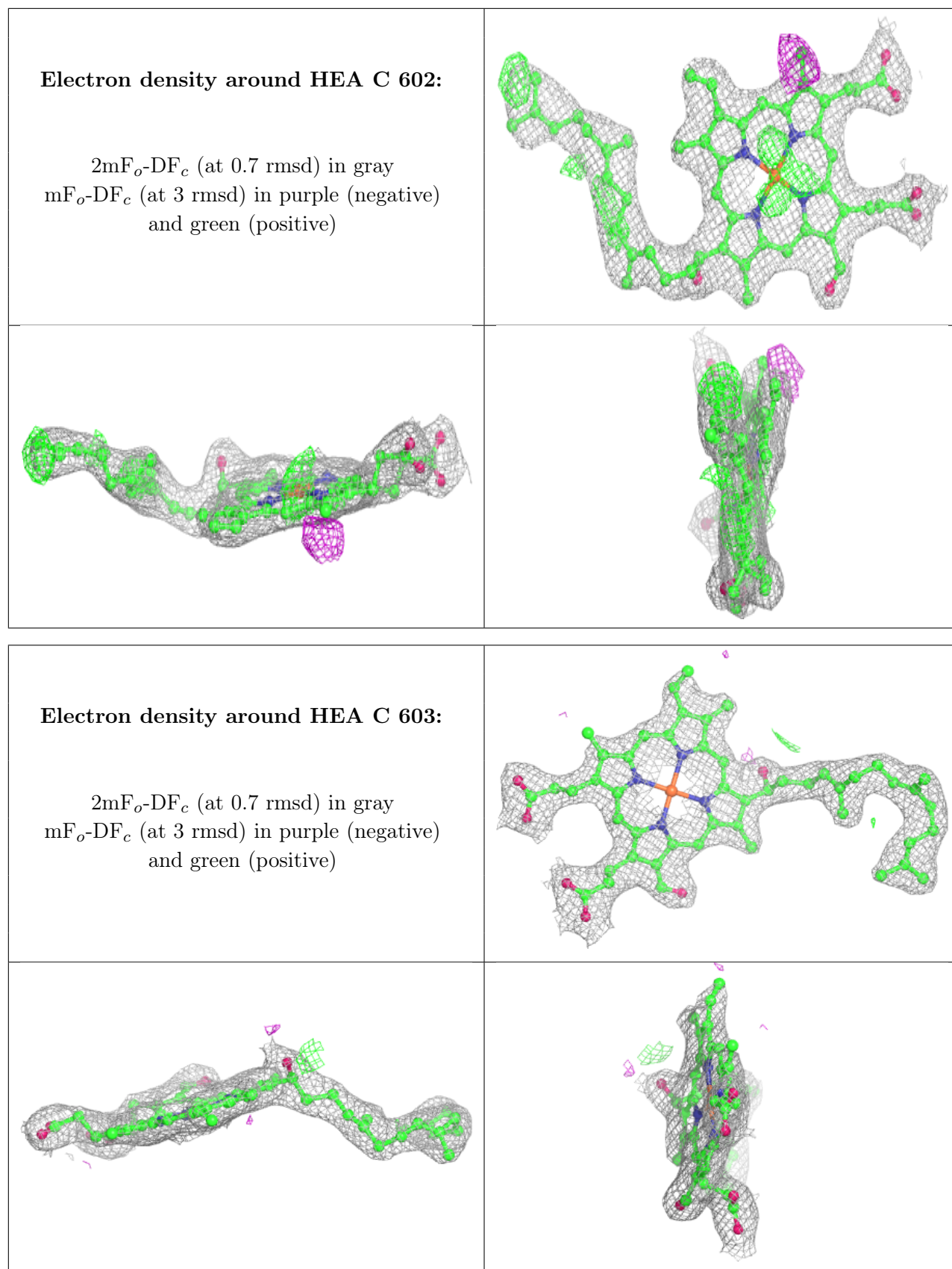
Electron density around HEA A 603:

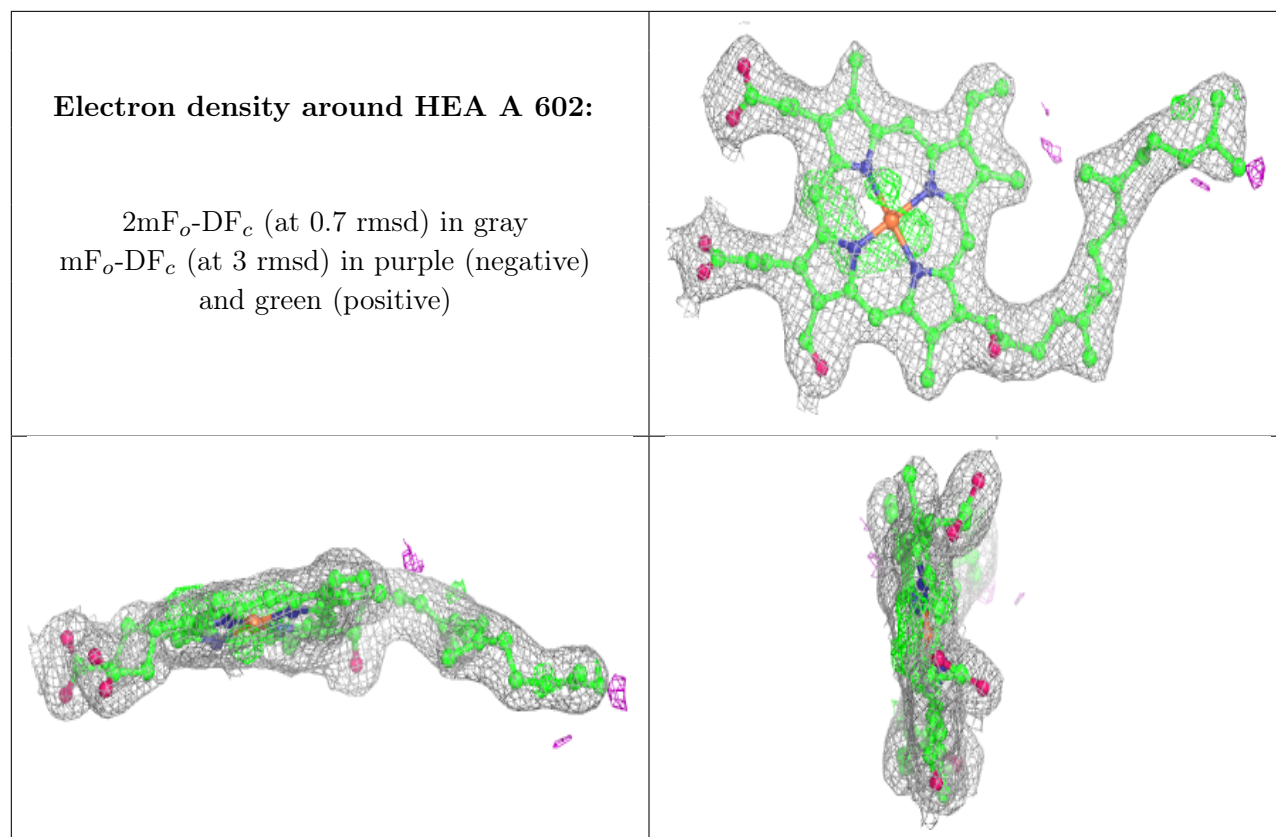
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around DMU A 608:**

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







6.5 Other polymers [i](#)

There are no such residues in this entry.