



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 01:56 AM EDT

PDB ID : 6PW1 / pdb_00006pw1
Title : Cytochrome c Oxidase delta 16
Authors : Liu, J.; Ferguson-Miller, S.
Deposited on : 2019-07-21
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

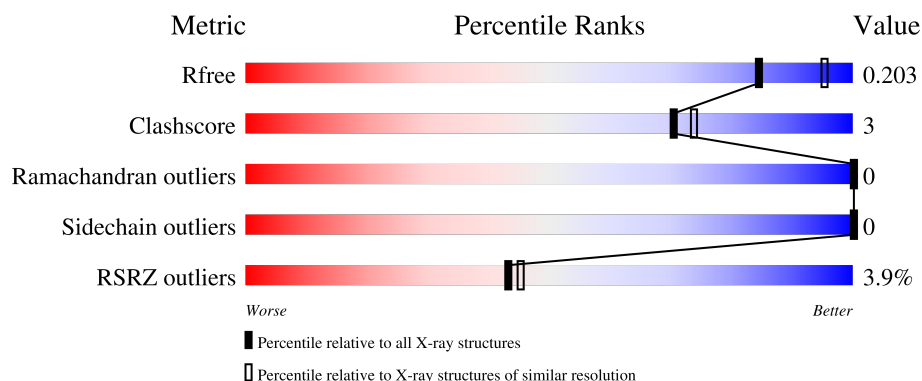
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	534	 3% 92% 8%
1	C	534	 6% 90% 10%
2	B	257	 2% 95% .
2	D	257	 3% 95% .
3	E	2	 50% 50%

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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
11	TRS	B	304	-	X	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 13526 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
1	A	534	Total	C	N	O	S	0	0	0
			4154	2780	650	694	30			
1	C	533	Total	C	N	O	S	0	0	0
			4164	2788	655	691	30			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	1	0	0
			2022	1319	333	364	6			
2	D	256	Total	C	N	O	S	0	0	0
			2003	1308	326	363	6			

There are 10 discrepancies between the modelled and reference sequences:

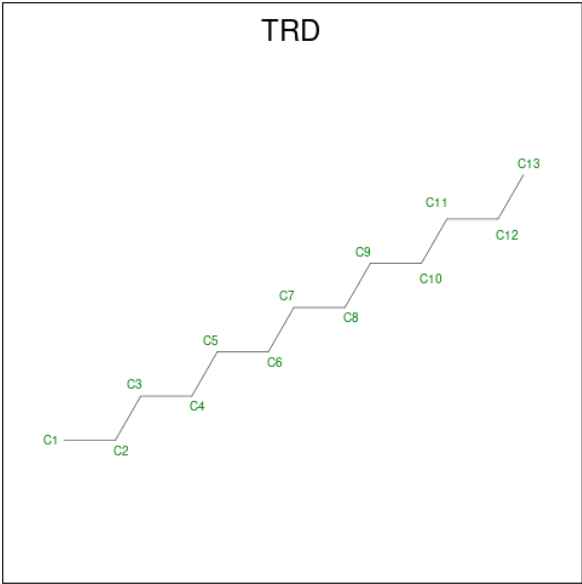
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	ALA	-	expression tag	UNP Q3J5G0
B	282	HIS	-	expression tag	UNP Q3J5G0
B	283	HIS	-	expression tag	UNP Q3J5G0
B	284	HIS	-	expression tag	UNP Q3J5G0
B	285	HIS	-	expression tag	UNP Q3J5G0
D	29	ALA	-	expression tag	UNP Q3J5G0
D	282	HIS	-	expression tag	UNP Q3J5G0
D	283	HIS	-	expression tag	UNP Q3J5G0
D	284	HIS	-	expression tag	UNP Q3J5G0
D	285	HIS	-	expression tag	UNP Q3J5G0

- 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 TRIDECANE (CCD ID: TRD) (formula: C₁₃H₂₈).



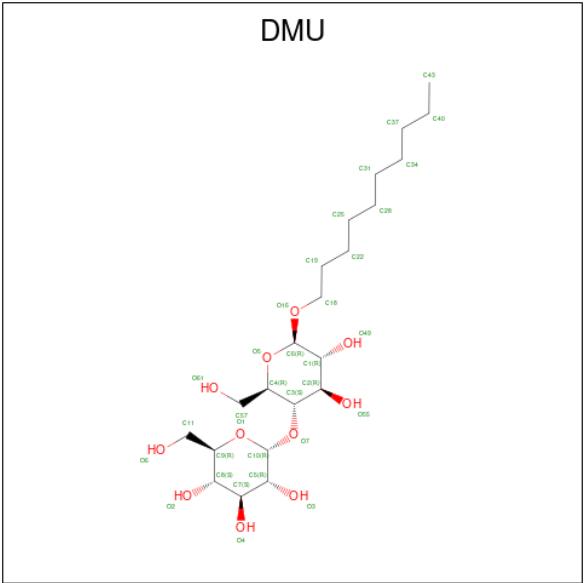
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			13	13		
4	A	1	Total	C	0	0
			13	13		
4	A	1	Total	C	0	0
			13	13		
4	A	1	Total	C	0	0
			13	13		
4	A	1	Total	C	0	0
			7	7		
4	A	1	Total	C	0	0
			13	13		
4	A	1	Total	C	0	0
			13	13		
4	A	1	Total	C	0	0
			13	13		
4	A	1	Total	C	0	0
			13	13		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

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

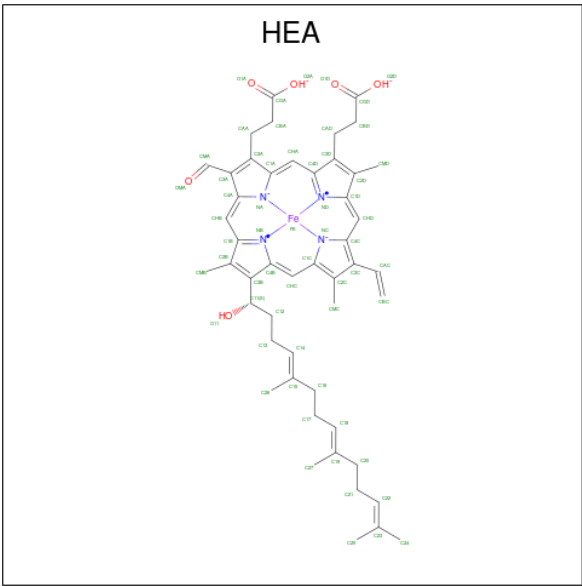
- Molecule 5 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 33 22 11	0	0
5	A	1	Total C O 33 22 11	0	0
5	A	1	Total C O 33 22 11	0	0
5	A	1	Total C O 33 22 11	0	0
5	B	1	Total C O 30 19 11	0	0
5	C	1	Total C O 23 17 6	0	0

- Molecule 6 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of

Interest" by depositor).



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

- Molecule 7 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		

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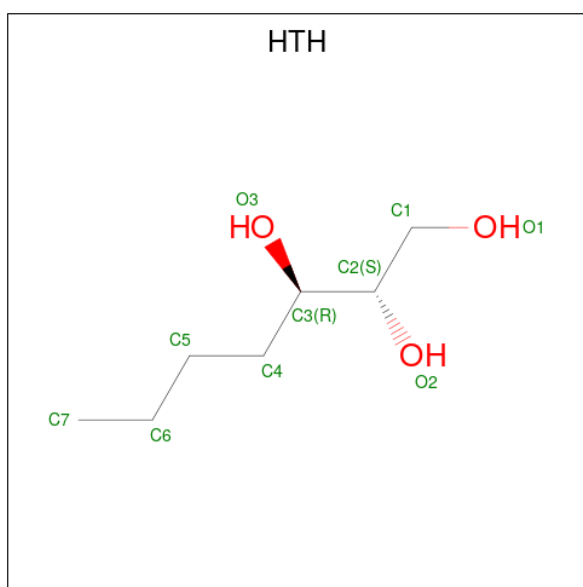
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Mg	0	0
			1	1		

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

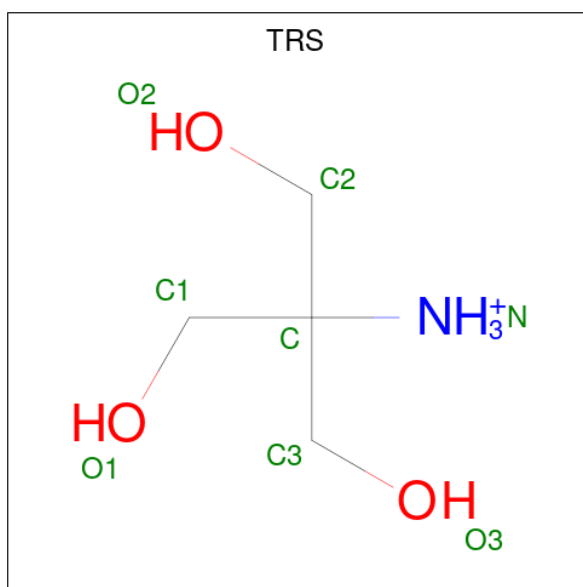
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Ca	0	0
			1	1		
9	C	1	Total	Ca	0	0
			1	1		

- Molecule 10 is (2S,3R)-heptane-1,2,3-triol (CCD ID: HTH) (formula: C₇H₁₆O₃).



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

- Molecule 11 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

- Molecule 12 is CADMIUM ION (CCD ID: 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		

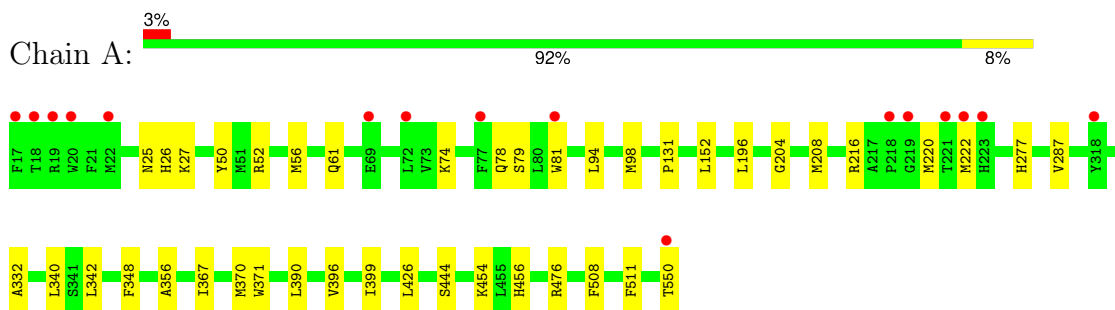
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	150	Total	O	0	0
			150	150		
13	B	124	Total	O	0	0
			124	124		
13	C	102	Total	O	0	0
			102	102		
13	D	122	Total	O	0	0
			122	122		

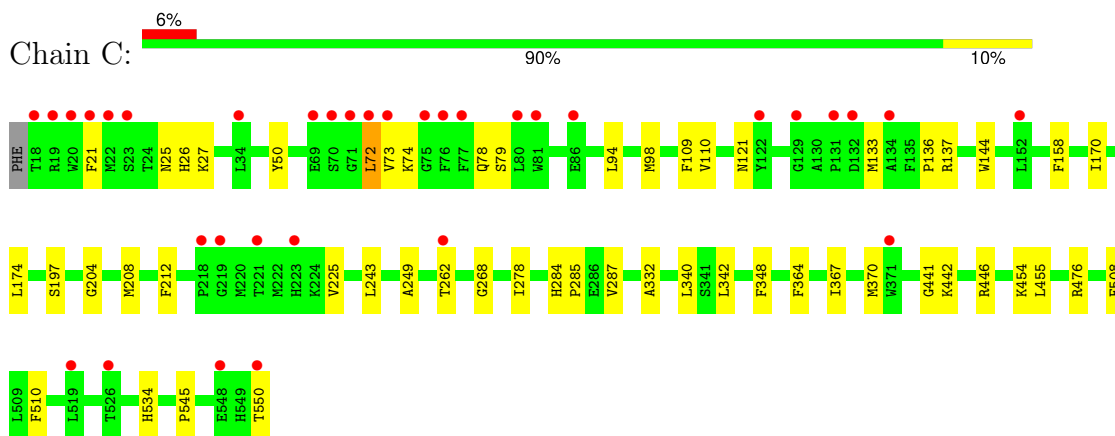
3 Residue-property plots [i](#)

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.

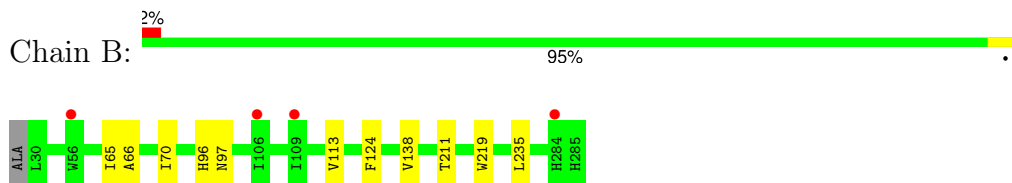
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 1: Cytochrome c oxidase subunit 1

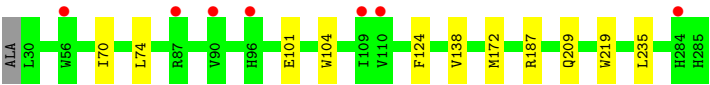


- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2





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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.31Å 130.00Å 177.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.96 – 2.10 34.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.96-2.10) 94.1 (34.96-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.180 , 0.204 0.179 , 0.203	Depositor DCC
R_{free} test set	5009 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13526	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMU, HTH, TRS, MG, GLC, TRD, HEA, CA, CD, CU

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	0.36	0/4306	0.54	0/5883
1	C	0.30	0/4318	0.52	3/5899 (0.1%)
2	B	0.33	0/2084	0.49	0/2852
2	D	0.30	0/2064	0.47	0/2828
All	All	0.32	0/12772	0.51	3/17462 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	VAL	N-CA-C	-5.33	107.63	112.96
1	C	72	LEU	CA-C-N	-5.08	116.09	121.84
1	C	72	LEU	C-N-CA	-5.08	116.09	121.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4154	0	4045	35	0
1	C	4164	0	4062	38	0
2	B	2022	0	1978	8	0
2	D	2003	0	1945	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	23	0	21	0	0
3	F	23	0	21	0	0
4	A	124	0	265	6	0
4	B	13	0	28	0	0
4	C	26	0	56	1	0
4	D	9	0	17	0	0
5	A	132	0	168	5	0
5	B	30	0	33	3	0
5	C	23	0	31	0	0
6	A	120	0	108	5	0
6	C	120	0	108	5	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	2	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	10	0	16	1	0
10	B	10	0	16	0	0
11	B	8	0	12	0	0
12	B	2	0	0	0	0
12	D	2	0	0	0	0
13	A	150	0	0	1	0
13	B	124	0	0	0	0
13	C	102	0	0	2	0
13	D	122	0	0	0	0
All	All	13526	0	12930	89	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 3.

