Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 06:37 AM EDT

PDB ID	:	6CI0 / pdb_00006ci0
Title	:	Catalytic core subunits (I and II) of cytochrome C oxidase from Rhodobacter sphaeroides with E101A (II) mutation
Authors	:	Liu, J.; Hiser, C.; Ferguson-Miller, S.
Deposited on	:	2018-02-23
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

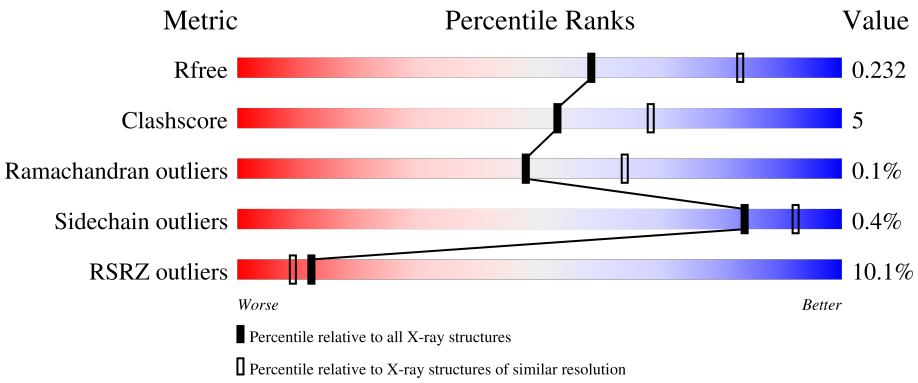
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	535	3%, 91%, 8%
1	C	535	21%, 84%, 15%, •
2	B	257	5%, 92%, 7%, •
2	D	257	7%, 96%, •
3	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	2	50% 50%
3	G	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	TRD	C	601	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 13231 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	2787	651	691	31	0	0	0
1	C	531	4094	2742	641	681	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	2013	1314	331	362	6	0	0	0
2	D	257	1995	1303	324	362	6	0	0	0

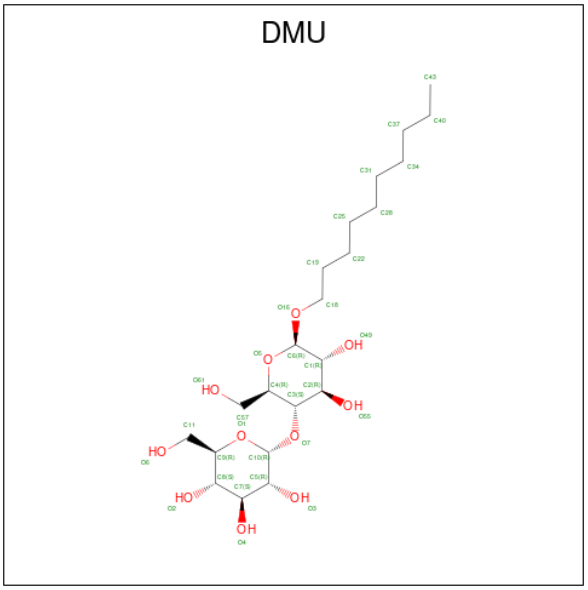
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	101	ALA	GLU	engineered mutation	UNP Q03736
B	282	HIS	-	expression tag	UNP Q03736
B	283	HIS	-	expression tag	UNP Q03736
B	284	HIS	-	expression tag	UNP Q03736
B	285	HIS	-	expression tag	UNP Q03736
D	101	ALA	GLU	engineered mutation	UNP Q03736
D	282	HIS	-	expression tag	UNP Q03736
D	283	HIS	-	expression tag	UNP Q03736
D	284	HIS	-	expression tag	UNP Q03736
D	285	HIS	-	expression tag	UNP Q03736

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

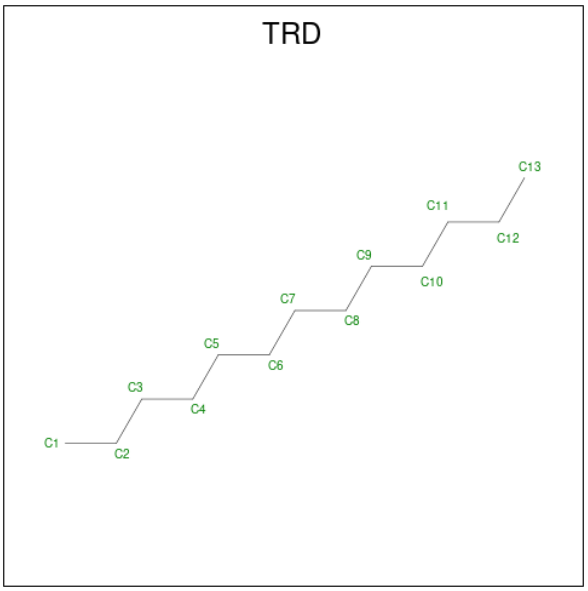
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	E	2	23	12	11	0	0	0
			Total	C	O			
3	F	2	23	12	11	0	0	0
			Total	C	O			
3	G	2	23	12	11	0	0	0

- Molecule 4 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	33	22	11	0	0
			Total	C	O		
4	A	1	33	22	11	0	0
			Total	C	O		
4	A	1	33	22	11	0	0
			Total	C	O		
4	A	1	33	22	11	0	0
			Total	C	O		
4	A	1	33	22	11	0	0
			Total	C	O		
4	D	1	30	19	11	0	0

- Molecule 5 is TRIDECANE (CCD ID: TRD) (formula: $C_{13}H_{28}$).



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

- Molecule 6 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

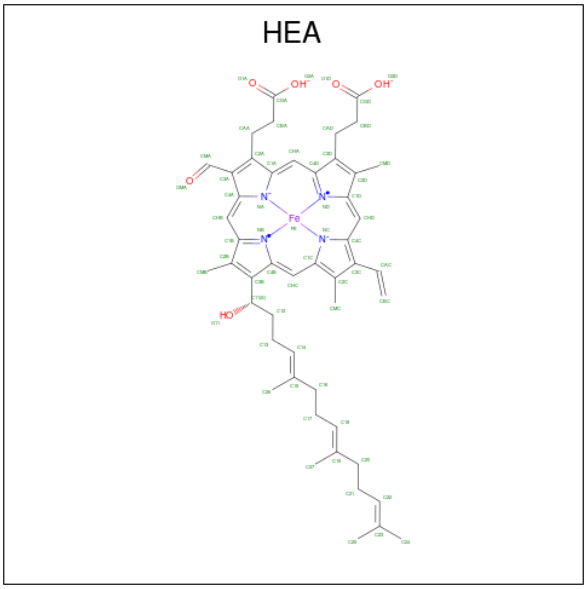
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 9 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

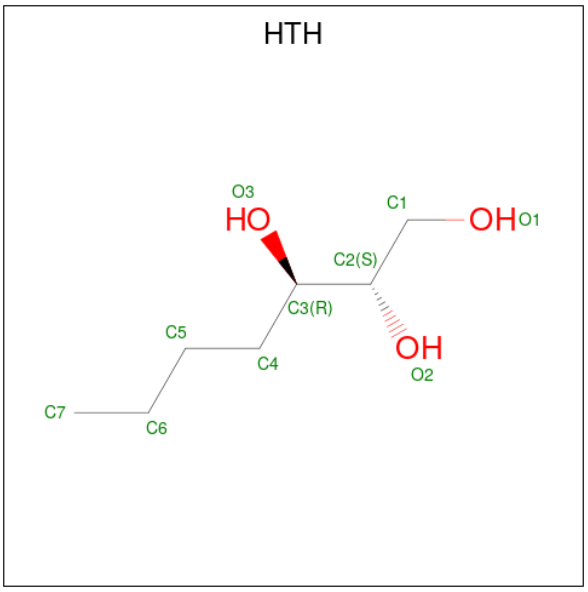


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
9	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
9	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
9	C	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
9	C	1	60	49	1	4	6	0	0

- Molecule 10 is CADMIUM ION (CCD ID: CD) (formula: Cd).

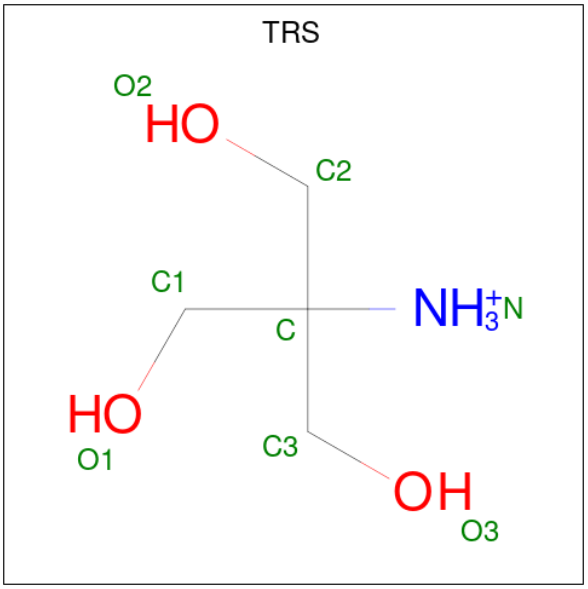
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
10	B	1	1	1	0	0
			Total	Cd		
10	D	1	1	1	0	0

- Molecule 11 is (2S,3R)-heptane-1,2,3-triol (CCD ID: HTH) (formula: $C_7H_{16}O_3$).



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

- Molecule 12 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



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

- Molecule 13 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
13	B	1	1	1	0	0

- Molecule 14 is water.