All (89) 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:27:LYS:HZ2	1:A:550:THR:HG22	1.34	0.92
1:C:170:ILE:HD11	1:C:174:LEU:HD22	1.56	0.86
5:A:614:DMU:O49	13:A:701:HOH:O	1.81	0.80
1:A:27:LYS:NZ	1:A:550:THR:HG22	1.98	0.78
1:C:170:ILE:CD1	1:C:174:LEU:HD22	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LYS:HZ2	1:C:550:THR:HG22	1.62	0.65
1:A:56:MET:HE1	5:A:614:DMU:H10	1.77	0.64
1:A:74:LYS:O	1:A:78:GLN:HG3	1.98	0.63
1:A:25:ASN:HD21	1:A:550:THR:CG2	2.10	0.63
1:C:21:PHE:HB3	1:C:144:TRP:HZ2	1.65	0.61
1:A:61:GLN:HG2	5:A:614:DMU:H32	1.82	0.60
1:C:74:LYS:O	1:C:78:GLN:HG3	2.01	0.60
1:A:454:LYS:HD3	4:A:604:TRD:H91	1.85	0.59
1:C:508:PHE:HB2	6:C:604:HEA:H261	1.86	0.58
1:C:367:ILE:HA	1:C:370:MET:HE2	1.86	0.58
1:A:287:VAL:HB	6:A:616:HEA:CAC	2.34	0.58
1:C:27:LYS:NZ	1:C:550:THR:HG22	2.20	0.57
1:A:390:LEU:HD13	1:A:426:LEU:HD12	1.86	0.57
6:A:615:HEA:HBC1	6:A:615:HEA:HMC1	1.85	0.57
1:A:367:ILE:HA	1:A:370:MET:HE2	1.87	0.56
1:C:136:PRO:HD2	1:C:137:ARG:HH12	1.71	0.56
6:C:604:HEA:HMC1	6:C:604:HEA:HBC1	1.89	0.55
1:C:287:VAL:HB	6:C:605:HEA:CAC	2.37	0.54
2:B:96:HIS:O	5:B:302:DMU:O61	2.23	0.52
1:A:52:ARG:NH2	6:A:615:HEA:OMA	2.42	0.52
1:C:50:TYR:OH	1:C:79:SER:HB3	2.09	0.52
1:A:508:PHE:HB2	6:A:615:HEA:H261	1.92	0.50
1:C:25:ASN:HD21	1:C:550:THR:CG2	2.24	0.50
1:C:26:HIS:CD2	1:C:550:THR:HG21	2.47	0.50
1:C:170:ILE:HD11	1:C:174:LEU:CD2	2.34	0.50
1:A:356:ALA:HB2	1:A:399:ILE:HD11	1.94	0.49
1:C:332:ALA:HB1	1:C:340:LEU:HD11	1.94	0.49
1:C:364:PHE:HB3	2:D:104:TRP:CE3	2.48	0.49
1:C:204:GLY:O	1:C:208:MET:HG2	2.13	0.49
1:A:94:LEU:O	1:A:98:MET:HG2	2.12	0.48
1:C:110:VAL:HG11	6:C:604:HEA:H271	1.94	0.48
1:C:476:ARG:HH21	4:C:601:TRD:H122	1.77	0.48
1:A:26:HIS:CD2	1:A:550:THR:HG21	2.48	0.48
1:C:121:ASN:OD1	1:C:133:MET:HE3	2.13	0.48
1:C:534:HIS:HD2	13:C:801:HOH:O	1.95	0.48
1:C:109:PHE:CE1	1:C:197:SER:HB2	2.50	0.47
1:C:342:LEU:HD21	2:D:124:PHE:CD2	2.49	0.46
1:A:204:GLY:O	1:A:208:MET:HG2	2.15	0.46
1:C:26:HIS:NE2	1:C:550:THR:HG21	2.30	0.46
1:A:25:ASN:HD21	1:A:550:THR:HG23	1.79	0.46
1:A:456:HIS:CE1	1:A:511:PHE:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:209:GLN:HB3	2:D:235:LEU:HD11	1.96	0.46
1:A:332:ALA:HB1	1:A:340:LEU:HD11	1.98	0.46
2:B:138:VAL:HG11	2:B:219:TRP:CD1	2.51	0.46
1:A:277:HIS:HB3	4:A:606:TRD:H81	1.99	0.45
1:A:476:ARG:HH21	4:A:609:TRD:H31	1.81	0.45
1:A:342:LEU:HD21	2:B:124:PHE:CD2	2.52	0.44
1:A:371:TRP:CD1	5:B:302:DMU:H9	2.52	0.44
1:C:442:LYS:O	1:C:545:PRO:HA	2.18	0.44
1:A:287:VAL:HB	6:A:616:HEA:C3C	2.48	0.43
5:A:614:DMU:H36	5:A:614:DMU:H2	1.33	0.43
1:C:262:THR:OG1	1:C:268:GLY:HA3	2.18	0.43
1:C:72:LEU:HD21	1:C:158:PHE:CE1	2.53	0.43
1:C:170:ILE:CD1	1:C:174:LEU:CD2	2.93	0.43
2:D:101:GLU:HA	2:D:104:TRP:CD1	2.53	0.43
10:A:620:HTH:H3	2:B:113:VAL:HA	2.01	0.43
1:C:455:LEU:HD23	1:C:510:PHE:CZ	2.54	0.43
2:D:70:ILE:O	2:D:74:LEU:HG	2.18	0.43
1:A:131:PRO:O	1:A:550:THR:OG1	2.36	0.43
1:C:332:ALA:HB3	1:C:348:PHE:CD2	2.54	0.43
1:C:212:PHE:CE2	1:C:225:VAL:HG11	2.54	0.43
1:A:332:ALA:HB3	1:A:348:PHE:CD2	2.54	0.42
4:A:607:TRD:H71	4:A:607:TRD:H42	1.61	0.42
2:B:97:ASN:ND2	5:B:302:DMU:H29	2.34	0.42
1:C:249:ALA:HB2	1:C:278:ILE:HG22	2.02	0.42
2:B:211:THR:HB	2:B:235:LEU:HD12	2.00	0.42
1:A:27:LYS:HZ2	1:A:550:THR:CG2	2.19	0.42
1:C:454:LYS:HE3	13:C:779:HOH:O	2.18	0.42
1:A:50:TYR:OH	1:A:79:SER:HB3	2.20	0.42
2:D:138:VAL:HG11	2:D:219:TRP:CD1	2.55	0.42
1:A:216:ARG:HD2	1:A:220:MET:O	2.20	0.41
1:C:441:GLY:HA2	1:C:446:ARG:O	2.19	0.41
1:A:396:VAL:HB	2:B:65:ILE:HB	2.02	0.41
1:A:444:SER:HB3	5:A:611:DMU:H8	2.01	0.41
1:C:94:LEU:O	1:C:98:MET:HG2	2.20	0.41
1:C:287:VAL:HB	6:C:605:HEA:C3C	2.50	0.41
2:D:172:MET:HE3	2:D:187:ARG:HG3	2.02	0.41
1:A:216:ARG:CZ	1:A:222:MET:HG3	2.51	0.41
1:C:243:LEU:HD13	1:C:243:LEU:HA	1.90	0.40
1:A:81:TRP:CZ2	4:A:601:TRD:H62	2.56	0.40
1:A:454:LYS:HD2	4:A:604:TRD:H133	2.04	0.40
1:C:284:HIS:HB3	1:C:285:PRO:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HD12	1:A:196:LEU:HD12	2.02	0.40
2:B:66:ALA:O	2:B:70:ILE:HG12	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	532/534 (100%)	520 (98%)	12 (2%)	0	100	100
1	C	531/534 (99%)	521 (98%)	10 (2%)	0	100	100
2	B	254/257 (99%)	246 (97%)	8 (3%)	0	100	100
2	D	254/257 (99%)	246 (97%)	8 (3%)	0	100	100
All	All	1571/1582 (99%)	1533 (98%)	38 (2%)	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	425/434 (98%)	425 (100%)	0	100	100
1	C	426/434 (98%)	426 (100%)	0	100	100
2	B	214/215 (100%)	214 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	210/215 (98%)	210 (100%)	0	100	100
All	All	1275/1298 (98%)	1275 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	139	ASN
2	B	53	GLN
2	B	88	ASN
2	B	96	HIS
2	B	125	ASN
2	B	170	ASN
2	B	179	GLN
2	B	251	GLN
1	C	67	HIS
1	C	78	GLN
1	C	163	ASN
2	D	170	ASN
2	D	251	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.50	0	17,17,17	0.49	0
3	GLC	E	2	3	11,11,12	0.56	0	15,15,17	1.22	1 (6%)
3	GLC	F	1	3	12,12,12	0.49	0	17,17,17	1.25	2 (11%)
3	GLC	F	2	3	11,11,12	0.74	0	15,15,17	1.80	3 (20%)

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	-	2/2/22/22	0/1/1/1
3	GLC	F	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	GLC	C1-C2-C3	4.92	116.81	109.64
3	E	2	GLC	C1-O5-C5	3.87	117.38	112.19
3	F	1	GLC	C4-C3-C2	-2.86	105.80	110.83
3	F	1	GLC	O4-C4-C5	2.79	116.19	109.32
3	F	2	GLC	O5-C1-C2	2.35	116.40	110.79
3	F	2	GLC	C3-C4-C5	-2.27	106.12	110.23

There are no chirality outliers.

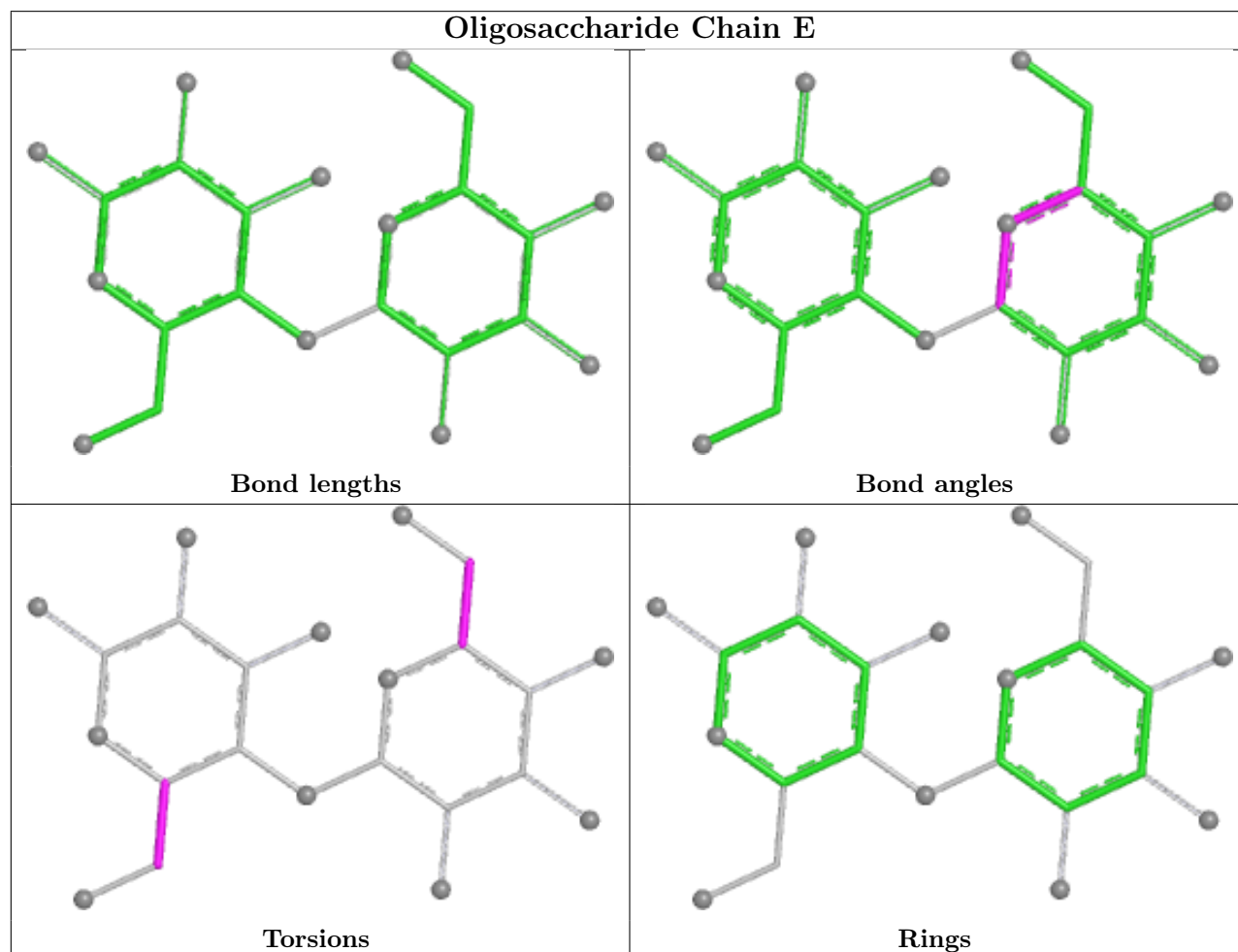
All (4) torsion outliers are listed below:

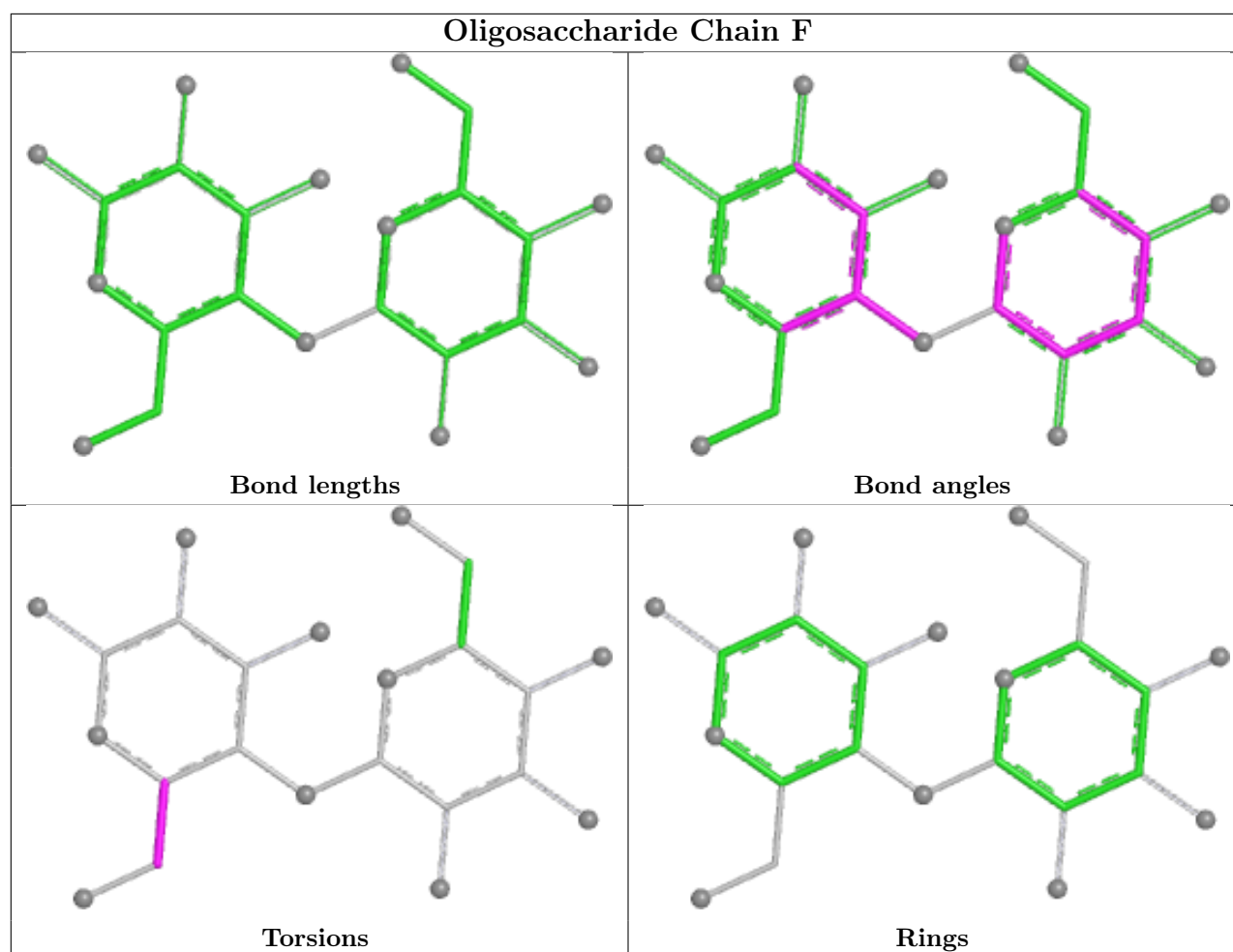
Mol	Chain	Res	Type	Atoms
3	F	1	GLC	O5-C5-C6-O6
3	F	1	GLC	C4-C5-C6-O6
3	E	2	GLC	O5-C5-C6-O6
3	E	1	GLC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 14 are monoatomic - leaving 27 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	$\# Z > 2$
4	TRD	A	601	-	12,12,12	0.14	0	11,11,11	0.65	0
6	HEA	A	615	1	67,67,67	2.30	24 (35%)	81,103,103	2.44	29 (35%)
6	HEA	C	605	1,13	67,67,67	2.43	26 (38%)	81,103,103	2.41	31 (38%)
5	DMU	C	603	-	23,23,34	1.83	6 (26%)	28,28,45	1.04	2 (7%)
4	TRD	A	602	-	12,12,12	0.17	0	11,11,11	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TRD	C	601	-	12,12,12	0.14	0	11,11,11	0.93	0
4	TRD	A	605	-	6,6,12	0.17	0	5,5,11	0.56	0
10	HTH	A	620	-	9,9,9	0.58	0	10,10,10	1.30	1 (10%)
11	TRS	B	304	-	7,7,7	0.34	0	9,9,9	1.28	1 (11%)
4	TRD	A	606	-	12,12,12	0.12	0	11,11,11	0.98	0
5	DMU	A	612	-	34,34,34	1.77	8 (23%)	45,45,45	1.26	4 (8%)
5	DMU	A	614	-	34,34,34	1.91	12 (35%)	45,45,45	1.91	11 (24%)
4	TRD	A	604	-	12,12,12	0.17	0	11,11,11	0.63	0
4	TRD	A	609	-	12,12,12	0.13	0	11,11,11	0.81	0
4	TRD	A	603	-	12,12,12	0.15	0	11,11,11	0.72	0
4	TRD	C	602	-	12,12,12	0.14	0	11,11,11	0.69	0
6	HEA	C	604	1	67,67,67	2.37	23 (34%)	81,103,103	2.42	30 (37%)
4	TRD	A	608	-	12,12,12	0.14	0	11,11,11	0.71	0
4	TRD	A	610	-	12,12,12	0.16	0	11,11,11	0.74	0
5	DMU	A	613	-	34,34,34	1.93	10 (29%)	45,45,45	1.40	6 (13%)
10	HTH	B	309	-	9,9,9	0.58	0	10,10,10	1.14	2 (20%)
5	DMU	A	611	-	34,34,34	1.94	13 (38%)	45,45,45	1.28	4 (8%)
5	DMU	B	302	-	31,31,34	1.97	12 (38%)	42,42,45	1.27	4 (9%)
4	TRD	A	607	-	12,12,12	0.09	0	11,11,11	0.87	0
4	TRD	B	301	-	12,12,12	0.15	0	11,11,11	0.76	0
6	HEA	A	616	1,13	67,67,67	2.31	24 (35%)	81,103,103	2.39	30 (37%)
4	TRD	D	301	-	8,8,12	0.12	0	7,7,11	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRD	A	601	-	-	0/10/10/10	-
6	HEA	A	615	1	-	6/36/76/76	-
6	HEA	C	605	1,13	-	5/36/76/76	-
5	DMU	C	603	-	-	5/15/35/59	0/1/1/2
4	TRD	A	602	-	-	2/10/10/10	-
4	TRD	C	601	-	-	3/10/10/10	-
4	TRD	A	605	-	-	1/4/4/10	-
10	HTH	A	620	-	-	6/10/10/10	-
11	TRS	B	304	-	-	9/9/9/9	-
4	TRD	A	606	-	-	3/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMU	A	612	-	-	3/19/59/59	0/2/2/2
5	DMU	A	614	-	-	8/19/59/59	0/2/2/2
4	TRD	A	604	-	-	5/10/10/10	-
4	TRD	A	609	-	-	3/10/10/10	-
4	TRD	A	603	-	-	4/10/10/10	-
4	TRD	C	602	-	-	2/10/10/10	-
6	HEA	C	604	1	-	4/36/76/76	-
4	TRD	A	608	-	-	7/10/10/10	-
4	TRD	A	610	-	-	3/10/10/10	-
5	DMU	A	613	-	-	6/19/59/59	0/2/2/2
10	HTH	B	309	-	-	5/10/10/10	-
5	DMU	A	611	-	-	13/19/59/59	0/2/2/2
5	DMU	B	302	-	-	8/16/56/59	0/2/2/2
4	TRD	A	607	-	-	4/10/10/10	-
4	TRD	B	301	-	-	3/10/10/10	-
6	HEA	A	616	1,13	-	5/36/76/76	-
4	TRD	D	301	-	-	1/6/6/10	-

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	605	HEA	FE-NB	5.74	2.12	1.94
6	C	604	HEA	C3B-C2B	5.55	1.47	1.34
6	C	605	HEA	FE-ND	5.36	2.11	1.94
6	A	616	HEA	FE-ND	5.11	2.10	1.94
6	C	605	HEA	C3B-C2B	5.08	1.46	1.34
6	A	616	HEA	C3B-C2B	5.06	1.46	1.34
6	A	615	HEA	C3B-C2B	4.95	1.46	1.34
6	C	604	HEA	FE-ND	4.90	2.10	1.94
6	A	616	HEA	FE-NB	4.89	2.10	1.94
6	C	604	HEA	FE-NC	4.88	2.11	1.95
6	A	615	HEA	FE-NB	4.86	2.09	1.94
6	C	604	HEA	FE-NB	4.80	2.09	1.94
6	C	605	HEA	FE-NC	4.76	2.10	1.95
6	C	604	HEA	CHD-C1D	4.68	1.47	1.38
6	C	604	HEA	C3D-C2D	4.59	1.46	1.36
6	A	615	HEA	FE-ND	4.58	2.09	1.94
6	A	615	HEA	C3D-C2D	4.56	1.46	1.36
5	C	603	DMU	O16-C6	-4.53	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	614	DMU	O16-C6	-4.52	1.32	1.40
6	C	605	HEA	CHD-C1D	4.50	1.47	1.38
6	C	605	HEA	C3D-C2D	4.49	1.46	1.36
6	A	616	HEA	C3D-C2D	4.43	1.46	1.36
6	A	615	HEA	CHC-C4B	4.42	1.47	1.38
6	A	615	HEA	FE-NC	4.42	2.09	1.95
6	A	616	HEA	CHD-C1D	4.36	1.47	1.38
6	C	605	HEA	C3A-C2A	4.31	1.47	1.37
6	C	605	HEA	CHC-C4B	4.28	1.47	1.38
6	A	616	HEA	C3A-C2A	4.27	1.46	1.37
6	A	616	HEA	FE-NC	4.23	2.09	1.95
6	C	604	HEA	C3A-C2A	4.14	1.46	1.37
6	C	605	HEA	CHB-C4A	4.14	1.46	1.38
6	C	604	HEA	CHC-C4B	4.13	1.46	1.38
6	C	604	HEA	CHA-C1A	4.13	1.46	1.38
6	A	616	HEA	CHC-C4B	4.12	1.46	1.38
5	A	612	DMU	O16-C6	-4.06	1.33	1.40
6	A	615	HEA	CHB-C4A	4.02	1.46	1.38
6	C	604	HEA	CHB-C4A	4.01	1.46	1.38
6	A	615	HEA	C1A-NA	4.01	1.47	1.39
6	A	616	HEA	C1A-NA	3.98	1.47	1.39
6	A	616	HEA	CHB-C4A	3.97	1.46	1.38
5	A	611	DMU	O16-C6	-3.96	1.33	1.40
5	A	613	DMU	O16-C6	-3.94	1.33	1.40
6	C	604	HEA	C1A-NA	3.93	1.47	1.39
6	A	615	HEA	CHD-C1D	3.91	1.46	1.38
6	A	616	HEA	CHA-C1A	3.90	1.46	1.38
6	A	615	HEA	C3A-C2A	3.89	1.46	1.37
5	B	302	DMU	O16-C6	-3.88	1.33	1.40
6	C	605	HEA	C1A-NA	3.83	1.46	1.39
5	A	611	DMU	O1-C9	3.83	1.53	1.44
6	C	605	HEA	C4A-NA	3.82	1.46	1.39
6	A	615	HEA	CHA-C1A	3.75	1.45	1.38
6	C	605	HEA	CHA-C1A	3.70	1.45	1.38
5	A	614	DMU	C11-C9	-3.69	1.39	1.51
6	A	616	HEA	C4A-NA	3.65	1.46	1.39
5	B	302	DMU	C11-C9	-3.61	1.39	1.51
5	A	613	DMU	C11-C9	-3.60	1.39	1.51
6	A	615	HEA	CHD-C4C	3.59	1.47	1.39
5	C	603	DMU	O7-C3	3.53	1.51	1.42
5	A	611	DMU	C11-C9	-3.50	1.40	1.51
5	B	302	DMU	O1-C9	3.50	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	616	HEA	CHB-C1B	3.49	1.47	1.39
6	C	604	HEA	C11-C3B	-3.49	1.47	1.51
6	C	605	HEA	CHC-C1C	3.48	1.47	1.39
6	C	604	HEA	CHC-C1C	3.48	1.47	1.39
6	A	616	HEA	CHC-C1C	3.46	1.47	1.39
5	A	614	DMU	O1-C9	3.45	1.52	1.44
5	A	613	DMU	O5-C6	3.44	1.50	1.41
6	C	605	HEA	CHD-C4C	3.41	1.47	1.39
5	A	613	DMU	O1-C9	3.40	1.52	1.44
6	A	615	HEA	CHC-C1C	3.35	1.46	1.39
6	C	605	HEA	CHB-C1B	3.34	1.46	1.39
6	C	604	HEA	CHD-C4C	3.33	1.46	1.39
6	A	615	HEA	C11-C3B	-3.31	1.47	1.51
5	A	612	DMU	C11-C9	-3.31	1.40	1.51
5	A	612	DMU	O1-C9	3.29	1.52	1.44
6	C	604	HEA	CHB-C1B	3.27	1.46	1.39
5	A	614	DMU	O5-C6	3.24	1.50	1.41
5	C	603	DMU	O5-C6	3.23	1.50	1.41
5	A	611	DMU	O5-C6	3.23	1.50	1.41
6	A	615	HEA	C4B-NB	-3.16	1.34	1.40
6	C	604	HEA	C4B-NB	-3.13	1.34	1.40
5	B	302	DMU	O5-C6	3.13	1.49	1.41
6	A	615	HEA	C4A-NA	3.10	1.45	1.39
6	A	616	HEA	CHD-C4C	3.05	1.46	1.39
5	A	613	DMU	O7-C3	3.03	1.51	1.43
5	A	611	DMU	O7-C3	3.02	1.51	1.43
6	C	604	HEA	C4A-NA	3.02	1.45	1.39
6	C	605	HEA	C1D-ND	-3.01	1.35	1.40
6	A	615	HEA	C1D-ND	-3.01	1.35	1.40
6	C	604	HEA	CHA-C4D	3.00	1.46	1.39
5	A	612	DMU	C8-C9	3.00	1.59	1.53
6	C	605	HEA	CHA-C4D	2.99	1.46	1.39
6	A	616	HEA	CHA-C4D	2.97	1.46	1.39
5	B	302	DMU	O7-C3	2.96	1.51	1.43
6	A	615	HEA	CHB-C1B	2.95	1.45	1.39
6	A	615	HEA	CHA-C4D	2.92	1.45	1.39
5	A	614	DMU	O7-C3	2.86	1.51	1.43
5	A	612	DMU	C2-C3	-2.84	1.44	1.52
5	A	612	DMU	O5-C6	2.78	1.49	1.41
6	A	616	HEA	C1D-ND	-2.76	1.35	1.40
5	B	302	DMU	C2-C3	-2.74	1.44	1.52
6	C	604	HEA	C1D-ND	-2.74	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	613	DMU	C2-C3	-2.73	1.44	1.52
6	C	605	HEA	C4B-NB	-2.72	1.35	1.40
6	C	605	HEA	C1C-C2C	2.67	1.49	1.43
6	C	604	HEA	C4C-NC	-2.62	1.34	1.39
6	A	615	HEA	C4C-NC	-2.61	1.34	1.39
6	C	605	HEA	C1C-NC	-2.60	1.34	1.39
6	C	604	HEA	C1C-C2C	2.60	1.49	1.43
5	A	613	DMU	O5-C4	2.60	1.50	1.44
5	A	614	DMU	O3-C5	2.59	1.49	1.43
5	A	611	DMU	O4-C7	2.58	1.49	1.43
5	B	302	DMU	C7-C5	-2.58	1.45	1.52
5	A	614	DMU	C7-C5	-2.57	1.45	1.52
6	C	605	HEA	C4C-NC	-2.56	1.34	1.39
5	A	611	DMU	C8-C9	2.55	1.58	1.53
5	A	611	DMU	C2-C3	-2.54	1.45	1.52
6	C	605	HEA	C4B-C3B	2.52	1.49	1.44
5	A	613	DMU	O4-C7	2.51	1.49	1.43
6	A	615	HEA	C1B-NB	-2.51	1.33	1.38
5	C	603	DMU	C2-C3	-2.47	1.45	1.52
5	A	611	DMU	O5-C4	2.46	1.50	1.44
5	A	611	DMU	C7-C5	-2.45	1.46	1.52
6	C	605	HEA	C11-C3B	-2.44	1.48	1.51
6	C	605	HEA	C4D-ND	-2.43	1.34	1.38
6	A	616	HEA	C1C-NC	-2.43	1.35	1.39
5	B	302	DMU	O4-C7	2.42	1.48	1.43
5	A	612	DMU	O4-C7	2.41	1.48	1.43
5	C	603	DMU	O5-C4	2.34	1.50	1.44
6	A	616	HEA	C1A-C2A	2.33	1.49	1.45
5	A	613	DMU	O55-C2	2.33	1.48	1.43
6	C	605	HEA	C1A-C2A	2.32	1.49	1.45
6	A	615	HEA	C1C-C2C	2.31	1.48	1.43
6	A	616	HEA	C4D-ND	-2.25	1.34	1.38
6	A	616	HEA	C1C-C2C	2.23	1.48	1.43
5	A	613	DMU	C7-C5	-2.21	1.46	1.52
5	A	614	DMU	C2-C3	-2.19	1.46	1.52
5	A	614	DMU	C8-C9	2.19	1.57	1.53
5	C	603	DMU	O55-C2	2.18	1.48	1.43
6	A	616	HEA	C4B-NB	-2.17	1.36	1.40
5	A	612	DMU	O7-C3	2.17	1.49	1.43
6	C	604	HEA	C1C-NC	-2.15	1.35	1.39
6	A	616	HEA	C4B-C3B	2.14	1.48	1.44
5	B	302	DMU	O5-C4	2.13	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	611	DMU	O1-C10	2.12	1.47	1.41
5	A	614	DMU	O55-C2	2.11	1.48	1.43
5	A	611	DMU	O3-C5	2.10	1.48	1.43
5	B	302	DMU	O55-C2	2.10	1.48	1.43
5	A	611	DMU	O55-C2	2.09	1.48	1.43
5	B	302	DMU	C8-C9	2.09	1.57	1.53
5	A	614	DMU	O1-C10	2.08	1.47	1.41
6	A	615	HEA	C4D-ND	-2.07	1.34	1.38
5	B	302	DMU	O1-C10	2.07	1.47	1.41
6	A	616	HEA	C11-C3B	-2.06	1.48	1.51
5	A	614	DMU	O5-C4	2.06	1.49	1.44
6	C	604	HEA	C4D-ND	-2.03	1.34	1.38
6	A	615	HEA	C1A-C2A	2.02	1.48	1.45
6	C	605	HEA	C3C-C4C	2.02	1.48	1.42