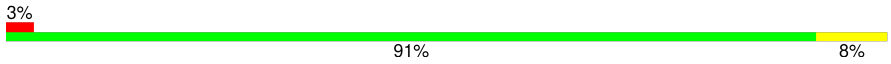
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
14	A	94	94	94	0	0
			Total	O		
14	B	69	69	69	0	0
			Total	O		
14	C	37	37	37	0	0
			Total	O		
14	D	42	42	42	0	0

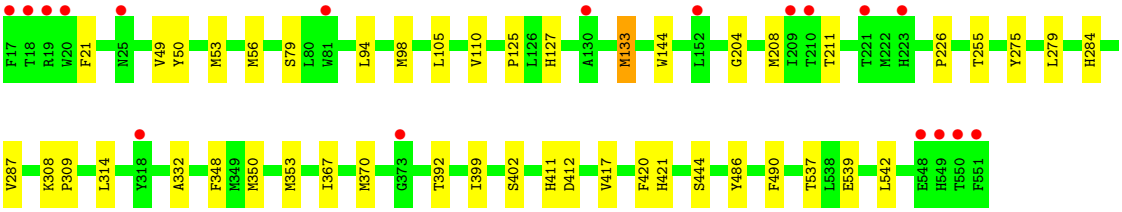
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome c oxidase subunit 1

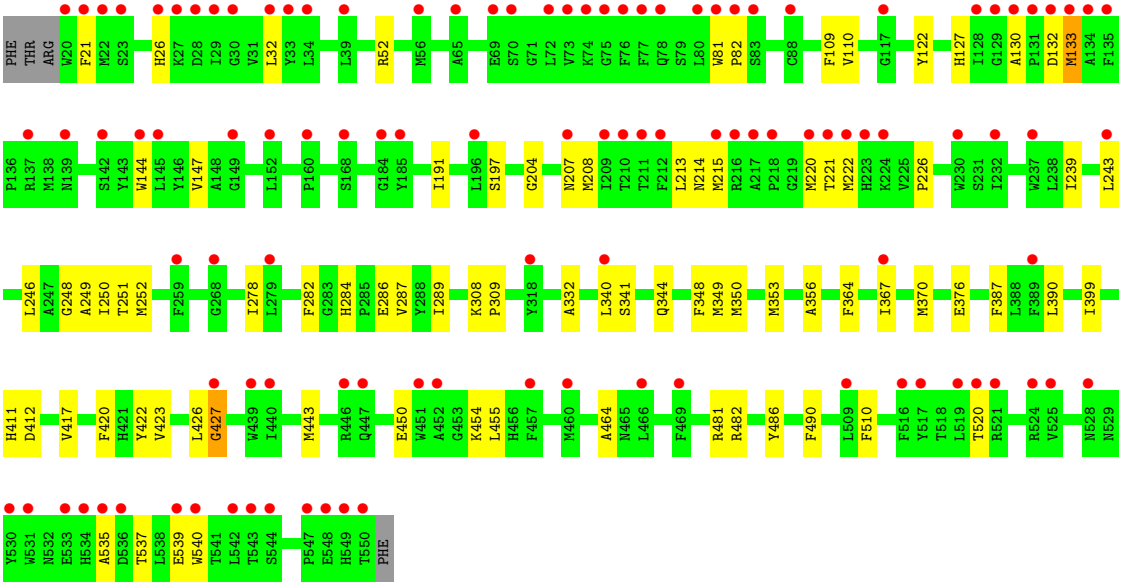
Chain A:





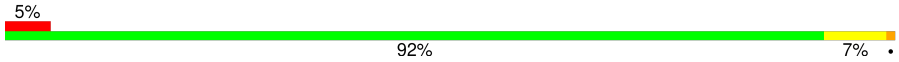
• Molecule 1: Cytochrome c oxidase subunit 1

Chain C:



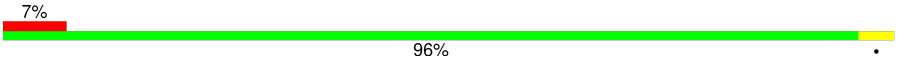
• Molecule 2: Cytochrome c oxidase subunit 2

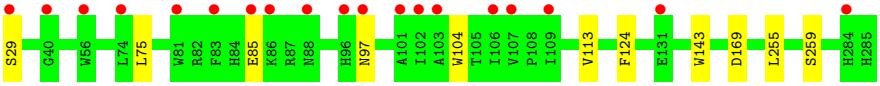
Chain B:



• Molecule 2: Cytochrome c oxidase subunit 2

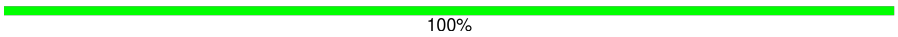
Chain D:





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

Chain E:

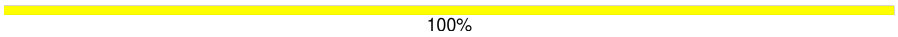


• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:

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

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	124.92Å 130.97Å 177.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.09 – 2.40 42.09 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.09-2.40) 92.5 (42.09-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.89 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.199 , 0.234 0.200 , 0.232	Depositor DCC
R_{free} test set	3901 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13231	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: TRD, K, HEA, CA, GLC, TRS, MG, CU, DMU, HTH, CD

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	0.27	0/4312	0.38	0/5892
1	C	0.24	0/4244	0.38	1/5804 (0.0%)
2	B	0.25	0/2074	0.37	0/2839
2	D	0.15	0/2056	0.35	0/2820
All	All	0.24	0/12686	0.37	1/17355 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	520	THR	OG1-CB-CG2	5.15	119.60	109.30

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	4054	36	0
1	C	4094	0	3968	64	0
2	B	2013	0	1972	15	0
2	D	1995	0	1929	9	0
3	E	23	0	21	0	0
3	F	23	0	21	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	23	0	21	1	0
4	A	165	0	210	4	0
4	D	30	0	33	2	0
5	A	98	0	209	4	0
5	B	39	0	84	3	0
5	C	13	0	28	0	0
5	D	22	0	45	1	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	A	120	0	108	8	0
9	C	120	0	108	7	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
11	B	30	0	48	1	0
12	B	8	0	11	0	0
13	B	1	0	0	0	0
14	A	94	0	0	0	0
14	B	69	0	0	0	0
14	C	37	0	0	1	0
14	D	42	0	0	0	0
All	All	13231	0	12870	129	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 5.

All (129) 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:125:PRO:HG3	1:A:133:MET:HE3	1.31	1.11
1:C:287:VAL:HG22	9:C:606:HEA:HAC	1.51	0.93
1:A:287:VAL:HG13	9:A:618:HEA:C3C	2.01	0.90
1:C:133:MET:HB3	1:C:207:ASN:HD21	1.41	0.85
1:A:125:PRO:CG	1:A:133:MET:HE3	2.07	0.84
1:A:125:PRO:HG3	1:A:133:MET:CE	2.10	0.81
1:C:133:MET:HG2	1:C:207:ASN:ND2	1.95	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:VAL:HG22	9:C:606:HEA:CAC	2.13	0.78
2:B:64:ILE:HD11	2:B:115:ILE:HD11	1.65	0.77
1:C:284:HIS:O	1:C:287:VAL:HG12	1.89	0.73
1:C:287:VAL:HG21	9:C:606:HEA:CHD	2.19	0.73
1:A:49:VAL:HG12	1:A:53:MET:HE2	1.72	0.70
4:A:604:DMU:H2	5:A:607:TRD:H121	1.75	0.69
1:C:133:MET:CB	1:C:207:ASN:HD21	2.08	0.66
1:C:81:TRP:CD2	1:C:82:PRO:HD2	2.32	0.65
2:B:278:TRP:HE1	5:B:302:TRD:H42	1.62	0.64
1:C:133:MET:CG	1:C:207:ASN:ND2	2.61	0.64
1:C:133:MET:HB3	1:C:207:ASN:ND2	2.13	0.63
1:A:255:THR:HG21	5:A:612:TRD:H22	1.80	0.63
2:B:196:THR:HB	5:B:302:TRD:H31	1.80	0.62
1:C:127:HIS:NE2	1:C:539:GLU:OE2	2.32	0.62
1:A:287:VAL:HG13	9:A:618:HEA:CAC	2.29	0.62
1:C:426:LEU:HD21	1:C:464:ALA:HB1	1.82	0.62
9:A:617:HEA:HMC1	9:A:617:HEA:HBC1	1.83	0.60
1:C:21:PHE:HA	1:C:32:LEU:HD11	1.82	0.60
1:A:314:LEU:HB2	11:B:310:HTH:H7A	1.83	0.60
1:C:287:VAL:CG2	9:C:606:HEA:HAC	2.29	0.59
9:C:605:HEA:HBC1	9:C:605:HEA:HMC3	1.84	0.59
1:A:287:VAL:CG1	9:A:618:HEA:C3C	2.78	0.59
1:C:411:HIS:NE2	1:C:412:ASP:OD1	2.36	0.58
1:C:133:MET:HG2	1:C:207:ASN:CG	2.28	0.57
1:C:387:PHE:HD2	1:C:427:GLY:O	1.86	0.57
1:C:450:GLU:OE1	1:C:454:LYS:NZ	2.37	0.56
9:C:605:HEA:HBC1	9:C:605:HEA:CMC	2.35	0.56
2:B:268:LYS:HD2	5:B:302:TRD:H71	1.88	0.56
1:C:411:HIS:NE2	14:C:701:HOH:O	2.33	0.55
1:C:133:MET:CB	1:C:207:ASN:ND2	2.70	0.54
1:C:364:PHE:HB3	2:D:104:TRP:CE3	2.42	0.54
1:A:444:SER:HB3	4:A:601:DMU:H8	1.89	0.54
1:C:367:ILE:HA	1:C:370:MET:HE2	1.88	0.53
1:A:204:GLY:O	1:A:208:MET:HG2	2.09	0.53
2:B:211:THR:HB	2:B:235:LEU:HD12	1.91	0.53
9:A:617:HEA:HBC1	9:A:617:HEA:CMC	2.40	0.52
1:A:50:TYR:HA	1:A:53:MET:HE3	1.89	0.52
1:A:275:TYR:OH	1:A:279:LEU:HD13	2.09	0.52
1:C:26:HIS:HD2	1:C:132:ASP:HA	1.74	0.52
1:C:282:PHE:CE1	1:C:286:GLU:HB2	2.44	0.52
1:C:422:TYR:HA	1:C:426:LEU:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:MET:HA	1:A:353:MET:HE3	1.91	0.51
1:A:411:HIS:NE2	1:A:412:ASP:OD2	2.44	0.51
1:C:387:PHE:CD2	1:C:427:GLY:O	2.63	0.51
1:A:133:MET:HE2	1:A:211:THR:HG21	1.92	0.51
1:C:350:MET:HA	1:C:353:MET:HE3	1.94	0.50
1:C:127:HIS:HB3	1:C:226:PRO:HG2	1.94	0.50
1:C:239:ILE:HA	1:C:243:LEU:HD13	1.94	0.50
1:A:539:GLU:HA	1:A:542:LEU:HD12	1.94	0.49
1:C:356:ALA:HB2	1:C:399:ILE:HD11	1.95	0.49
1:C:252:MET:HE1	1:C:278:ILE:HD13	1.95	0.48
1:C:537:THR:OG1	1:C:539:GLU:OE1	2.32	0.48
1:A:127:HIS:HB3	1:A:226:PRO:HG2	1.97	0.47
1:A:332:ALA:HB3	1:A:348:PHE:CG	2.49	0.47
1:A:392:THR:HG22	2:B:69:THR:HG22	1.96	0.47
1:C:332:ALA:HB3	1:C:348:PHE:CG	2.49	0.47
1:C:81:TRP:CE3	1:C:82:PRO:HD2	2.50	0.47
1:C:286:GLU:HA	1:C:289:ILE:HD12	1.97	0.47
1:C:349:MET:HG2	1:C:353:MET:HE2	1.97	0.47
1:A:308:LYS:HG3	1:A:309:PRO:HD2	1.96	0.46
2:B:100:LEU:HD12	2:B:100:LEU:O	2.14	0.46
1:C:204:GLY:O	1:C:208:MET:HG2	2.15	0.46
1:C:191:ILE:HG23	1:C:250:ILE:HB	1.96	0.46
1:A:21:PHE:HB3	1:A:144:TRP:HZ2	1.80	0.46
5:A:612:TRD:H71	5:A:612:TRD:H42	1.68	0.46
1:A:50:TYR:OH	1:A:79:SER:HB3	2.15	0.46
2:D:124:PHE:HB3	3:F:2:GLC:H3	1.98	0.46
2:B:138:VAL:HG11	2:B:219:TRP:CD1	2.51	0.46
1:A:367:ILE:HA	1:A:370:MET:HE2	1.99	0.45
1:C:221:THR:OG1	1:C:222:MET:N	2.50	0.45
1:C:486:TYR:CD1	1:C:490:PHE:HB2	2.52	0.44
1:A:537:THR:OG1	1:A:539:GLU:OE1	2.33	0.44
1:C:220:MET:HE3	1:C:220:MET:HB2	1.93	0.44
1:A:56:MET:HE1	4:A:604:DMU:H7	1.99	0.44
1:C:110:VAL:HG11	9:C:605:HEA:H271	1.99	0.44
1:C:248:GLY:O	1:C:251:THR:HG22	2.17	0.44
1:A:417:VAL:HG13	1:A:421:HIS:CE1	2.52	0.44
1:C:144:TRP:HA	1:C:147:VAL:HG12	2.00	0.44
1:C:390:LEU:HD13	1:C:426:LEU:HB3	2.00	0.44
2:D:113:VAL:HA	5:D:303:TRD:H52	2.00	0.44
1:C:390:LEU:HD13	1:C:426:LEU:HD13	2.00	0.44
1:A:486:TYR:CD1	1:A:490:PHE:HB2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:LEU:C	1:C:214:ASN:HD22	2.26	0.43
1:C:249:ALA:HB2	1:C:278:ILE:HG22	2.00	0.43
1:C:109:PHE:CE1	1:C:197:SER:HB2	2.53	0.43
1:C:122:TYR:CZ	1:C:443:MET:HG2	2.54	0.43
1:C:246:LEU:HD22	1:C:282:PHE:CZ	2.53	0.43
1:C:417:VAL:HA	1:C:420:PHE:CE2	2.54	0.43
4:A:604:DMU:H10	5:A:606:TRD:H52	2.00	0.43
1:C:341:SER:OG	1:C:344:GLN:HG3	2.18	0.43
1:A:105:LEU:O	1:A:110:VAL:HG23	2.19	0.43
1:A:284:HIS:O	1:A:287:VAL:HB	2.19	0.43
2:D:75:LEU:HD12	2:D:75:LEU:HA	1.89	0.43
1:C:482:ARG:HD3	2:D:255:LEU:HB2	2.02	0.42
2:B:100:LEU:HD12	2:B:100:LEU:C	2.45	0.42
1:C:535:ALA:HB1	1:C:540:TRP:CD1	2.55	0.42
2:D:143:TRP:CG	2:D:259:SER:HB2	2.55	0.42
1:A:94:LEU:O	1:A:98:MET:HG2	2.19	0.42
2:B:97:ASN:ND2	4:D:301:DMU:H29	2.34	0.42
1:C:332:ALA:HB1	1:C:340:LEU:HD11	2.00	0.42
1:C:130:ALA:HB2	1:C:215:MET:O	2.20	0.42
2:B:98:SER:N	2:B:99:PRO:HD2	2.35	0.41
9:A:618:HEA:CMC	9:A:618:HEA:HBC1	2.50	0.41
1:A:399:ILE:O	1:A:402:SER:OG	2.36	0.41
1:A:420:PHE:CD2	9:A:618:HEA:HAD1	2.55	0.41
2:B:98:SER:OG	2:B:99:PRO:HD3	2.20	0.41
1:C:376:GLU:HG2	2:D:85:GLU:OE1	2.20	0.41
4:D:301:DMU:H38	4:D:301:DMU:H28	1.66	0.41
2:B:143:TRP:CG	2:B:259:SER:HB2	2.55	0.41
1:C:539:GLU:OE1	1:C:539:GLU:N	2.49	0.41
2:D:169:ASP:OD1	2:D:169:ASP:N	2.54	0.41
2:B:61:ILE:O	2:B:65:ILE:HG12	2.21	0.40
1:C:308:LYS:HG3	1:C:309:PRO:HD2	2.03	0.40
1:A:21:PHE:HB3	1:A:144:TRP:CZ2	2.55	0.40
1:C:455:LEU:HD23	1:C:510:PHE:CZ	2.56	0.40
1:C:537:THR:HG1	1:C:539:GLU:CD	2.28	0.40
1:A:417:VAL:HG13	1:A:421:HIS:HE1	1.87	0.40
2:B:104:TRP:CD1	2:B:104:TRP:C	2.99	0.40
1:A:287:VAL:CG1	9:A:618:HEA:C4C	2.99	0.40
1:C:412:ASP:HA	1:C:481:ARG:HD3	2.04	0.40
1:C:420:PHE:HA	1:C:423:VAL:HG22	2.03	0.40
2:D:97:ASN:ND2	3:G:1:GLC:H62	2.36	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	533/535 (100%)	518 (97%)	15 (3%)	0	100	100
1	C	529/535 (99%)	514 (97%)	14 (3%)	1 (0%)	43	58
2	B	254/257 (99%)	246 (97%)	7 (3%)	1 (0%)	30	43
2	D	255/257 (99%)	246 (96%)	9 (4%)	0	100	100
All	All	1571/1584 (99%)	1524 (97%)	45 (3%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	97	ASN
1	C	427	GLY

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	424/435 (98%)	423 (100%)	1 (0%)	87	94
1	C	414/435 (95%)	412 (100%)	2 (0%)	81	91
2	B	212/215 (99%)	211 (100%)	1 (0%)	81	91
2	D	208/215 (97%)	207 (100%)	1 (0%)	81	91
All	All	1258/1300 (97%)	1253 (100%)	5 (0%)	84	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	MET
2	B	100	LEU
1	C	52	ARG
1	C	133	MET
2	D	29	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	91	ASN
1	A	140	ASN
1	A	165	GLN
1	A	276	GLN
1	A	534	HIS
2	B	170	ASN
2	B	203	ASN
2	B	251	GLN
1	C	87	ASN
1	C	93	HIS
1	C	207	ASN
1	C	214	ASN
1	C	465	ASN
1	C	534	HIS
2	D	125	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)

6 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	0.45	0
3	GLC	E	2	3	11,11,12	0.58	0	15,15,17	0.56	0
3	GLC	F	1	3	12,12,12	0.50	0	17,17,17	0.47	0
3	GLC	F	2	3	11,11,12	0.55	0	15,15,17	0.82	1 (6%)
3	GLC	G	1	3	12,12,12	0.53	0	17,17,17	0.51	0
3	GLC	G	2	3	11,11,12	0.54	0	15,15,17	0.91	1 (6%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2	GLC	C1-O5-C5	2.78	115.91	112.19
3	F	2	GLC	C1-O5-C5	2.57	115.63	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