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	605	HEA	C3D-C4D-ND	6.46	116.60	110.35
6	A	616	HEA	C3D-C4D-ND	6.26	116.40	110.35
6	A	615	HEA	C2B-C1B-NB	5.95	116.78	109.90
6	C	604	HEA	C2B-C1B-NB	5.82	116.63	109.90
5	A	614	DMU	C10-O7-C3	-5.76	104.32	117.98
6	C	604	HEA	C3C-C2C-C1C	-5.73	100.41	107.17
6	A	615	HEA	C3D-C4D-ND	5.63	115.79	110.35
6	C	605	HEA	C2B-C1B-NB	5.62	116.40	109.90
6	C	604	HEA	C3D-C4D-ND	5.59	115.75	110.35
6	A	616	HEA	C2D-C1D-ND	5.47	116.13	109.84
6	A	615	HEA	C3C-C2C-C1C	-5.36	100.85	107.17
6	C	604	HEA	C2D-C1D-ND	5.32	115.96	109.84
6	C	605	HEA	C2D-C1D-ND	5.22	115.84	109.84
6	C	605	HEA	C3C-C4C-NC	5.22	114.19	109.80
5	A	614	DMU	C1-C2-C3	5.20	121.47	109.68
6	C	605	HEA	C3C-C2C-C1C	-5.19	101.06	107.17
6	A	615	HEA	C3C-C4C-NC	5.16	114.15	109.80
6	C	605	HEA	C3B-C4B-NB	5.15	115.76	109.84
6	A	616	HEA	C2A-C1A-NA	5.12	115.26	110.32
6	A	616	HEA	C2B-C1B-NB	5.04	115.73	109.90
6	C	604	HEA	C3C-C4C-NC	4.96	113.97	109.80
6	A	616	HEA	C3B-C4B-NB	4.92	115.49	109.84
6	A	615	HEA	C2A-C1A-NA	4.87	115.02	110.32
6	A	616	HEA	C3C-C4C-NC	4.84	113.88	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	615	HEA	C3B-C4B-NB	4.80	115.36	109.84
6	A	616	HEA	C3C-C2C-C1C	-4.79	101.52	107.17
6	A	615	HEA	C2D-C1D-ND	4.67	115.21	109.84
6	A	616	HEA	C1D-C2D-C3D	-4.66	102.08	106.98
6	A	616	HEA	C3A-C2A-C1A	-4.61	102.68	107.05
6	C	604	HEA	C2A-C1A-NA	4.60	114.76	110.32
6	C	604	HEA	C1B-C2B-C3B	-4.57	101.50	106.80
6	C	605	HEA	C1D-C2D-C3D	-4.52	102.22	106.98
6	A	615	HEA	C3A-C2A-C1A	-4.46	102.82	107.05
6	C	604	HEA	C3B-C4B-NB	4.43	114.94	109.84
6	A	615	HEA	C1D-C2D-C3D	-4.43	102.32	106.98
6	A	616	HEA	CAD-CBD-CGD	-4.43	101.92	113.67
6	C	604	HEA	C1D-C2D-C3D	-4.41	102.35	106.98
6	C	604	HEA	C3A-C2A-C1A	-4.32	102.95	107.05
6	C	605	HEA	C2A-C1A-NA	4.31	114.48	110.32
6	A	615	HEA	C1B-C2B-C3B	-4.23	101.89	106.80
5	A	614	DMU	C6-C1-C2	4.15	118.75	110.01
6	C	604	HEA	O11-C11-C3B	-4.02	103.88	111.26
6	A	615	HEA	C13-C12-C11	-4.02	107.97	114.39
6	C	605	HEA	CAD-CBD-CGD	-4.02	103.00	113.67
6	C	605	HEA	C3A-C2A-C1A	-4.02	103.25	107.05
5	A	613	DMU	C10-C5-C7	3.98	118.37	110.01
5	A	614	DMU	C2-C3-C4	3.90	119.58	110.93
6	C	604	HEA	C2C-C1C-NC	3.82	116.27	110.14
6	A	615	HEA	CHB-C1B-C2B	-3.72	119.16	125.03
6	C	605	HEA	C2C-C1C-NC	3.71	116.09	110.14
6	C	605	HEA	C1B-C2B-C3B	-3.69	102.52	106.80
6	C	604	HEA	C13-C12-C11	-3.68	108.51	114.39
10	A	620	HTH	C5-C4-C3	-3.65	108.13	114.11
6	A	616	HEA	CHA-C4D-C3D	-3.60	119.53	124.77
5	A	613	DMU	C8-C7-C5	3.59	117.13	110.83
6	A	616	HEA	C2C-C1C-NC	3.54	115.81	110.14
6	A	615	HEA	C2C-C1C-NC	3.53	115.81	110.14
6	A	615	HEA	C13-C14-C15	-3.43	119.77	127.62
6	A	615	HEA	CAD-CBD-CGD	-3.38	104.69	113.67
6	C	604	HEA	CHB-C1B-C2B	-3.34	119.76	125.03
5	B	302	DMU	O5-C4-C3	3.29	116.53	109.72
5	A	611	DMU	O5-C6-C1	-3.26	103.66	110.37
5	A	613	DMU	O16-C6-C1	3.19	113.12	108.27
6	A	615	HEA	CHA-C4D-C3D	-3.16	120.16	124.77
6	C	605	HEA	CHA-C4D-C3D	-3.14	120.19	124.77
6	A	616	HEA	C4A-NA-C1A	-3.12	100.74	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	615	HEA	C4A-NA-C1A	-3.12	100.74	105.82
5	A	612	DMU	C10-O7-C3	-3.11	110.60	117.98
5	A	611	DMU	C18-O16-C6	3.11	119.00	113.68
6	C	605	HEA	CBA-CAA-C2A	-3.11	103.94	112.53
6	C	605	HEA	CMB-C2B-C1B	3.09	129.87	125.03
6	A	615	HEA	O11-C11-C3B	-3.06	105.65	111.26
6	A	616	HEA	C4B-C3B-C2B	-3.02	102.36	107.44
5	A	611	DMU	O5-C4-C3	3.01	115.94	109.72
6	A	616	HEA	CBA-CAA-C2A	-2.98	104.29	112.53
5	B	302	DMU	C10-O7-C3	-2.96	110.97	117.98
6	A	616	HEA	CHB-C1B-C2B	-2.94	120.39	125.03
6	C	605	HEA	C4D-C3D-C2D	-2.93	102.62	106.89
5	C	603	DMU	O5-C4-C3	2.91	115.74	109.72
5	A	612	DMU	O1-C9-C8	-2.90	104.47	109.70
6	A	616	HEA	C1B-C2B-C3B	-2.88	103.47	106.80
6	A	615	HEA	CHA-C1A-NA	-2.85	121.34	124.45
6	C	605	HEA	C4B-C3B-C2B	-2.81	102.72	107.44
11	B	304	TRS	C1-C-N	2.80	115.31	108.17
6	A	615	HEA	C27-C19-C20	2.76	120.02	115.23
5	A	611	DMU	C10-O7-C3	-2.72	111.53	117.98
6	C	604	HEA	C13-C14-C15	-2.72	121.40	127.62
6	C	604	HEA	CMD-C2D-C1D	2.70	129.26	125.03
6	C	605	HEA	C4A-NA-C1A	-2.70	101.42	105.82
6	A	616	HEA	C4D-C3D-C2D	-2.70	102.96	106.89
5	B	302	DMU	O5-C6-C1	-2.70	104.83	110.37
6	C	604	HEA	CAD-CBD-CGD	-2.69	106.53	113.67
6	C	604	HEA	C4D-C3D-C2D	-2.68	102.99	106.89
5	B	302	DMU	C57-C4-C3	-2.67	105.86	113.38
6	C	604	HEA	C4A-NA-C1A	-2.67	101.47	105.82
6	A	616	HEA	C27-C19-C20	2.63	119.79	115.23
6	C	604	HEA	CHA-C4D-C3D	-2.62	120.95	124.77
6	A	615	HEA	CBA-CAA-C2A	-2.60	105.34	112.53
5	A	614	DMU	O7-C10-C5	2.60	114.48	108.09
6	C	604	HEA	CHA-C1A-NA	-2.57	121.65	124.45
5	A	614	DMU	O1-C10-C5	2.55	115.61	110.37
6	A	615	HEA	CMD-C2D-C1D	2.54	129.00	125.03
6	A	615	HEA	C4B-C3B-C2B	-2.53	103.18	107.44
6	A	615	HEA	C4D-C3D-C2D	-2.53	103.21	106.89
6	C	604	HEA	C17-C18-C19	-2.51	121.88	127.62
6	C	604	HEA	CBA-CAA-C2A	-2.48	105.66	112.53
6	A	616	HEA	O11-C11-C3B	-2.48	106.71	111.26
5	A	613	DMU	O5-C4-C3	2.48	114.84	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	603	DMU	O5-C6-C1	-2.46	105.31	110.37
6	A	616	HEA	CHB-C4A-NA	-2.43	121.81	124.45
6	C	605	HEA	C27-C19-C20	2.41	119.42	115.23
6	A	616	HEA	C1D-ND-C4D	-2.39	102.37	105.21
5	A	613	DMU	O5-C6-C1	-2.39	105.46	110.37
6	A	615	HEA	CMC-C2C-C1C	2.38	129.04	125.42
6	C	605	HEA	C4C-C3C-C2C	-2.38	104.34	107.30
6	A	616	HEA	CHC-C1C-C2C	-2.36	120.57	127.43
6	C	605	HEA	CHB-C1B-C2B	-2.36	121.30	125.03
5	A	612	DMU	O5-C6-C1	-2.35	105.55	110.37
6	C	605	HEA	CMD-C2D-C1D	2.31	128.64	125.03
5	A	612	DMU	O61-C57-C4	-2.30	103.52	111.33
6	A	616	HEA	CHD-C1D-C2D	-2.26	120.52	126.95
6	C	604	HEA	C4B-C3B-C2B	-2.25	103.65	107.44
5	A	614	DMU	O55-C2-C1	-2.25	105.06	110.38
6	C	605	HEA	CHC-C1C-C2C	-2.25	120.89	127.43
5	A	614	DMU	O5-C4-C3	2.24	114.36	109.72
6	C	605	HEA	C4B-NB-C1B	-2.23	102.56	105.21
6	C	605	HEA	C13-C14-C15	-2.21	122.56	127.62
5	A	613	DMU	O4-C7-C8	-2.20	105.19	110.38
6	C	605	HEA	C26-C15-C16	2.20	119.04	115.23
6	A	616	HEA	CMD-C2D-C1D	2.19	128.46	125.03
6	A	615	HEA	C17-C18-C19	-2.18	122.63	127.62
6	A	616	HEA	C4C-C3C-C2C	-2.17	104.61	107.30
6	C	604	HEA	C25-C23-C24	2.16	119.56	114.59
6	C	604	HEA	CAA-C2A-C1A	2.15	129.23	124.85
6	A	615	HEA	CAA-C2A-C1A	2.15	129.23	124.85
6	A	616	HEA	CHA-C1A-NA	-2.15	122.11	124.45
6	C	605	HEA	C1D-ND-C4D	-2.15	102.66	105.21
6	C	604	HEA	CHC-C1C-C2C	-2.15	121.19	127.43
5	A	614	DMU	O1-C9-C11	2.13	111.71	106.44
6	C	604	HEA	C21-C22-C23	-2.12	120.58	127.64
6	A	616	HEA	CMB-C2B-C1B	2.11	128.33	125.03
6	A	616	HEA	CAA-C2A-C1A	2.10	129.13	124.85
6	A	615	HEA	CAA-CBA-CGA	-2.09	108.11	113.67
6	A	616	HEA	O1A-CGA-CBA	-2.08	116.49	123.09
6	C	604	HEA	CHD-C1D-C2D	-2.08	121.04	126.95
6	C	605	HEA	CHA-C1A-NA	-2.08	122.19	124.45
10	B	309	HTH	C5-C4-C3	-2.07	110.72	114.11
6	A	615	HEA	C4B-NB-C1B	-2.05	102.78	105.21
6	C	605	HEA	CHC-C4B-NB	-2.05	121.83	124.37
6	C	605	HEA	CHB-C1B-NB	-2.03	122.24	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	614	DMU	O3-C5-C7	2.03	115.16	110.38
5	A	614	DMU	O49-C1-C2	-2.03	105.59	110.38
6	C	605	HEA	CHD-C1D-C2D	-2.03	121.18	126.95
6	C	604	HEA	CMC-C2C-C3C	2.02	131.29	126.55
10	B	309	HTH	C4-C3-C2	-2.01	108.89	113.73

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	302	DMU	O5-C6-O16-C18
10	A	620	HTH	C1-C2-C3-O3
10	A	620	HTH	C1-C2-C3-C4
10	A	620	HTH	O2-C2-C3-O3
10	A	620	HTH	O2-C2-C3-C4
10	B	309	HTH	O1-C1-C2-O2
11	B	304	TRS	C1-C-C3-O3
11	B	304	TRS	C2-C-C3-O3
11	B	304	TRS	N-C-C3-O3
5	A	614	DMU	C2-C3-O7-C10
10	B	309	HTH	O1-C1-C2-C3
5	B	302	DMU	C3-C4-C57-O61
5	A	613	DMU	O5-C4-C57-O61
5	B	302	DMU	O5-C4-C57-O61
5	A	611	DMU	O5-C4-C57-O61
5	A	611	DMU	C3-C4-C57-O61
5	A	611	DMU	O6-C11-C9-O1
5	A	614	DMU	C4-C3-O7-C10
5	C	603	DMU	O16-C18-C19-C22
5	A	614	DMU	O16-C18-C19-C22
10	B	309	HTH	O3-C3-C4-C5
5	B	302	DMU	O16-C18-C19-C22
5	A	614	DMU	O6-C11-C9-O1
5	A	611	DMU	C31-C34-C37-C40
4	A	608	TRD	C6-C7-C8-C9
4	A	609	TRD	C11-C10-C9-C8
4	D	301	TRD	C3-C4-C5-C6
5	B	302	DMU	C19-C18-O16-C6
4	A	610	TRD	C6-C7-C8-C9
4	A	604	TRD	C4-C5-C6-C7
5	A	611	DMU	C25-C28-C31-C34
11	B	304	TRS	C3-C-C1-O1

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Mol	Chain	Res	Type	Atoms
4	A	608	TRD	C7-C8-C9-C10
5	A	611	DMU	C22-C25-C28-C31
4	A	607	TRD	C7-C8-C9-C10
4	A	606	TRD	C9-C10-C11-C12
5	A	614	DMU	C34-C37-C40-C43
4	A	603	TRD	C3-C4-C5-C6
5	A	611	DMU	O16-C18-C19-C22
5	C	603	DMU	C3-C4-C57-O61
4	A	604	TRD	C9-C10-C11-C12
4	A	607	TRD	C6-C7-C8-C9
5	B	302	DMU	C18-C19-C22-C25
5	A	611	DMU	O6-C11-C9-C8
10	B	309	HTH	C2-C3-C4-C5
4	C	601	TRD	C3-C4-C5-C6
4	A	609	TRD	C4-C5-C6-C7
6	A	615	HEA	C14-C15-C16-C17
5	A	611	DMU	C19-C22-C25-C28
4	C	601	TRD	C11-C10-C9-C8
6	C	604	HEA	C26-C15-C16-C17
4	B	301	TRD	C1-C2-C3-C4
5	A	614	DMU	C19-C18-O16-C6
5	B	302	DMU	C22-C25-C28-C31
5	A	611	DMU	C34-C37-C40-C43
5	A	612	DMU	C31-C34-C37-C40
6	C	604	HEA	C14-C15-C16-C17
11	B	304	TRS	N-C-C1-O1
4	C	602	TRD	C7-C8-C9-C10
5	C	603	DMU	C25-C28-C31-C34
6	A	615	HEA	C26-C15-C16-C17
4	A	603	TRD	C10-C11-C12-C13
4	A	608	TRD	C10-C11-C12-C13
5	A	611	DMU	C18-C19-C22-C25
4	A	603	TRD	C11-C10-C9-C8
4	A	606	TRD	C11-C10-C9-C8
4	A	608	TRD	C3-C4-C5-C6
4	A	608	TRD	C11-C10-C9-C8
4	A	610	TRD	C11-C10-C9-C8
5	A	613	DMU	C3-C4-C57-O61
4	C	601	TRD	C1-C2-C3-C4
5	B	302	DMU	C25-C28-C31-C34
5	A	613	DMU	C25-C28-C31-C34
5	A	611	DMU	C19-C18-O16-C6