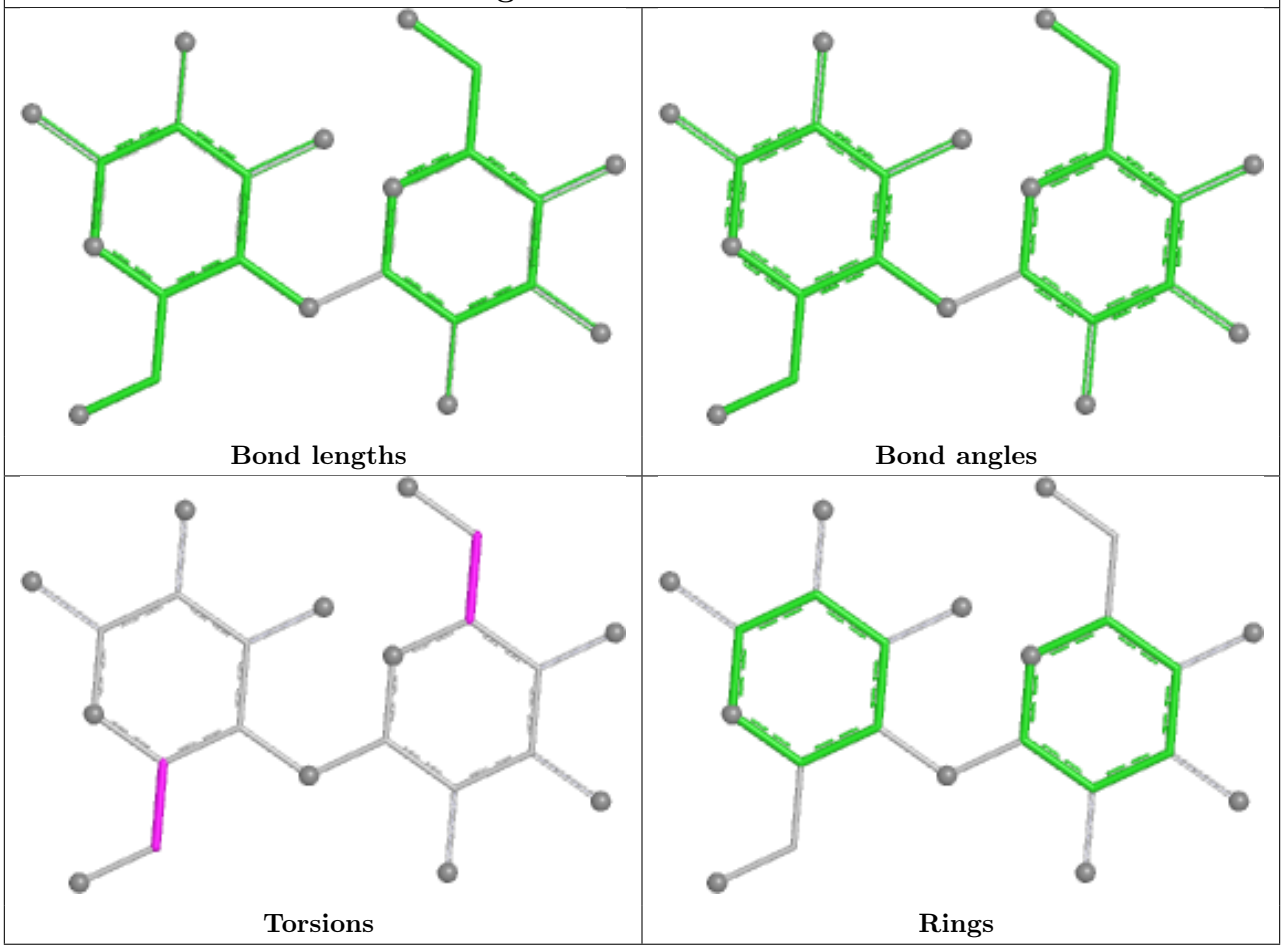
There are no ring outliers.

2 monomers are involved in 2 short contacts:

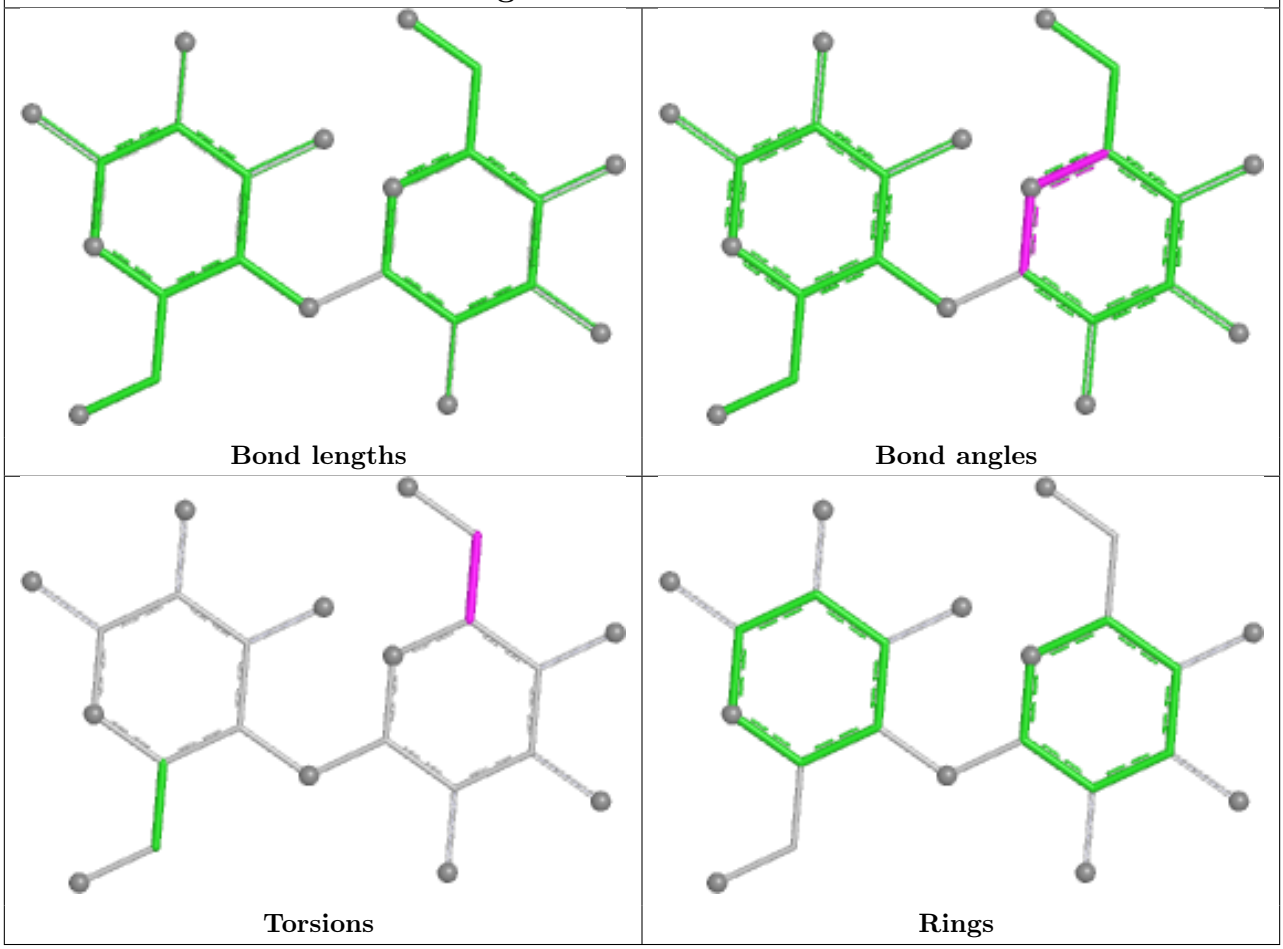
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	GLC	1	0
3	F	2	GLC	1	0

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

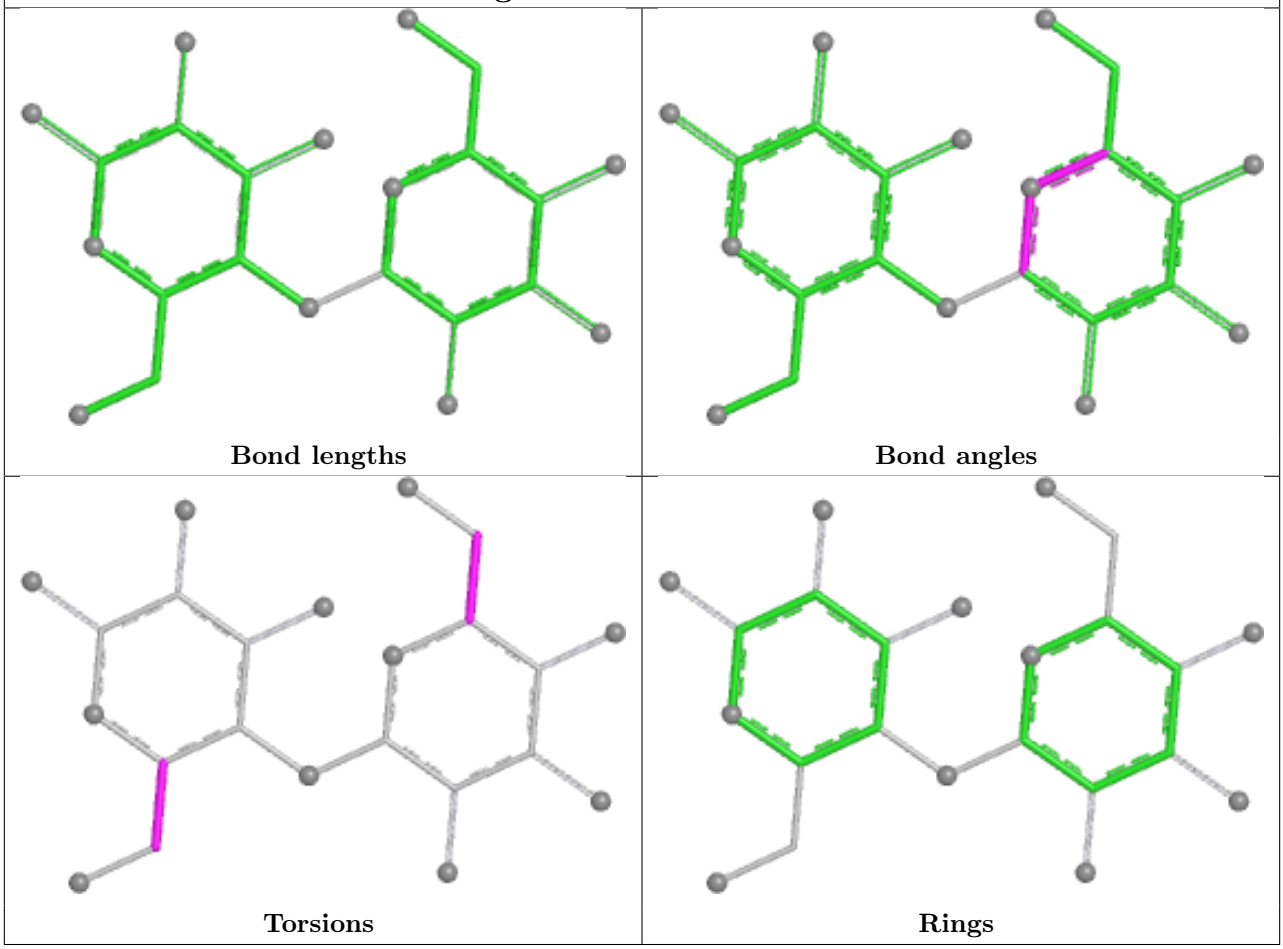
Oligosaccharide Chain E



Oligosaccharide Chain F



Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 41 ligands modelled in this entry, 13 are monoatomic - leaving 28 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	TRD	A	608	-	12,12,12	0.11	0	11,11,11	0.78	0
5	TRD	A	606	-	12,12,12	0.10	0	11,11,11	0.81	0
5	TRD	B	303	-	12,12,12	0.10	0	11,11,11	0.81	0
5	TRD	A	607	-	12,12,12	0.10	0	11,11,11	0.85	0
12	TRS	B	311	13	7,7,7	0.51	0	9,9,9	0.66	0
5	TRD	A	609	-	12,12,12	0.10	0	11,11,11	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	HTH	B	308	-	9,9,9	0.45	0	10,10,10	1.31	1 (10%)
4	DMU	A	602	-	34,34,34	1.91	10 (29%)	45,45,45	1.06	3 (6%)
5	TRD	C	601	-	12,12,12	0.18	0	11,11,11	0.54	0
5	TRD	B	302	-	12,12,12	0.14	0	11,11,11	0.57	0
9	HEA	C	606	14,1	67,67,67	2.50	26 (38%)	81,103,103	2.43	33 (40%)
9	HEA	A	618	14,1	67,67,67	2.21	25 (37%)	81,103,103	2.56	33 (40%)
9	HEA	C	605	1	67,67,67	2.11	25 (37%)	81,103,103	2.67	34 (41%)
5	TRD	A	610	-	6,6,12	0.15	0	5,5,11	0.55	0
5	TRD	B	301	-	12,12,12	0.09	0	11,11,11	0.83	0
4	DMU	D	301	-	31,31,34	2.01	12 (38%)	42,42,45	1.09	2 (4%)
11	HTH	B	310	-	9,9,9	0.52	0	10,10,10	1.17	1 (10%)
4	DMU	A	603	-	34,34,34	1.91	12 (35%)	45,45,45	1.24	5 (11%)
5	TRD	D	302	-	12,12,12	0.10	0	11,11,11	0.82	0
4	DMU	A	604	-	34,34,34	1.95	11 (32%)	45,45,45	1.16	5 (11%)
5	TRD	D	303	-	8,8,12	0.10	0	7,7,11	0.77	0
9	HEA	A	617	1	67,67,67	2.15	22 (32%)	81,103,103	2.79	37 (45%)
4	DMU	A	601	-	34,34,34	1.95	12 (35%)	45,45,45	1.08	1 (2%)
5	TRD	A	613	-	12,12,12	0.10	0	11,11,11	0.79	0
4	DMU	A	605	-	34,34,34	1.89	11 (32%)	45,45,45	1.32	6 (13%)
11	HTH	B	309	-	9,9,9	0.56	0	10,10,10	1.28	1 (10%)
5	TRD	A	612	-	12,12,12	0.09	0	11,11,11	0.83	0
5	TRD	A	611	-	12,12,12	0.09	0	11,11,11	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TRD	A	608	-	-	1/10/10/10	-
5	TRD	A	606	-	-	0/10/10/10	-
5	TRD	B	303	-	-	4/10/10/10	-
5	TRD	A	607	-	-	0/10/10/10	-
12	TRS	B	311	13	-	6/9/9/9	-
5	TRD	A	609	-	-	3/10/10/10	-
11	HTH	B	308	-	-	7/10/10/10	-
4	DMU	A	602	-	-	3/19/59/59	0/2/2/2
5	TRD	C	601	-	-	4/10/10/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TRD	B	302	-	-	5/10/10/10	-
9	HEA	C	606	14,1	-	7/36/76/76	-
9	HEA	A	618	14,1	-	6/36/76/76	-
9	HEA	C	605	1	-	8/36/76/76	-
5	TRD	A	610	-	-	1/4/4/10	-
5	TRD	B	301	-	-	2/10/10/10	-
4	DMU	D	301	-	-	8/16/56/59	0/2/2/2
11	HTH	B	310	-	-	7/10/10/10	-
4	DMU	A	603	-	-	8/19/59/59	0/2/2/2
5	TRD	D	302	-	-	3/10/10/10	-
4	DMU	A	604	-	-	11/19/59/59	0/2/2/2
5	TRD	D	303	-	-	3/6/6/10	-
9	HEA	A	617	1	-	7/36/76/76	-
4	DMU	A	601	-	-	9/19/59/59	0/2/2/2
5	TRD	A	613	-	-	5/10/10/10	-
4	DMU	A	605	-	-	6/19/59/59	0/2/2/2
11	HTH	B	309	-	-	7/10/10/10	-
5	TRD	A	612	-	-	4/10/10/10	-
5	TRD	A	611	-	-	3/10/10/10	-