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Mol	Chain	Res	Type	Atoms
5	A	613	DMU	C19-C18-O16-C6
4	A	607	TRD	C3-C4-C5-C6
5	C	603	DMU	C19-C22-C25-C28
4	A	604	TRD	C6-C7-C8-C9
11	B	304	TRS	C2-C-C1-O1
11	B	304	TRS	C1-C-C2-O2
4	A	610	TRD	C7-C8-C9-C10
4	A	602	TRD	C9-C10-C11-C12
5	A	611	DMU	O5-C6-O16-C18
4	A	607	TRD	C9-C10-C11-C12
4	A	608	TRD	C9-C10-C11-C12
10	A	620	HTH	O3-C3-C4-C5
10	B	309	HTH	C4-C5-C6-C7
10	A	620	HTH	C4-C5-C6-C7
4	A	608	TRD	C1-C2-C3-C4
5	A	614	DMU	O6-C11-C9-C8
5	C	603	DMU	C19-C18-O16-C6
4	A	609	TRD	C3-C4-C5-C6
4	A	602	TRD	C11-C10-C9-C8
4	B	301	TRD	C7-C8-C9-C10
11	B	304	TRS	C3-C-C2-O2
4	A	603	TRD	C1-C2-C3-C4
5	A	613	DMU	C28-C31-C34-C37
4	C	602	TRD	C6-C7-C8-C9
6	A	616	HEA	CAA-CBA-CGA-O1A
5	A	613	DMU	C22-C25-C28-C31
6	C	605	HEA	CAD-CBD-CGD-O2D
6	A	616	HEA	CAD-CBD-CGD-O1D
6	C	605	HEA	CAD-CBD-CGD-O1D
6	A	616	HEA	CAA-CBA-CGA-O2A
4	A	604	TRD	C1-C2-C3-C4
6	C	604	HEA	CAD-CBD-CGD-O2D
6	A	616	HEA	CAD-CBD-CGD-O2D
5	A	612	DMU	C3-C4-C57-O61
4	B	301	TRD	C5-C6-C7-C8
6	A	615	HEA	CAD-CBD-CGD-O2D
4	A	606	TRD	C7-C8-C9-C10
6	C	604	HEA	CAD-CBD-CGD-O1D
6	A	615	HEA	CAD-CBD-CGD-O1D
5	A	614	DMU	C18-C19-C22-C25
6	A	615	HEA	C2C-C3C-CAC-CBC
4	A	604	TRD	C10-C11-C12-C13

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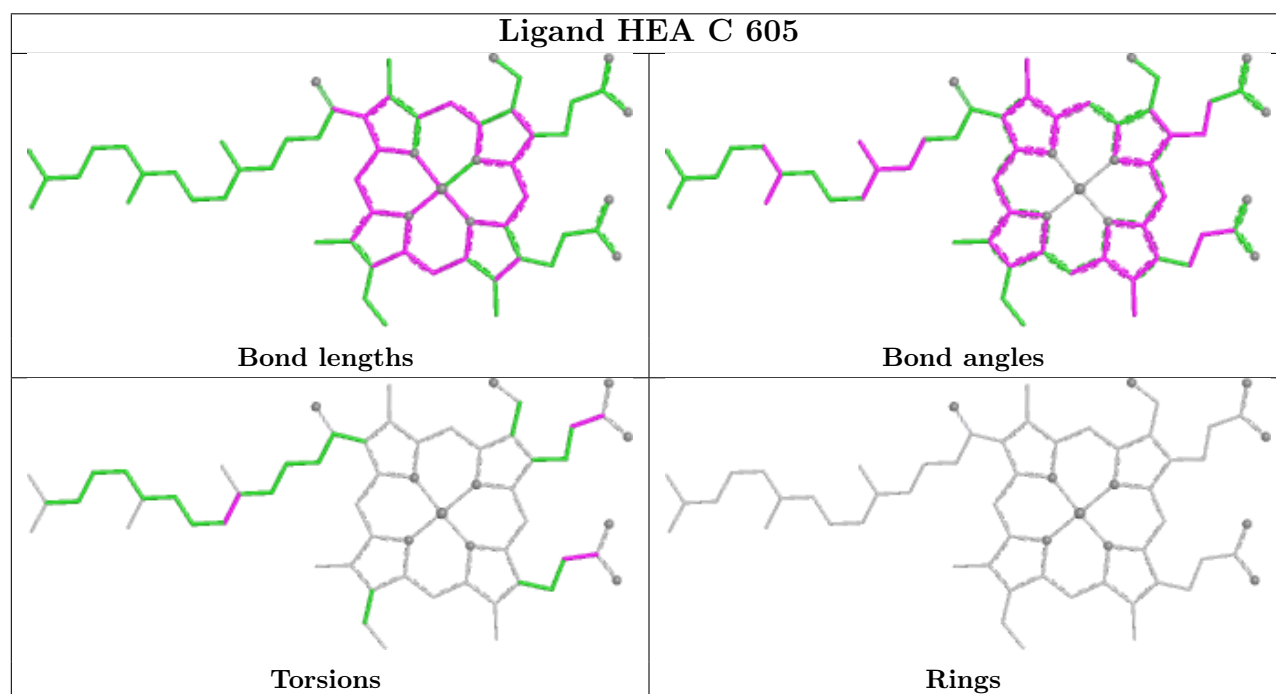
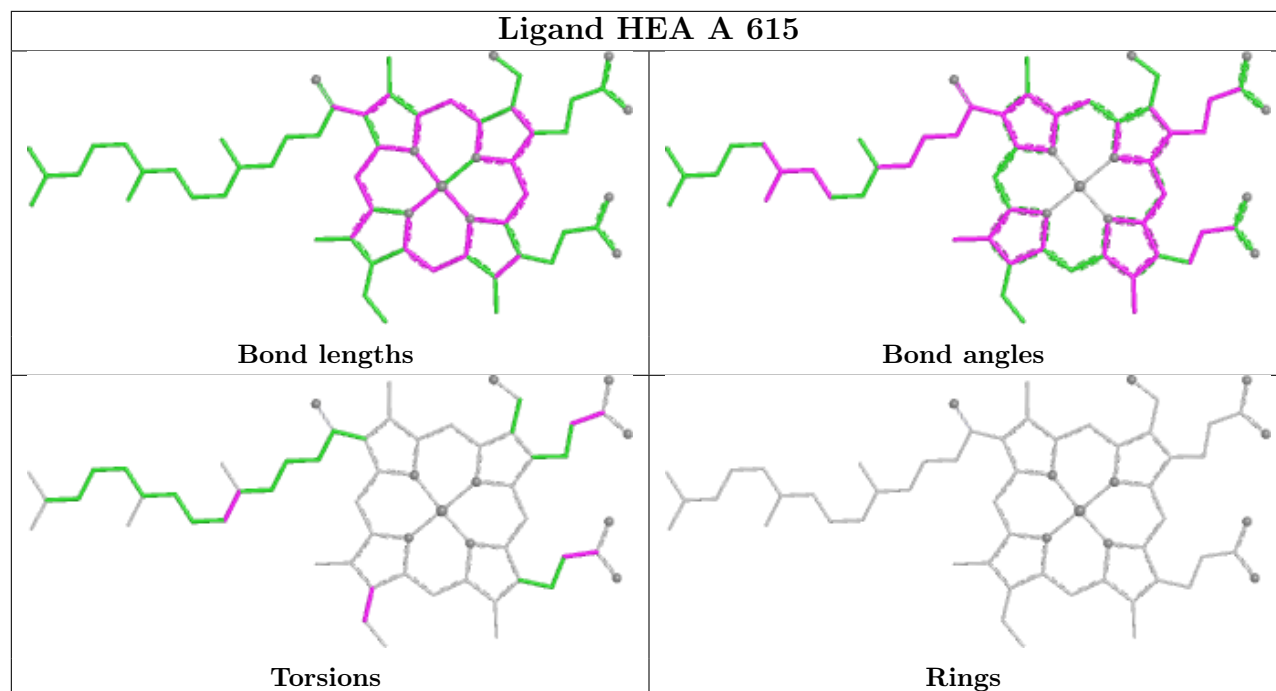
Mol	Chain	Res	Type	Atoms
6	C	605	HEA	CAA-CBA-CGA-O1A
6	C	605	HEA	C26-C15-C16-C17
6	C	605	HEA	CAA-CBA-CGA-O2A
6	A	616	HEA	C26-C15-C16-C17
6	A	615	HEA	CAA-CBA-CGA-O1A
11	B	304	TRS	N-C-C2-O2
4	A	605	TRD	C1-C2-C3-C4
5	A	612	DMU	C18-C19-C22-C25

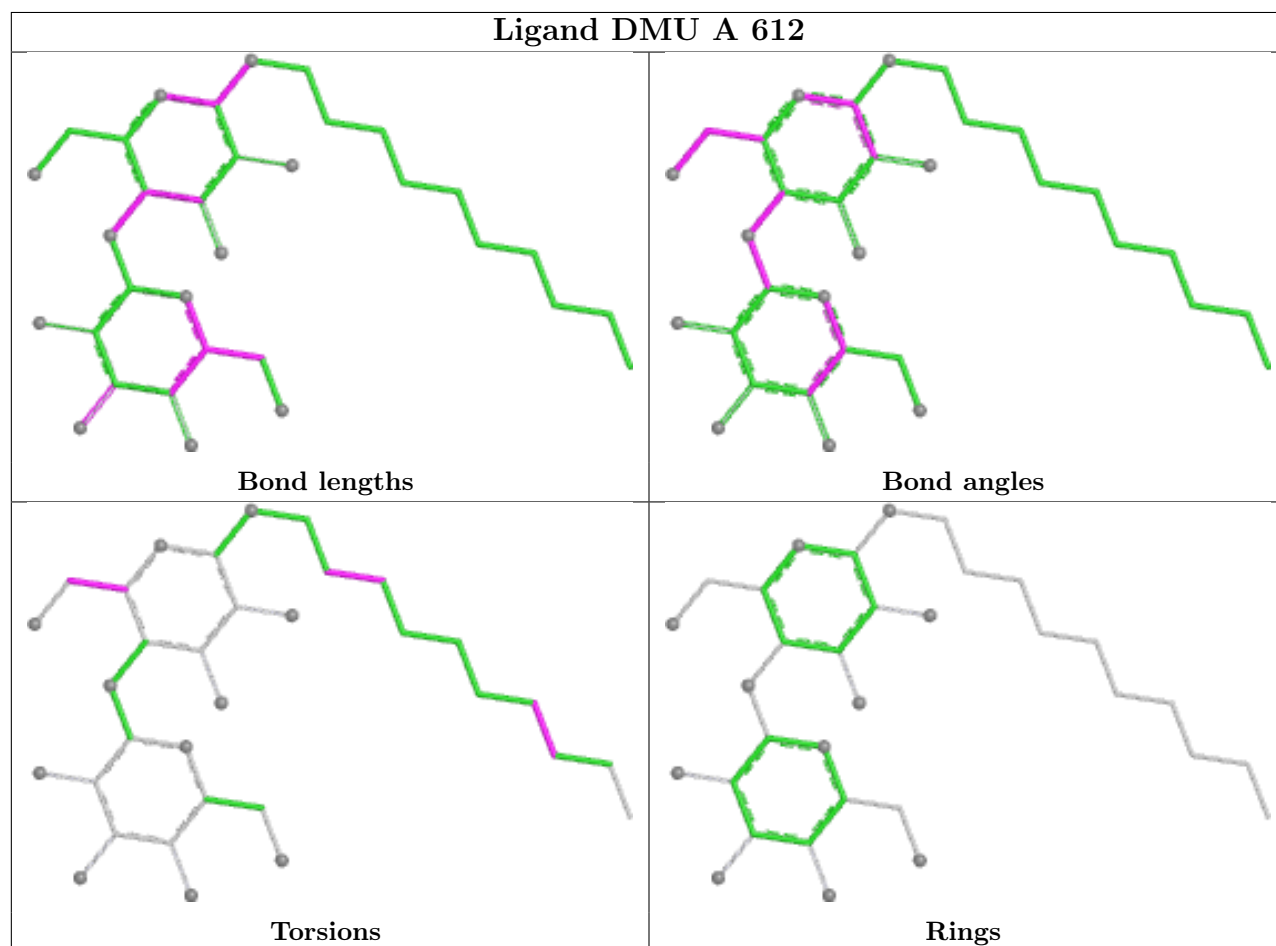
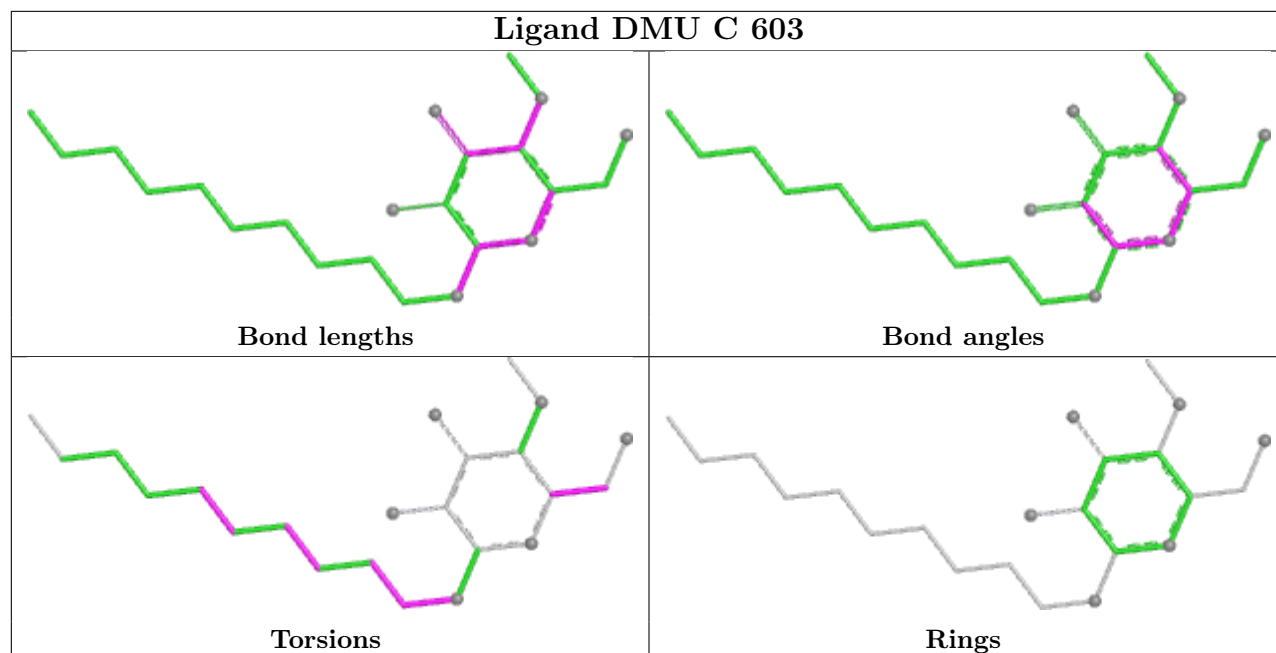
There are no ring outliers.