All (166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	606	HEA	FE-NB	5.68	2.12	1.94
9	C	606	HEA	FE-ND	5.53	2.11	1.94
9	C	606	HEA	C3B-C2B	5.31	1.46	1.34
9	C	606	HEA	FE-NC	5.21	2.12	1.95
9	C	606	HEA	C3D-C2D	4.95	1.47	1.36
9	A	617	HEA	C1D-ND	-4.95	1.31	1.40
9	C	605	HEA	C1D-ND	-4.94	1.31	1.40
9	A	617	HEA	C4B-NB	-4.78	1.32	1.40
4	A	602	DMU	O16-C6	-4.74	1.32	1.40
9	A	618	HEA	FE-NB	4.70	2.09	1.94
9	C	606	HEA	C3A-C2A	4.69	1.47	1.37
9	C	606	HEA	CHD-C1D	4.69	1.47	1.38
4	A	601	DMU	O16-C6	-4.65	1.32	1.40
9	A	618	HEA	C1A-NA	-4.64	1.30	1.39
4	A	603	DMU	O16-C6	-4.48	1.32	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	DMU	O16-C6	-4.48	1.32	1.40
9	C	606	HEA	CHC-C4B	4.47	1.47	1.38
4	A	605	DMU	O16-C6	-4.39	1.32	1.40
9	C	605	HEA	C4B-NB	-4.38	1.32	1.40
4	D	301	DMU	O16-C6	-4.38	1.32	1.40
9	A	618	HEA	FE-ND	4.32	2.08	1.94
9	C	606	HEA	C4A-NA	4.31	1.47	1.39
9	C	606	HEA	CHB-C4A	4.30	1.46	1.38
9	C	606	HEA	C1A-NA	4.30	1.47	1.39
9	C	605	HEA	C3B-C2B	4.28	1.44	1.34
9	C	605	HEA	C4C-NC	-4.24	1.31	1.39
9	A	617	HEA	FE-ND	4.23	2.07	1.94
9	A	617	HEA	C4C-NC	-4.21	1.31	1.39
9	C	606	HEA	CHA-C1A	4.19	1.46	1.38
9	A	618	HEA	C1D-ND	-4.17	1.33	1.40
9	A	618	HEA	C3B-C2B	4.16	1.44	1.34
9	A	617	HEA	C3B-C2B	4.01	1.43	1.34
9	C	605	HEA	C11-C3B	-3.96	1.46	1.51
9	A	617	HEA	C1B-NB	-3.94	1.31	1.38
9	C	605	HEA	C1B-NB	-3.78	1.31	1.38
9	A	618	HEA	C4C-NC	-3.76	1.32	1.39
9	A	617	HEA	C11-C3B	-3.72	1.46	1.51
9	C	605	HEA	C3D-C2D	3.71	1.44	1.36
4	A	604	DMU	O1-C9	3.70	1.53	1.44
4	D	301	DMU	C11-C9	-3.69	1.39	1.51
9	A	618	HEA	C4B-NB	-3.67	1.33	1.40
9	C	606	HEA	CHD-C4C	3.66	1.47	1.39
4	A	602	DMU	C11-C9	-3.66	1.39	1.51
4	A	605	DMU	C11-C9	-3.65	1.39	1.51
9	C	605	HEA	FE-ND	3.65	2.06	1.94
4	A	601	DMU	C11-C9	-3.64	1.39	1.51
4	A	604	DMU	C11-C9	-3.64	1.39	1.51
9	A	617	HEA	FE-NB	3.63	2.06	1.94
4	A	603	DMU	C11-C9	-3.62	1.39	1.51
9	A	617	HEA	C1C-NC	-3.62	1.32	1.39
4	A	601	DMU	O1-C9	3.62	1.53	1.44
9	C	605	HEA	FE-NB	3.61	2.06	1.94
9	A	618	HEA	C3A-C2A	3.60	1.45	1.37
9	A	618	HEA	CHD-C1D	3.59	1.45	1.38
4	D	301	DMU	O1-C9	3.56	1.53	1.44
4	A	603	DMU	O1-C9	3.52	1.53	1.44
9	C	605	HEA	C3A-C2A	3.47	1.45	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	606	HEA	CHC-C1C	3.47	1.47	1.39
4	A	605	DMU	O1-C9	3.46	1.52	1.44
9	C	606	HEA	CHB-C1B	3.46	1.47	1.39
9	A	617	HEA	CHC-C4B	3.43	1.45	1.38
9	A	618	HEA	C4D-ND	-3.41	1.32	1.38
9	A	617	HEA	O2D-CGD	-3.39	1.19	1.30
9	C	606	HEA	CHA-C4D	3.39	1.46	1.39
9	A	617	HEA	CHB-C4A	3.36	1.45	1.38
4	A	602	DMU	O1-C9	3.36	1.52	1.44
9	A	617	HEA	O2A-CGA	-3.36	1.19	1.30
9	A	618	HEA	CHB-C4A	3.34	1.44	1.38
9	C	605	HEA	CHD-C1D	3.33	1.45	1.38
9	A	618	HEA	O2D-CGD	-3.33	1.19	1.30
9	A	618	HEA	CHC-C4B	3.31	1.45	1.38
9	A	618	HEA	C11-C3B	-3.30	1.47	1.51
9	A	618	HEA	C1C-NC	-3.27	1.33	1.39
9	A	618	HEA	FE-NC	3.27	2.05	1.95
9	C	605	HEA	FE-NC	3.26	2.05	1.95
9	A	617	HEA	CHD-C1D	3.26	1.45	1.38
4	A	601	DMU	O5-C6	3.23	1.50	1.41
9	A	618	HEA	C1B-NB	-3.22	1.32	1.38
9	A	618	HEA	FE-NA	3.22	2.05	1.95
9	A	618	HEA	O2A-CGA	-3.21	1.20	1.30
4	A	603	DMU	O5-C6	3.19	1.50	1.41
4	A	605	DMU	O5-C6	3.18	1.50	1.41
4	D	301	DMU	O5-C6	3.18	1.50	1.41
9	C	605	HEA	CHC-C4B	3.14	1.44	1.38
4	A	604	DMU	O5-C6	3.14	1.49	1.41
9	A	617	HEA	C4D-ND	-3.13	1.32	1.38
9	A	617	HEA	C3D-C2D	3.11	1.43	1.36
9	C	605	HEA	C1C-NC	-3.10	1.33	1.39
4	A	602	DMU	O5-C6	3.07	1.49	1.41
9	C	605	HEA	CHA-C1A	3.06	1.44	1.38
9	C	605	HEA	CHB-C4A	3.06	1.44	1.38
9	A	618	HEA	CHC-C1C	3.03	1.46	1.39
9	A	617	HEA	FE-NC	3.02	2.05	1.95
9	A	618	HEA	CHB-C1B	2.94	1.45	1.39
9	A	618	HEA	CHA-C1A	2.93	1.44	1.38
9	C	605	HEA	C1A-NA	2.91	1.45	1.39
4	A	604	DMU	O7-C3	2.88	1.51	1.43
9	A	618	HEA	C3D-C2D	2.88	1.43	1.36
9	C	605	HEA	O2D-CGD	-2.86	1.21	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	605	HEA	C4A-NA	2.84	1.45	1.39
9	A	617	HEA	CHA-C1A	2.81	1.43	1.38
4	D	301	DMU	O7-C3	2.80	1.51	1.43
4	A	604	DMU	C7-C5	-2.78	1.45	1.52
9	A	617	HEA	C3A-C2A	2.76	1.43	1.37
4	A	602	DMU	O7-C3	2.74	1.50	1.43
9	C	605	HEA	C4D-ND	-2.74	1.33	1.38
4	A	601	DMU	O7-C3	2.72	1.50	1.43
4	A	603	DMU	O7-C3	2.68	1.50	1.43
4	A	605	DMU	O7-C3	2.68	1.50	1.43
4	A	602	DMU	C2-C3	-2.65	1.45	1.52
4	A	602	DMU	O4-C7	2.63	1.49	1.43
4	A	601	DMU	C7-C5	-2.63	1.45	1.52
4	A	603	DMU	C7-C5	-2.63	1.45	1.52
4	D	301	DMU	C7-C5	-2.63	1.45	1.52
4	A	601	DMU	C2-C3	-2.62	1.45	1.52
9	C	605	HEA	CHC-C1C	2.61	1.45	1.39
4	A	603	DMU	C2-C3	-2.61	1.45	1.52
9	A	617	HEA	CHC-C1C	2.61	1.45	1.39
9	C	606	HEA	C4B-C3B	2.59	1.49	1.44
9	C	605	HEA	O2A-CGA	-2.55	1.22	1.30
4	A	601	DMU	O4-C7	2.55	1.49	1.43
9	C	606	HEA	C1D-ND	-2.54	1.35	1.40
4	A	604	DMU	O4-C7	2.53	1.49	1.43
4	A	605	DMU	C7-C5	-2.53	1.45	1.52
4	D	301	DMU	C2-C3	-2.53	1.45	1.52
4	A	602	DMU	C7-C5	-2.50	1.45	1.52
9	A	617	HEA	CHD-C4C	2.50	1.45	1.39
9	C	605	HEA	CHB-C1B	2.50	1.44	1.39
9	C	606	HEA	C1C-C2C	2.50	1.49	1.43
9	C	606	HEA	C4B-NB	-2.50	1.35	1.40
4	D	301	DMU	O4-C7	2.49	1.49	1.43
9	C	606	HEA	C1D-C2D	2.48	1.49	1.44
4	A	605	DMU	C2-C3	-2.46	1.45	1.52
4	A	601	DMU	C8-C9	2.40	1.58	1.53
4	A	604	DMU	C2-C3	-2.40	1.45	1.52
4	A	604	DMU	O1-C10	2.37	1.47	1.41
9	C	606	HEA	C3C-C4C	2.34	1.49	1.42
9	A	617	HEA	CHB-C1B	2.33	1.44	1.39
4	A	605	DMU	O4-C7	2.32	1.48	1.43
4	A	603	DMU	O4-C7	2.27	1.48	1.43
9	A	618	HEA	CHD-C4C	2.25	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	606	HEA	C11-C3B	-2.23	1.48	1.51
9	A	618	HEA	CHA-C4D	2.22	1.44	1.39
4	A	605	DMU	O5-C4	2.21	1.49	1.44
4	A	602	DMU	C8-C9	2.21	1.57	1.53
9	C	605	HEA	CHD-C4C	2.17	1.44	1.39
9	C	606	HEA	C1B-C2B	2.16	1.48	1.44
4	A	605	DMU	C8-C9	2.15	1.57	1.53
4	D	301	DMU	C8-C9	2.15	1.57	1.53
4	D	301	DMU	O55-C2	2.13	1.48	1.43
4	A	604	DMU	O55-C2	2.12	1.48	1.43
4	A	601	DMU	O5-C4	2.12	1.49	1.44
4	A	605	DMU	O55-C2	2.11	1.48	1.43
4	A	604	DMU	C8-C9	2.10	1.57	1.53
9	C	605	HEA	CHA-C4D	2.10	1.44	1.39
4	A	603	DMU	O1-C10	2.08	1.47	1.41
4	A	601	DMU	O55-C2	2.07	1.48	1.43
4	A	602	DMU	O55-C2	2.07	1.48	1.43
4	A	603	DMU	O5-C4	2.07	1.49	1.44
4	D	301	DMU	O5-C4	2.06	1.49	1.44
4	A	603	DMU	O3-C5	2.06	1.48	1.43
4	A	603	DMU	O55-C2	2.05	1.48	1.43
4	A	601	DMU	O3-C5	2.02	1.47	1.43
9	C	606	HEA	C1A-C2A	2.01	1.48	1.45
4	D	301	DMU	O1-C10	2.00	1.47	1.41
9	C	606	HEA	C4D-C3D	2.00	1.48	1.45