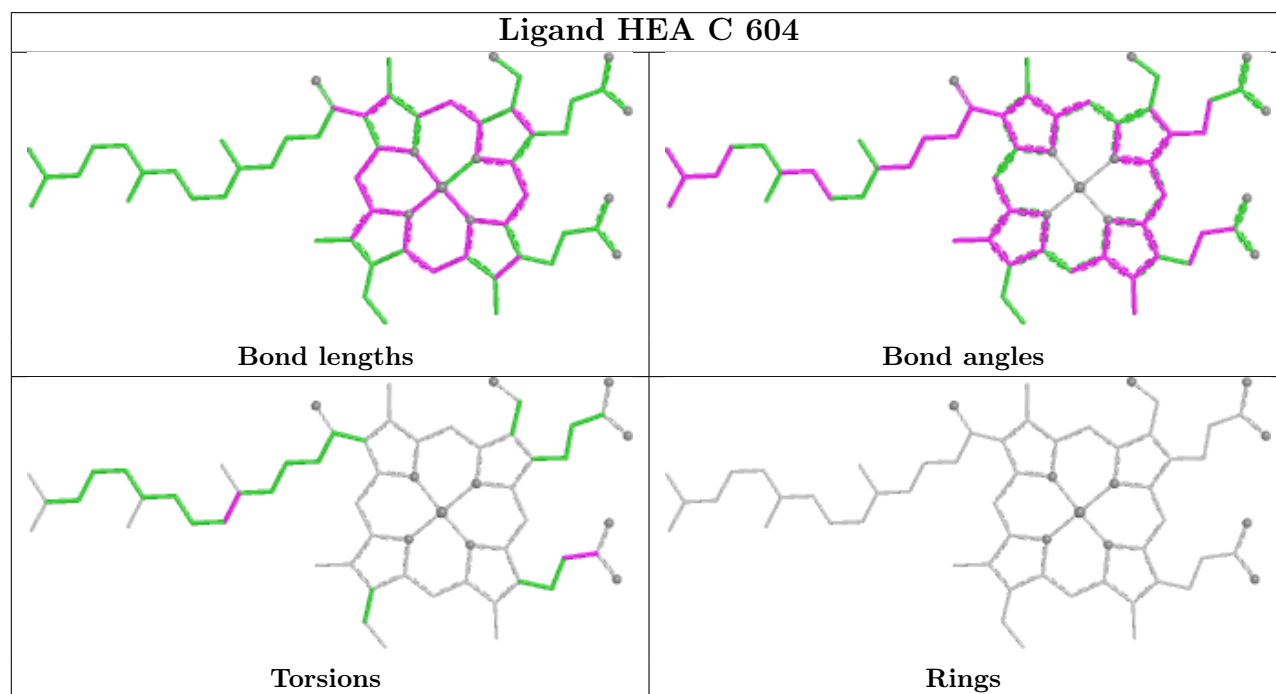
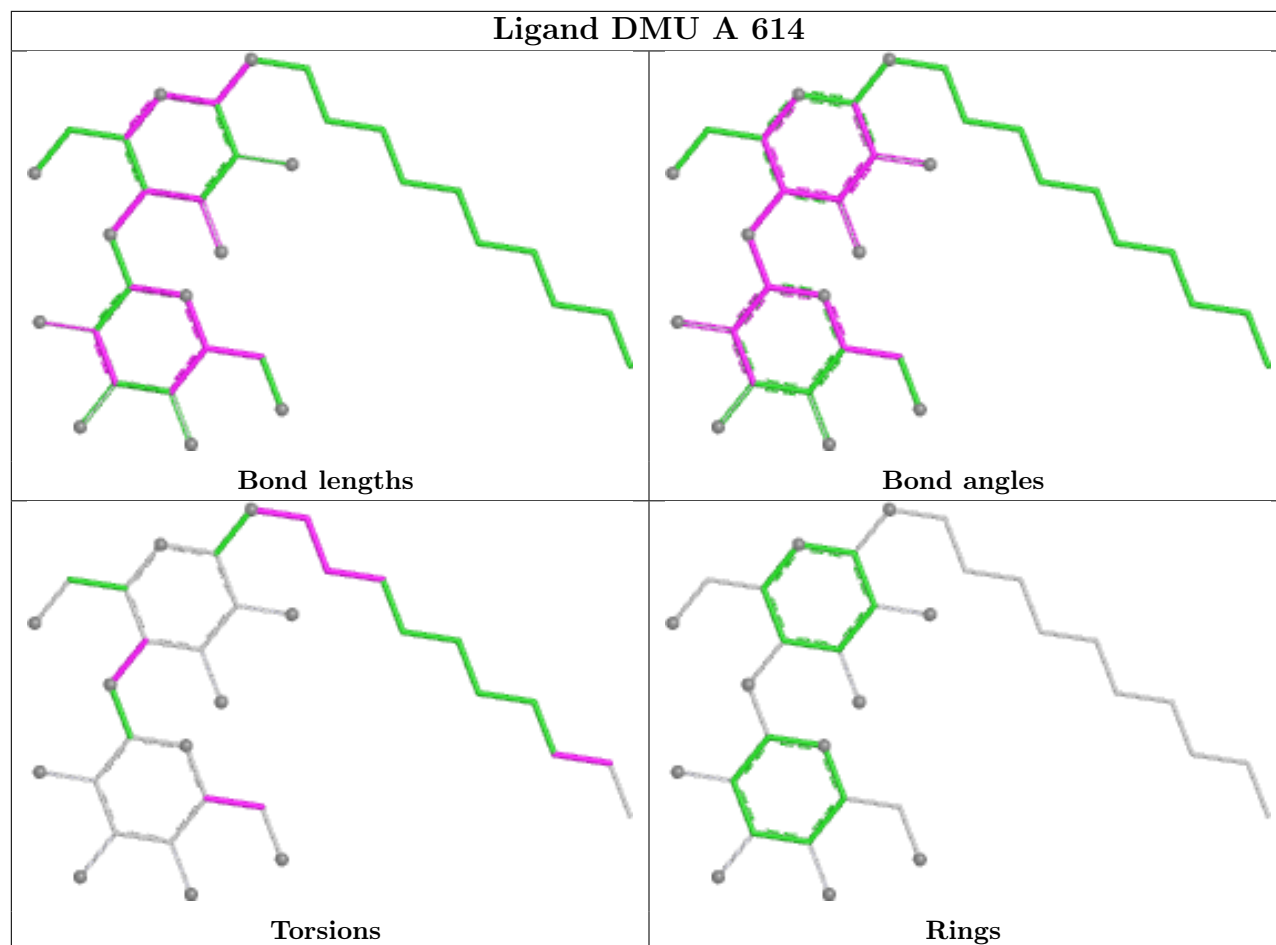
14 monomers are involved in 26 short contacts:

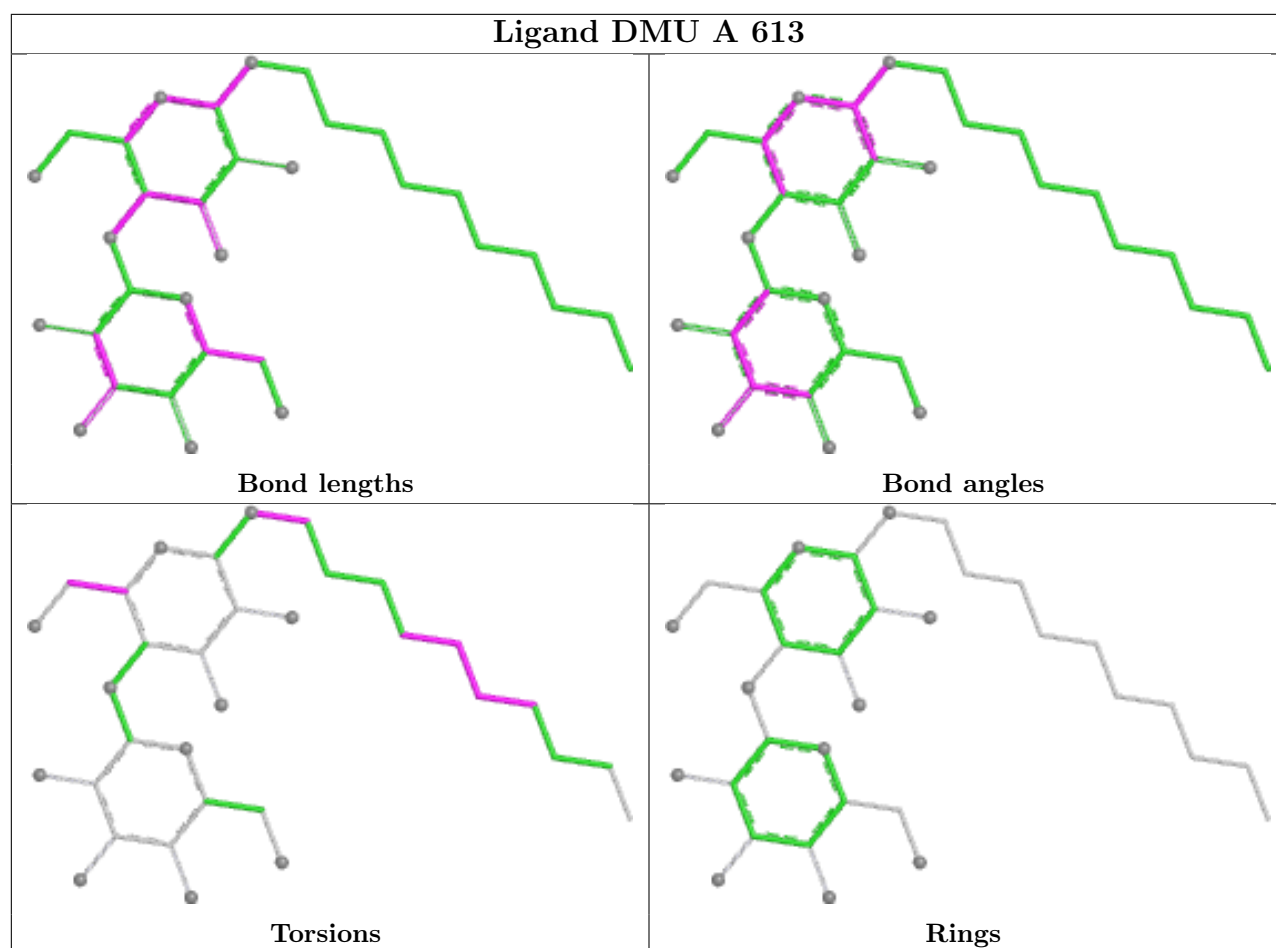
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	TRD	1	0
6	A	615	HEA	3	0
6	C	605	HEA	2	0
4	C	601	TRD	1	0
10	A	620	HTH	1	0
4	A	606	TRD	1	0
5	A	614	DMU	4	0
4	A	604	TRD	2	0
4	A	609	TRD	1	0
6	C	604	HEA	3	0
5	A	611	DMU	1	0
5	B	302	DMU	3	0
4	A	607	TRD	1	0
6	A	616	HEA	2	0

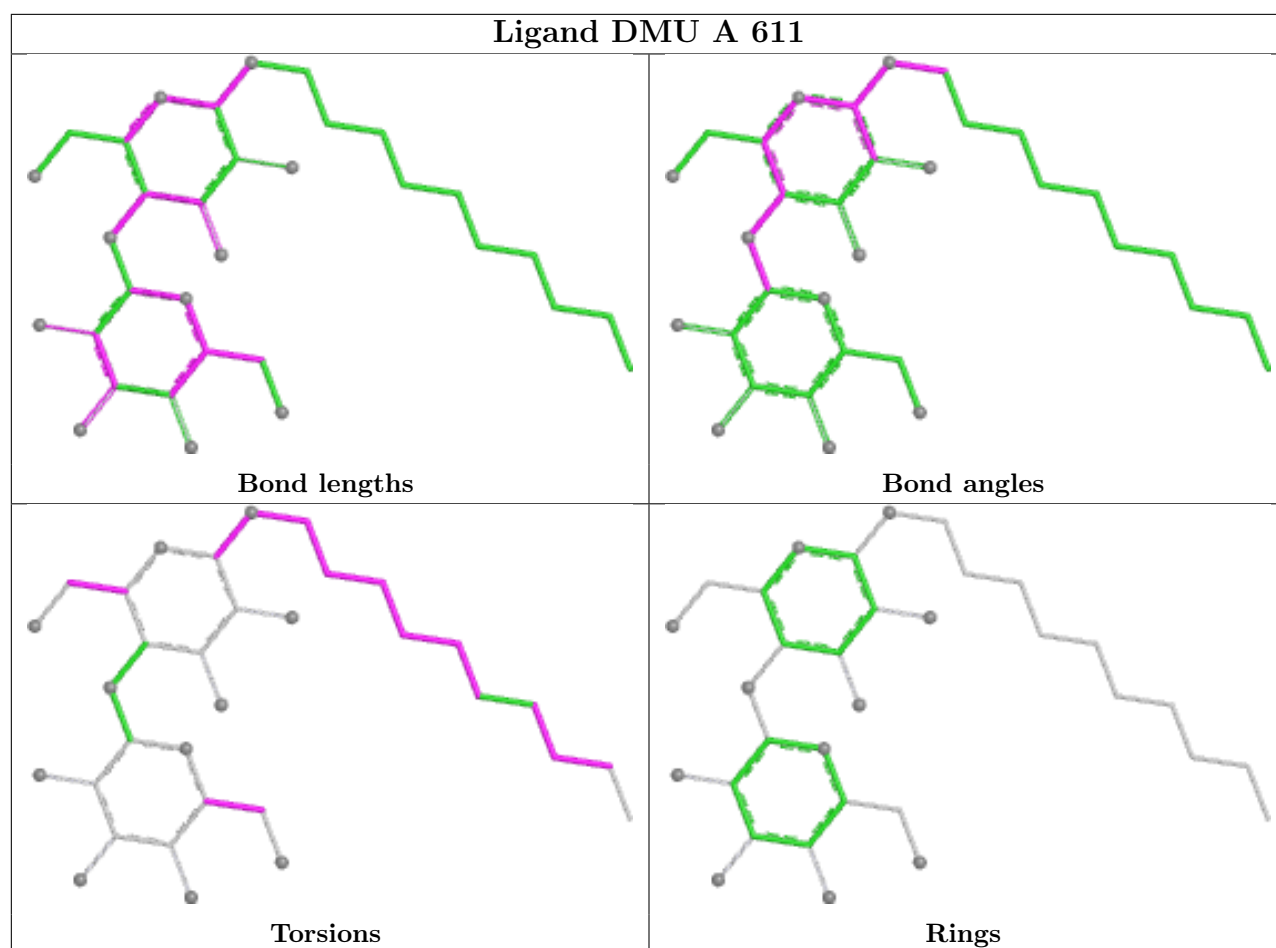
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