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	617	HEA	C3D-C4D-ND	9.24	119.28	110.35
9	C	605	HEA	C3D-C4D-ND	7.56	117.66	110.35
9	A	618	HEA	C3D-C4D-ND	7.43	117.53	110.35
9	C	605	HEA	C3B-C4B-NB	6.45	117.26	109.84
9	C	606	HEA	C3D-C4D-ND	6.31	116.45	110.35
9	A	617	HEA	C2D-C1D-ND	6.27	117.05	109.84
9	A	618	HEA	C2D-C1D-ND	6.20	116.97	109.84
9	C	605	HEA	C3C-C4C-NC	5.95	114.81	109.80
9	A	617	HEA	C2B-C1B-NB	5.95	116.78	109.90
9	C	605	HEA	C2B-C1B-NB	5.94	116.78	109.90
9	C	605	HEA	C2D-C1D-ND	5.88	116.60	109.84
9	A	618	HEA	C3B-C4B-NB	5.86	116.58	109.84
9	A	617	HEA	C3C-C2C-C1C	-5.81	100.32	107.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	606	HEA	C2B-C1B-NB	5.69	116.49	109.90
9	C	606	HEA	C3B-C4B-NB	5.68	116.37	109.84
9	A	617	HEA	C3B-C4B-NB	5.68	116.36	109.84
9	A	617	HEA	C3C-C4C-NC	5.66	114.56	109.80
9	C	605	HEA	C3C-C2C-C1C	-5.55	100.62	107.17
9	A	618	HEA	C2B-C1B-NB	5.41	116.16	109.90
9	C	606	HEA	C3C-C2C-C1C	-5.34	100.87	107.17
9	C	606	HEA	C3C-C4C-NC	5.27	114.24	109.80
9	A	618	HEA	C3C-C2C-C1C	-5.09	101.17	107.17
9	C	606	HEA	C2D-C1D-ND	5.08	115.67	109.84
9	A	618	HEA	C3C-C4C-NC	4.95	113.96	109.80
9	C	605	HEA	C2A-C1A-NA	4.82	114.98	110.32
9	A	618	HEA	CHB-C4A-NA	4.72	129.59	124.45
9	A	618	HEA	C4A-NA-C1A	4.69	113.47	105.82
9	C	606	HEA	C2A-C1A-NA	4.56	114.73	110.32
9	A	618	HEA	C1D-C2D-C3D	-4.50	102.25	106.98
9	A	617	HEA	C4D-C3D-C2D	-4.49	100.36	106.89
9	A	618	HEA	C3A-C2A-C1A	-4.48	102.81	107.05
9	A	617	HEA	C3A-C2A-C1A	-4.43	102.86	107.05
9	C	606	HEA	C2C-C1C-NC	4.29	117.02	110.14
9	A	617	HEA	C1D-ND-C4D	-4.23	100.20	105.21
9	C	605	HEA	C4D-C3D-C2D	-4.20	100.77	106.89
9	C	606	HEA	C1D-C2D-C3D	-4.14	102.62	106.98
9	A	617	HEA	C13-C14-C15	-4.07	118.32	127.62
9	A	618	HEA	CHA-C1A-NA	4.05	128.87	124.45
9	C	605	HEA	C2C-C1C-NC	3.96	116.50	110.14
9	A	617	HEA	C1B-C2B-C3B	-3.92	102.25	106.80
9	A	617	HEA	CHA-C4D-C3D	-3.90	119.09	124.77
9	A	617	HEA	O11-C11-C3B	-3.85	104.20	111.26
9	C	605	HEA	C1B-C2B-C3B	-3.83	102.36	106.80
9	A	617	HEA	C2C-C1C-NC	3.79	116.21	110.14
9	A	617	HEA	CAD-C3D-C4D	3.78	131.28	124.70
9	A	617	HEA	C1D-C2D-C3D	-3.68	103.11	106.98
9	C	606	HEA	C1B-C2B-C3B	-3.63	102.59	106.80
9	A	618	HEA	C4B-C3B-C2B	-3.56	101.45	107.44
9	C	605	HEA	CAD-C3D-C4D	3.56	130.90	124.70
9	A	618	HEA	C1D-ND-C4D	-3.52	101.03	105.21
9	C	605	HEA	C3A-C2A-C1A	-3.52	103.72	107.05
9	C	605	HEA	C1D-C2D-C3D	-3.51	103.29	106.98
9	C	605	HEA	C13-C14-C15	-3.48	119.65	127.62
9	A	618	HEA	C2C-C1C-NC	3.44	115.65	110.14
9	C	606	HEA	C3A-C2A-C1A	-3.42	103.81	107.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	603	DMU	C10-O7-C3	-3.41	109.88	117.98
9	C	605	HEA	CHA-C4D-ND	-3.41	120.75	124.42
9	A	617	HEA	CMD-C2D-C1D	3.40	130.35	125.03
9	C	605	HEA	C4B-C3B-C2B	-3.39	101.74	107.44
9	C	605	HEA	C4A-NA-C1A	-3.35	100.35	105.82
9	C	605	HEA	C27-C19-C20	3.30	120.95	115.23
4	A	601	DMU	C10-O7-C3	-3.27	110.23	117.98
11	B	309	HTH	C5-C4-C3	-3.25	108.79	114.11
4	A	605	DMU	O5-C4-C3	3.25	116.44	109.72
9	C	605	HEA	C13-C12-C11	-3.24	109.22	114.39
9	A	618	HEA	C4D-C3D-C2D	-3.22	102.21	106.89
4	A	602	DMU	C10-O7-C3	-3.21	110.37	117.98
9	C	606	HEA	CBA-CAA-C2A	-3.16	103.78	112.53
9	C	605	HEA	C17-C18-C19	-3.15	120.41	127.62
9	A	617	HEA	C4B-C3B-C2B	-3.13	102.17	107.44
9	C	605	HEA	O11-C11-C3B	-3.13	105.53	111.26
9	A	617	HEA	C17-C18-C19	-3.09	120.56	127.62
9	C	606	HEA	C4D-C3D-C2D	-3.05	102.45	106.89
9	A	617	HEA	CMC-C2C-C1C	3.04	130.05	125.42
9	A	618	HEA	C13-C14-C15	-3.02	120.71	127.62
9	A	617	HEA	C12-C11-C3B	3.01	116.83	112.12
9	A	618	HEA	CMB-C2B-C1B	3.00	129.72	125.03
9	C	606	HEA	C4B-C3B-C2B	-3.00	102.40	107.44
9	C	605	HEA	C1D-ND-C4D	-2.99	101.66	105.21
9	A	618	HEA	C27-C19-C20	2.99	120.41	115.23
9	C	606	HEA	C13-C14-C15	-2.97	120.82	127.62
9	A	618	HEA	CMD-C2D-C1D	2.96	129.65	125.03
9	A	617	HEA	CAA-C2A-C1A	2.90	130.76	124.85
9	A	618	HEA	C1B-C2B-C3B	-2.88	103.46	106.80
9	A	617	HEA	C13-C12-C11	-2.88	109.80	114.39
9	C	606	HEA	CAD-CBD-CGD	-2.86	106.08	113.67
9	C	606	HEA	C26-C15-C16	2.86	120.19	115.23
9	C	606	HEA	C4A-NA-C1A	-2.85	101.18	105.82
4	A	605	DMU	C10-O7-C3	-2.85	111.22	117.98
9	A	617	HEA	CHB-C1B-NB	-2.85	121.36	124.42
9	C	605	HEA	C4B-NB-C1B	-2.84	101.84	105.21
9	A	617	HEA	C27-C19-C20	2.84	120.16	115.23
11	B	310	HTH	C5-C4-C3	-2.83	109.47	114.11
9	C	605	HEA	CHB-C1B-C2B	-2.82	120.58	125.03
11	B	308	HTH	C5-C4-C3	-2.80	109.53	114.11
9	A	618	HEA	CHA-C4D-C3D	-2.78	120.72	124.77
9	C	606	HEA	C27-C19-C20	2.76	120.02	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	605	DMU	O5-C6-C1	-2.75	104.72	110.37
9	A	618	HEA	CAD-C3D-C4D	2.74	129.48	124.70
4	D	301	DMU	C10-O7-C3	-2.72	111.53	117.98
4	A	604	DMU	O1-C10-C5	2.71	115.94	110.37
9	C	605	HEA	CHC-C4B-C3B	-2.69	119.01	125.80
9	A	617	HEA	O2A-CGA-CBA	2.69	122.49	114.00
4	A	605	DMU	O16-C6-C1	2.68	112.35	108.27
4	A	605	DMU	C2-C3-C4	2.65	116.81	110.93
4	A	604	DMU	O5-C6-C1	-2.65	104.93	110.37
9	C	606	HEA	CHC-C1C-C2C	-2.63	119.78	127.43
9	A	618	HEA	CHC-C1C-C2C	-2.63	119.78	127.43
4	A	602	DMU	O1-C9-C8	-2.63	104.96	109.70
9	A	617	HEA	CHA-C4D-ND	-2.60	121.63	124.42
9	C	606	HEA	C13-C12-C11	-2.59	110.25	114.39
9	C	606	HEA	C4B-NB-C1B	-2.59	102.14	105.21
9	C	606	HEA	CMB-C2B-C1B	2.58	129.07	125.03
9	C	605	HEA	CHC-C1C-C2C	-2.53	120.07	127.43
9	A	618	HEA	CHA-C4D-ND	-2.51	121.73	124.42
9	A	618	HEA	CHD-C1D-C2D	-2.47	119.92	126.95
9	A	617	HEA	CHA-C1A-NA	2.43	127.10	124.45
9	A	618	HEA	C4B-NB-C1B	-2.43	102.33	105.21
9	C	606	HEA	CMD-C2D-C1D	2.41	128.80	125.03
9	C	606	HEA	C17-C18-C19	-2.39	122.16	127.62
9	A	618	HEA	CHA-C1A-C2A	-2.39	121.09	124.86
9	C	605	HEA	CHD-C1D-C2D	-2.39	120.17	126.95
9	C	606	HEA	CHA-C4D-C3D	-2.37	121.33	124.77
9	A	617	HEA	C4B-NB-C1B	-2.36	102.42	105.21
4	A	603	DMU	O5-C4-C3	2.35	114.59	109.72
9	A	617	HEA	CHC-C4B-C3B	-2.35	119.88	125.80
9	C	605	HEA	CHA-C1A-NA	-2.34	121.91	124.45
9	C	605	HEA	CBA-CAA-C2A	-2.33	106.09	112.53
4	A	604	DMU	O5-C4-C3	2.33	114.53	109.72
9	A	617	HEA	C4A-C3A-C2A	2.31	108.82	106.81
9	C	606	HEA	CHB-C1B-C2B	-2.30	121.40	125.03
4	A	602	DMU	O5-C6-C1	-2.29	105.67	110.37
9	A	618	HEA	CHC-C4B-NB	-2.27	121.55	124.37
9	C	605	HEA	CMD-C2D-C1D	2.27	128.59	125.03
4	A	605	DMU	C1-C2-C3	2.26	114.80	109.68
4	A	603	DMU	O1-C9-C8	-2.25	105.65	109.70
4	A	603	DMU	O16-C6-C1	2.23	111.66	108.27
4	D	301	DMU	C1-C2-C3	2.23	114.73	109.68
9	C	605	HEA	CHA-C4D-C3D	-2.19	121.57	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	618	HEA	CHB-C1B-NB	-2.18	122.08	124.42
9	C	605	HEA	CAD-CBD-CGD	-2.16	107.93	113.67
9	A	618	HEA	CBA-CAA-C2A	-2.16	106.56	112.53
4	A	604	DMU	C1-C2-C3	2.15	114.56	109.68
9	A	618	HEA	CBC-CAC-C3C	-2.15	116.79	127.53
9	C	606	HEA	CHB-C1B-NB	-2.15	122.11	124.42
9	A	618	HEA	CAD-CBD-CGD	-2.14	107.99	113.67
9	A	617	HEA	OMA-CMA-C3A	-2.11	120.87	125.62
9	A	617	HEA	CBA-CAA-C2A	-2.10	106.73	112.53
9	C	606	HEA	C4C-C3C-C2C	-2.10	104.69	107.30
4	A	604	DMU	C10-O7-C3	-2.09	113.03	117.98
9	A	618	HEA	CHB-C1B-C2B	-2.07	121.75	125.03
9	A	617	HEA	CHD-C1D-C2D	-2.06	121.08	126.95
9	A	617	HEA	CMB-C2B-C1B	2.06	128.25	125.03
9	A	617	HEA	CHD-C1D-ND	-2.05	121.83	124.37
9	C	606	HEA	CHA-C4D-ND	-2.05	122.22	124.42
9	C	605	HEA	C27-C19-C18	-2.05	118.37	123.63
9	C	606	HEA	C25-C23-C24	2.04	119.29	114.59
4	A	603	DMU	O1-C9-C11	2.04	111.50	106.44
9	C	605	HEA	C4C-C3C-C2C	-2.04	104.77	107.30
9	C	606	HEA	C1D-ND-C4D	-2.03	102.81	105.21
9	C	606	HEA	CMC-C2C-C1C	2.02	128.50	125.42
9	A	617	HEA	CHB-C1B-C2B	-2.01	121.86	125.03