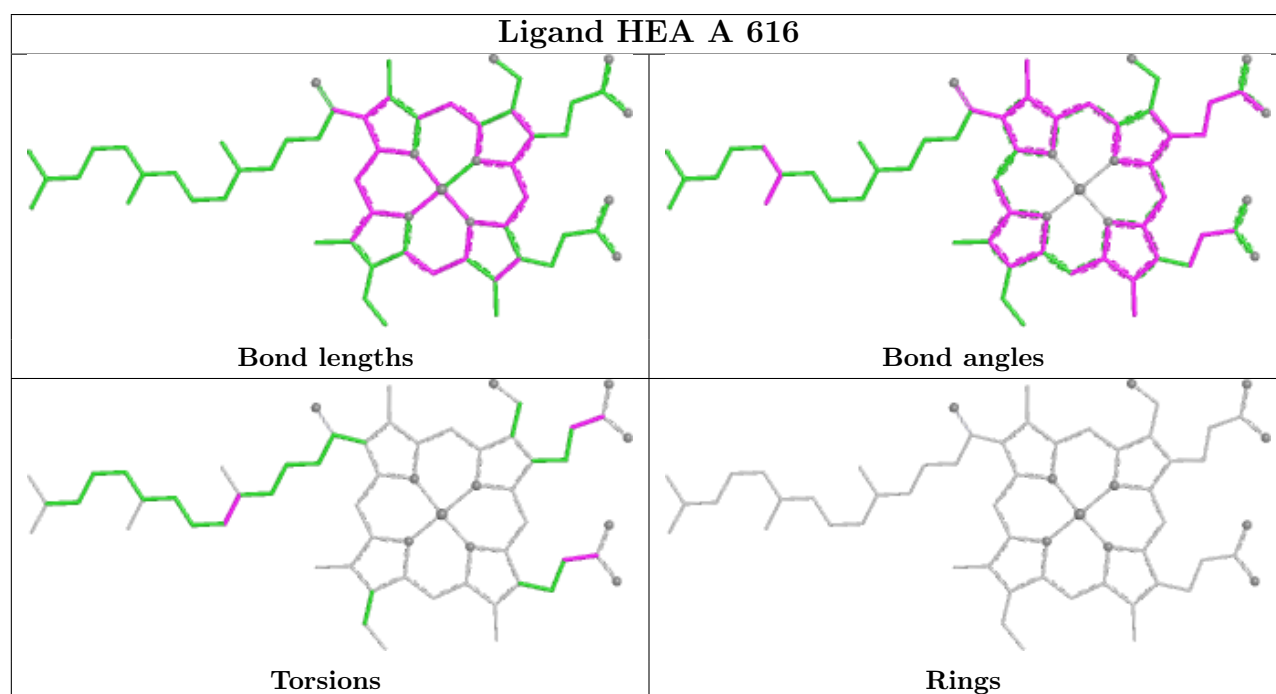
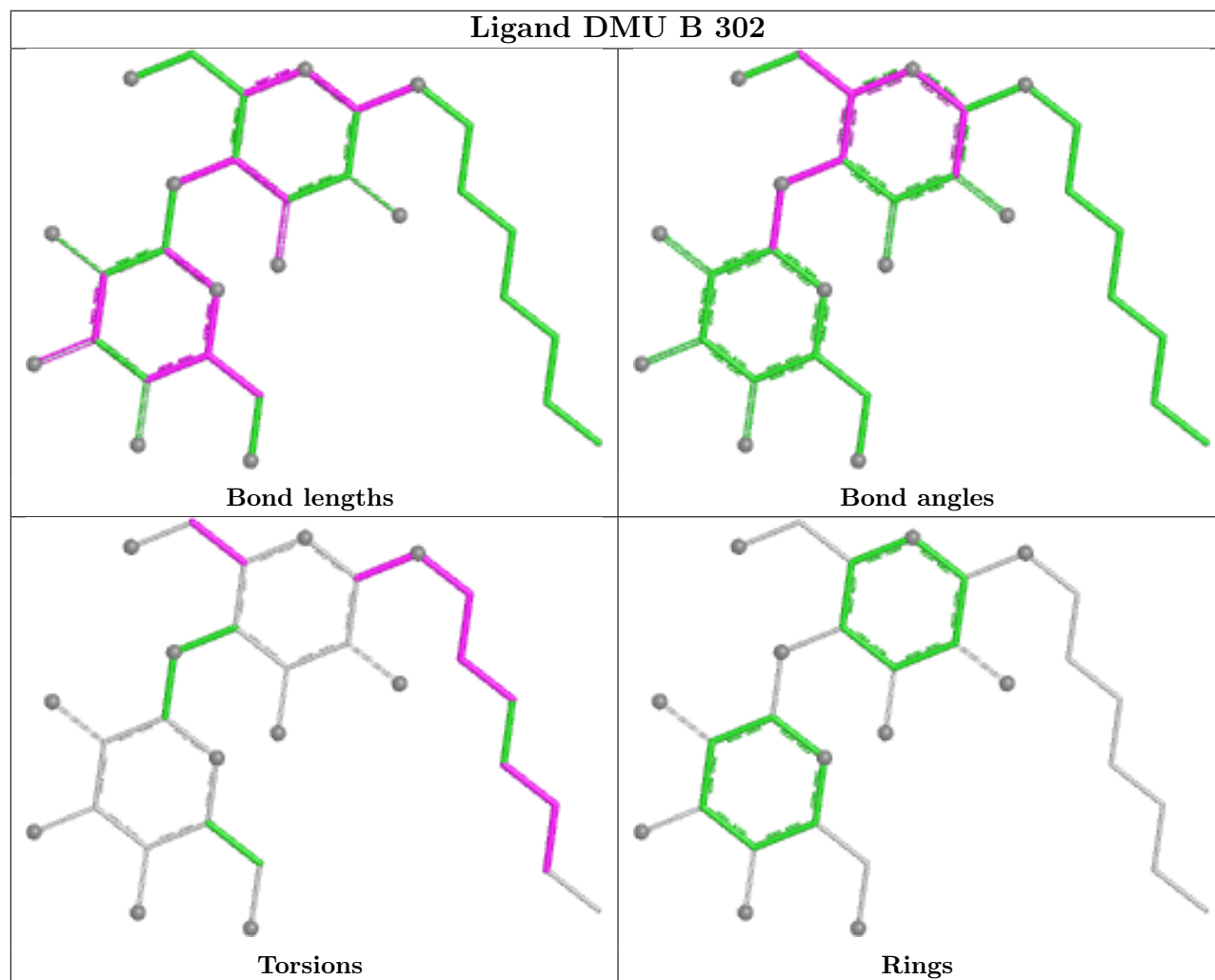












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	534/534 (100%)	0.00	16 (2%) 52 55	24, 34, 54, 92	0
1	C	533/534 (99%)	0.41	34 (6%) 25 27	27, 41, 64, 88	0
2	B	256/257 (99%)	0.03	4 (1%) 70 73	24, 37, 50, 59	1 (0%)
2	D	256/257 (99%)	0.24	7 (2%) 56 59	28, 40, 57, 67	0
All	All	1579/1582 (99%)	0.18	61 (3%) 43 45	24, 38, 57, 92	1 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	TRP	6.6
1	C	86	GLU	4.6
2	D	284	HIS	4.4
1	A	219	GLY	4.4
1	A	17	PHE	4.2
2	D	56	TRP	4.1
2	B	284	HIS	4.1
1	C	81	TRP	3.9
1	C	18	THR	3.9
1	A	222	MET	3.9
1	C	20	TRP	3.7
1	C	72	LEU	3.6
1	C	550	THR	3.6
1	C	219	GLY	3.6
2	B	109	ILE	3.5
1	C	21	PHE	3.5
1	A	218	PRO	3.5
1	C	76	PHE	3.4
1	A	19	ARG	3.3
1	A	72	LEU	3.3
1	C	69	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	221	THR	3.1
1	A	22	MET	3.1
1	A	550	THR	3.1
2	D	109	ILE	3.1
1	C	77	PHE	3.0
1	C	71	GLY	3.0
2	B	56	TRP	3.0
1	C	75	GLY	2.9
1	C	526	THR	2.9
1	C	23	SER	2.8
1	C	80	LEU	2.8
1	A	81	TRP	2.8
1	A	223	HIS	2.7
1	A	18	THR	2.7
1	C	218	PRO	2.7
1	C	70	SER	2.6
1	C	34	LEU	2.6
2	D	96	HIS	2.6
1	C	19	ARG	2.6
2	D	87	ARG	2.6
1	A	69	GLU	2.5
1	A	318	TYR	2.5
1	C	221	THR	2.5
1	C	548	GLU	2.4
1	C	131	PRO	2.4
2	B	106	ILE	2.3
1	C	519	LEU	2.2
1	C	122	TYR	2.2
1	C	132	ASP	2.2
2	D	90	VAL	2.1
2	D	110	VAL	2.1
1	C	134	ALA	2.1
1	A	77	PHE	2.1
1	C	22	MET	2.1
1	C	223	HIS	2.1
1	C	73	VAL	2.0
1	C	371	TRP	2.0
1	C	152	LEU	2.0
1	C	262	THR	2.0
1	C	129	GLY	2.0

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

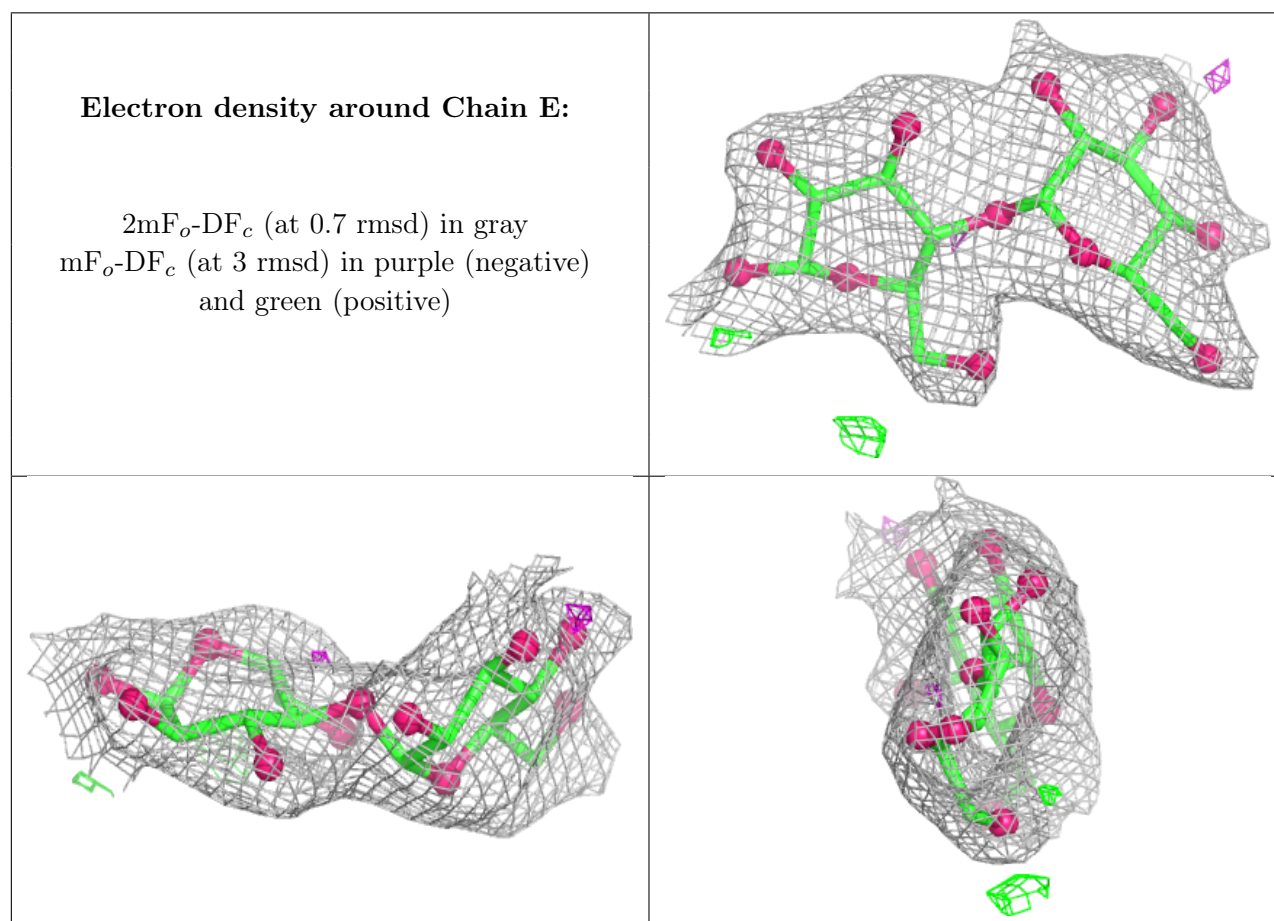
There are no non-standard protein/DNA/RNA residues in this entry.

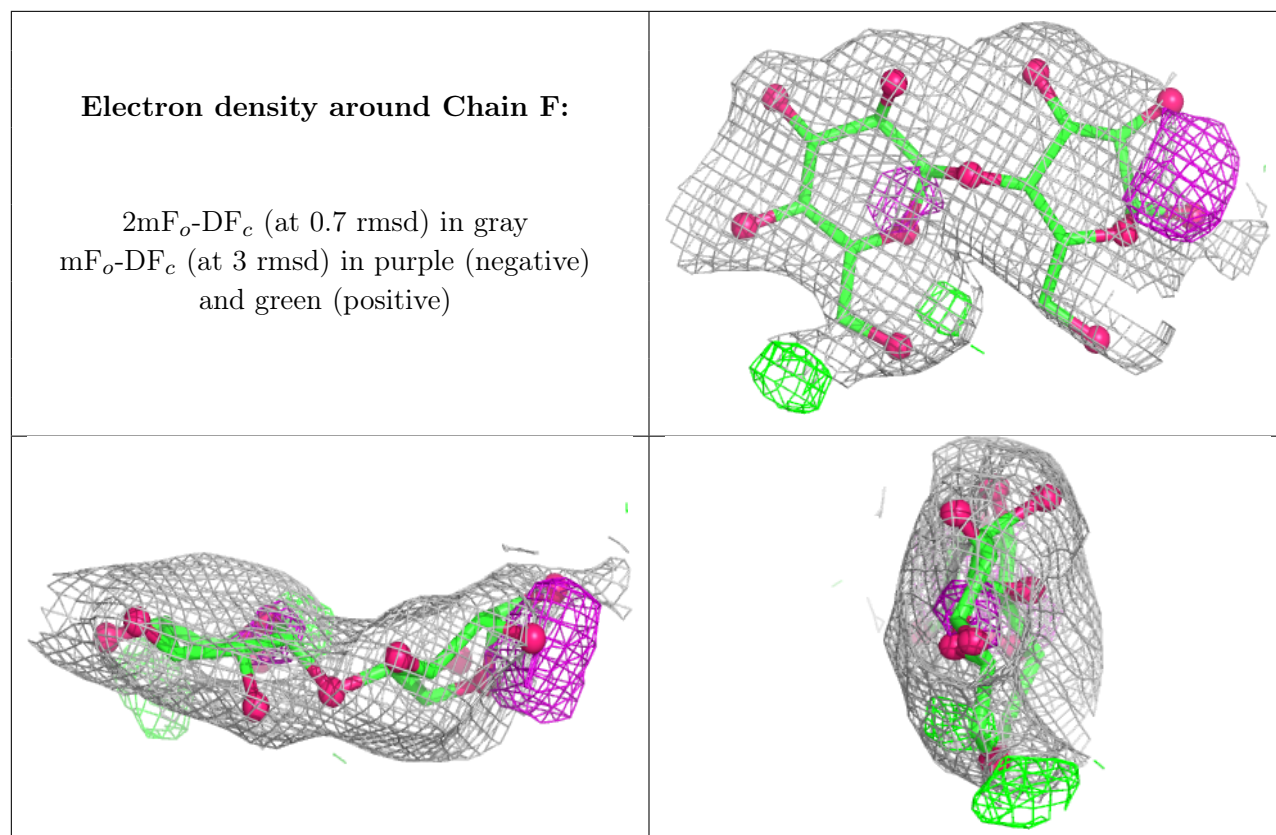
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
3	GLC	F	1	12/12	0.69	0.16	71,74,76,79	0
3	GLC	F	2	11/12	0.69	0.14	69,76,80,81	0
3	GLC	E	2	11/12	0.78	0.12	66,68,72,74	0
3	GLC	E	1	12/12	0.81	0.10	68,75,81,82	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
4	TRD	A	605	7/13	0.62	0.28	51,55,59,59	0
10	HTH	A	620	10/10	0.65	0.25	42,51,59,71	0
4	TRD	A	602	13/13	0.66	0.25	50,56,64,65	0
4	TRD	A	610	13/13	0.67	0.24	47,53,58,59	0
4	TRD	A	604	13/13	0.67	0.25	45,52,57,58	0
4	TRD	A	608	13/13	0.70	0.28	50,55,70,72	0
4	TRD	A	607	13/13	0.74	0.21	52,61,66,66	0
5	DMU	A	611	33/33	0.75	0.17	43,73,102,108	0
4	TRD	B	301	13/13	0.75	0.22	52,57,61,66	0
11	TRS	B	304	8/8	0.76	0.16	52,59,64,71	0
5	DMU	C	603	23/33	0.77	0.17	49,73,86,91	0
4	TRD	C	602	13/13	0.77	0.22	59,64,72,72	0
5	DMU	A	614	33/33	0.77	0.17	44,59,75,81	0
4	TRD	A	601	13/13	0.78	0.23	51,55,68,68	0

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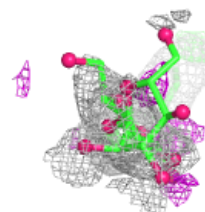
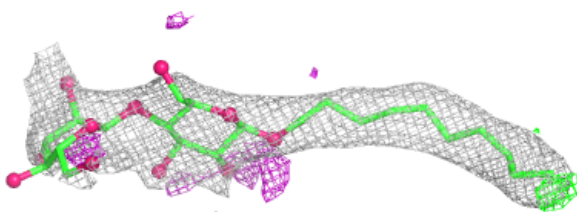
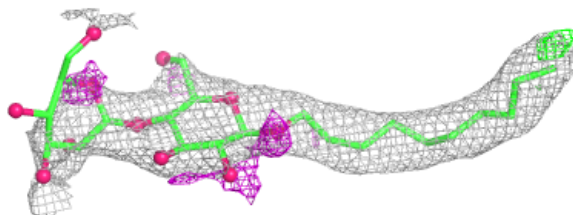
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	TRD	A	603	13/13	0.79	0.20	44,50,63,66	0
4	TRD	A	606	13/13	0.81	0.19	46,52,63,64	0
5	DMU	A	613	33/33	0.82	0.13	47,61,67,70	0
5	DMU	B	302	30/33	0.83	0.14	46,57,62,67	0
4	TRD	C	601	13/13	0.83	0.18	41,45,46,52	0
4	TRD	A	609	13/13	0.85	0.18	37,43,49,54	0
4	TRD	D	301	9/13	0.91	0.14	48,50,53,55	0
10	HTH	B	309	10/10	0.92	0.17	39,48,51,60	10
5	DMU	A	612	33/33	0.92	0.10	26,35,48,52	0
12	CD	B	308	1/1	0.95	0.06	57,57,57,57	1
9	CA	C	608	1/1	0.98	0.04	33,33,33,33	0
6	HEA	A	615	60/60	0.98	0.07	20,25,30,33	0
6	HEA	A	616	60/60	0.98	0.06	23,27,36,39	0
6	HEA	C	604	60/60	0.98	0.08	24,30,38,45	0
6	HEA	C	605	60/60	0.98	0.07	26,31,40,43	0
8	MG	A	618	1/1	0.99	0.04	15,15,15,15	0
8	MG	C	607	1/1	0.99	0.09	19,19,19,19	0
9	CA	A	619	1/1	0.99	0.02	28,28,28,28	0
12	CD	B	307	1/1	0.99	0.03	40,40,40,40	0
7	CU	C	606	1/1	0.99	0.02	34,34,34,34	0
12	CD	D	305	1/1	0.99	0.03	39,39,39,39	0
12	CD	D	306	1/1	0.99	0.04	62,62,62,62	1
7	CU	B	306	1/1	1.00	0.01	25,25,25,25	0
7	CU	A	617	1/1	1.00	0.01	30,30,30,30	0
7	CU	D	303	1/1	1.00	0.01	31,31,31,31	0
7	CU	D	304	1/1	1.00	0.01	31,31,31,31	0
7	CU	B	305	1/1	1.00	0.01	25,25,25,25	0

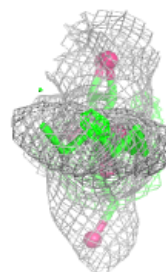
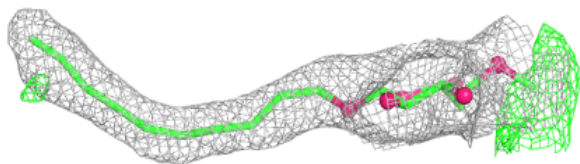
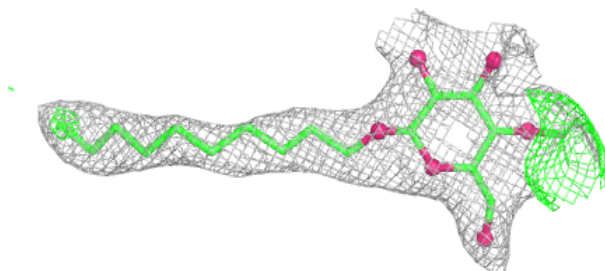
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DMU A 611:

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

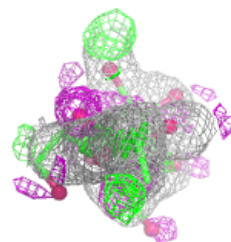
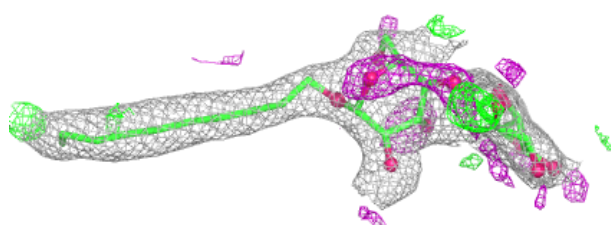
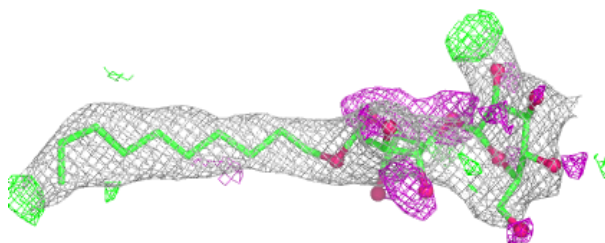
**Electron density around DMU C 603:**

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

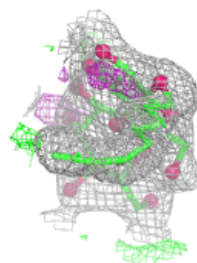
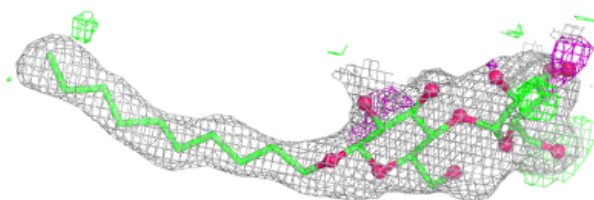
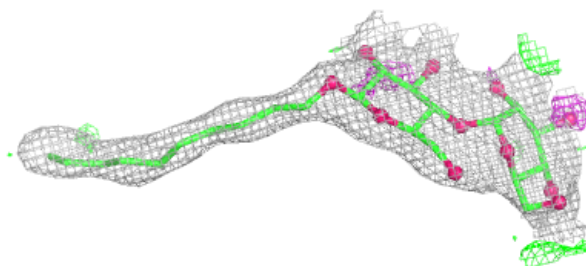


Electron density around DMU A 614:

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

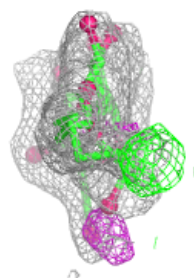
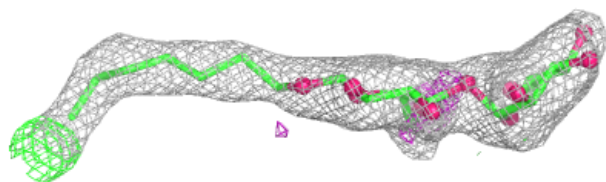
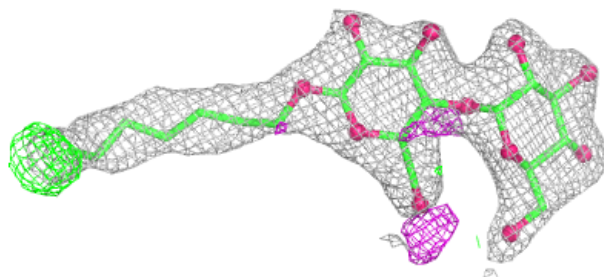
**Electron density around DMU A 613:**

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and green (positive)

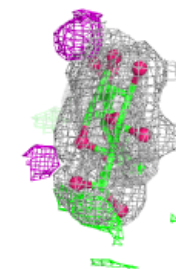
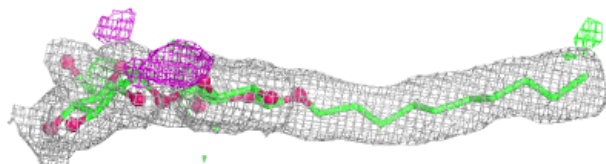
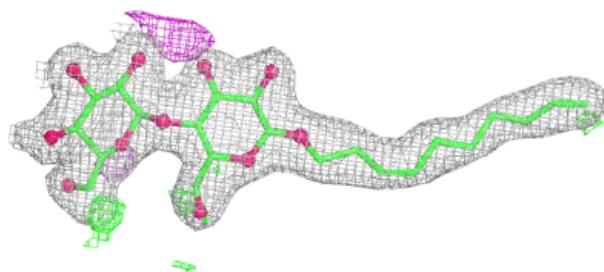


Electron density around DMU B 302:

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

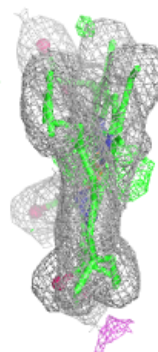
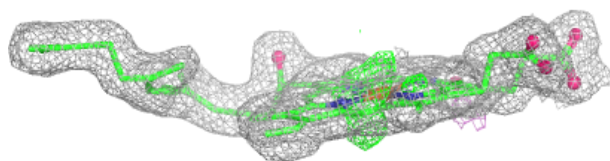
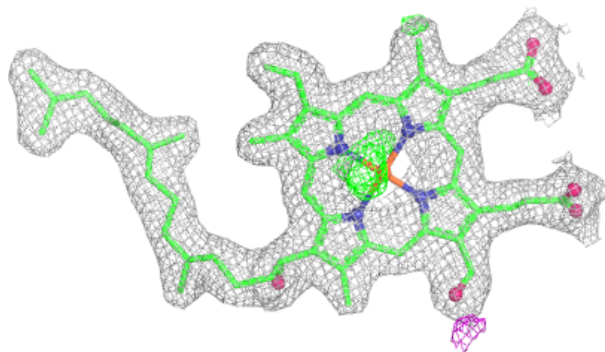
**Electron density around DMU A 612:**

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

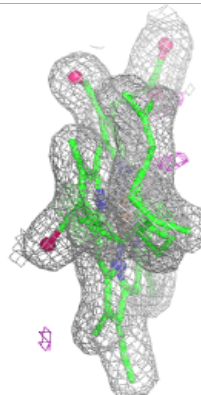
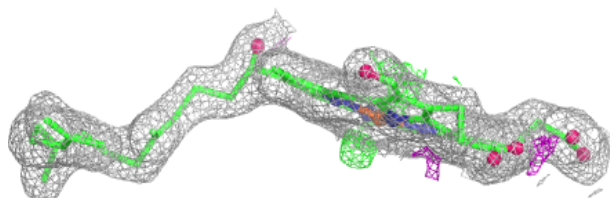
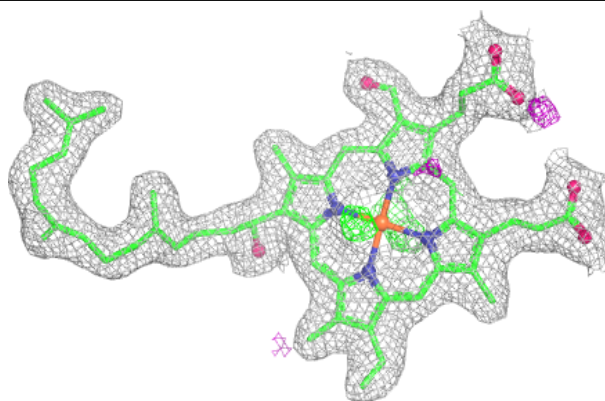


Electron density around HEA A 615:

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

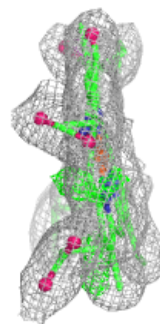
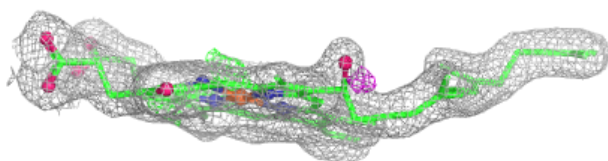
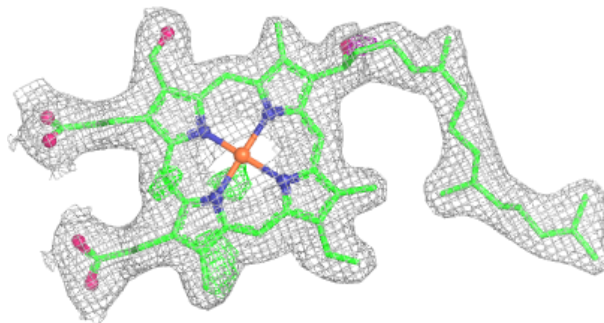
**Electron density around HEA A 616:**

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

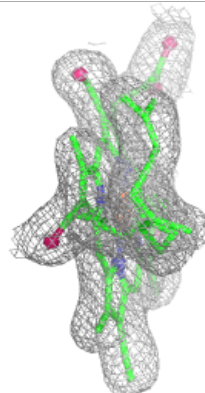
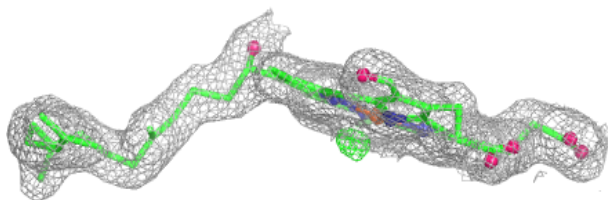
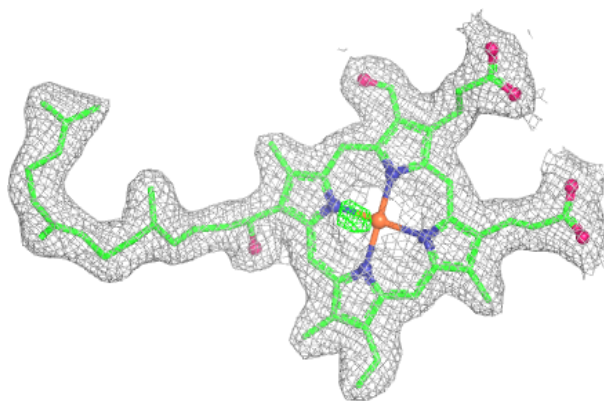


Electron density around HEA C 604:

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

**Electron density around HEA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.