There are no chirality outliers.

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	DMU	C19-C18-O16-C6
9	A	617	HEA	C19-C20-C21-C22
11	B	308	HTH	O1-C1-C2-C3
11	B	308	HTH	C1-C2-C3-O3
11	B	308	HTH	O2-C2-C3-C4
11	B	309	HTH	C1-C2-C3-O3
11	B	309	HTH	C1-C2-C3-C4
11	B	309	HTH	O2-C2-C3-O3
11	B	309	HTH	O2-C2-C3-C4
11	B	310	HTH	O1-C1-C2-O2
11	B	310	HTH	O1-C1-C2-C3
11	B	310	HTH	C1-C2-C3-O3
11	B	310	HTH	C1-C2-C3-C4
11	B	310	HTH	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	B	310	HTH	O2-C2-C3-C4
12	B	311	TRS	C1-C-C3-O3
12	B	311	TRS	C2-C-C3-O3
4	A	604	DMU	O1-C10-O7-C3
11	B	308	HTH	O1-C1-C2-O2
4	D	301	DMU	O5-C4-C57-O61
4	A	603	DMU	O5-C4-C57-O61
4	A	603	DMU	O6-C11-C9-O1
4	D	301	DMU	C3-C4-C57-O61
9	C	605	HEA	C19-C20-C21-C22
4	A	604	DMU	C3-C4-C57-O61
4	A	603	DMU	O6-C11-C9-C8
4	D	301	DMU	O5-C6-O16-C18
4	A	604	DMU	O5-C4-C57-O61
4	A	604	DMU	O16-C18-C19-C22
4	A	603	DMU	C3-C4-C57-O61
5	B	302	TRD	C4-C5-C6-C7
4	A	605	DMU	O16-C18-C19-C22
5	B	303	TRD	C11-C10-C9-C8
5	A	611	TRD	C11-C10-C9-C8
5	B	303	TRD	C9-C10-C11-C12
4	A	601	DMU	C19-C18-O16-C6
4	D	301	DMU	C19-C18-O16-C6
4	A	601	DMU	O16-C18-C19-C22
5	A	611	TRD	C7-C8-C9-C10
4	A	601	DMU	C22-C25-C28-C31
5	A	612	TRD	C6-C7-C8-C9
4	A	601	DMU	C19-C22-C25-C28
5	D	303	TRD	C3-C4-C5-C6
4	A	605	DMU	C25-C28-C31-C34
11	B	309	HTH	O1-C1-C2-O2
5	A	609	TRD	C9-C10-C11-C12
5	A	612	TRD	C7-C8-C9-C10
4	A	601	DMU	O5-C4-C57-O61
5	B	301	TRD	C11-C10-C9-C8
5	A	613	TRD	C9-C10-C11-C12
4	A	602	DMU	C3-C4-C57-O61
4	A	601	DMU	C31-C34-C37-C40
11	B	308	HTH	O2-C2-C3-O3
4	A	604	DMU	C31-C34-C37-C40
4	A	605	DMU	C19-C22-C25-C28
4	A	604	DMU	O6-C11-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	301	DMU	O16-C18-C19-C22
9	C	605	HEA	C2A-C3A-CMA-OMA
5	A	613	TRD	C7-C8-C9-C10
5	A	609	TRD	C10-C11-C12-C13
9	A	618	HEA	C3B-C11-C12-C13
5	A	613	TRD	C1-C2-C3-C4
4	D	301	DMU	C22-C25-C28-C31
5	B	302	TRD	C6-C7-C8-C9
5	A	613	TRD	C6-C7-C8-C9
11	B	308	HTH	O3-C3-C4-C5
11	B	309	HTH	O1-C1-C2-C3
4	A	605	DMU	C34-C37-C40-C43
12	B	311	TRS	N-C-C3-O3
4	A	605	DMU	O5-C4-C57-O61
5	A	611	TRD	C9-C10-C11-C12
5	A	612	TRD	C11-C10-C9-C8
11	B	308	HTH	C2-C3-C4-C5
9	C	605	HEA	C26-C15-C16-C17
5	C	601	TRD	C9-C10-C11-C12
4	A	604	DMU	O6-C11-C9-O1
4	A	603	DMU	C18-C19-C22-C25
9	C	605	HEA	C14-C15-C16-C17
5	B	302	TRD	C5-C6-C7-C8
5	B	303	TRD	C4-C5-C6-C7
5	B	301	TRD	C6-C7-C8-C9
9	C	605	HEA	C4A-C3A-CMA-OMA
12	B	311	TRS	C1-C-C2-O2
9	A	617	HEA	C26-C15-C16-C17
4	A	601	DMU	C28-C31-C34-C37
5	A	610	TRD	C1-C2-C3-C4
4	A	601	DMU	C18-C19-C22-C25
4	A	603	DMU	C19-C18-O16-C6
9	A	617	HEA	C14-C15-C16-C17
4	A	602	DMU	C25-C28-C31-C34
4	A	603	DMU	C19-C22-C25-C28
9	C	606	HEA	CAD-CBD-CGD-O1D
4	A	602	DMU	O5-C4-C57-O61
11	B	309	HTH	C3-C4-C5-C6
5	D	303	TRD	C6-C7-C8-C9
5	B	302	TRD	C9-C10-C11-C12
5	C	601	TRD	C2-C3-C4-C5
5	A	613	TRD	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	C	606	HEA	CAD-CBD-CGD-O2D
5	D	302	TRD	C4-C5-C6-C7
9	A	618	HEA	CAD-CBD-CGD-O2D
4	A	601	DMU	C34-C37-C40-C43
4	D	301	DMU	C18-C19-C22-C25
9	C	605	HEA	CAD-CBD-CGD-O2D
5	D	303	TRD	C5-C6-C7-C8
9	A	618	HEA	CAD-CBD-CGD-O1D
9	C	606	HEA	CAA-CBA-CGA-O1A
9	A	617	HEA	CAD-CBD-CGD-O2D
5	A	608	TRD	C3-C4-C5-C6
9	C	605	HEA	CAD-CBD-CGD-O1D
12	B	311	TRS	C3-C-C2-O2
4	A	604	DMU	C2-C3-O7-C10
9	A	617	HEA	CAD-CBD-CGD-O1D
9	A	618	HEA	CAA-CBA-CGA-O1A
5	D	302	TRD	C3-C4-C5-C6
9	C	606	HEA	C3B-C11-C12-C13
9	C	606	HEA	CAA-CBA-CGA-O2A
5	A	609	TRD	C4-C5-C6-C7
11	B	310	HTH	C3-C4-C5-C6
5	D	302	TRD	C6-C7-C8-C9
9	C	606	HEA	C26-C15-C16-C17
4	A	604	DMU	O5-C6-O16-C18
9	A	618	HEA	CAA-CBA-CGA-O2A
5	C	601	TRD	C5-C6-C7-C8
4	A	605	DMU	C28-C31-C34-C37
5	A	612	TRD	C4-C5-C6-C7
5	B	303	TRD	C10-C11-C12-C13
4	A	604	DMU	C4-C3-O7-C10
9	A	618	HEA	O11-C11-C12-C13
9	C	606	HEA	O11-C11-C12-C13
12	B	311	TRS	N-C-C2-O2
9	A	617	HEA	CAA-CBA-CGA-O2A
4	D	301	DMU	O6-C11-C9-C8
9	C	605	HEA	CAA-CBA-CGA-O2A
4	A	603	DMU	C22-C25-C28-C31
5	C	601	TRD	C7-C8-C9-C10
5	B	302	TRD	C7-C8-C9-C10
9	A	617	HEA	CAA-CBA-CGA-O1A

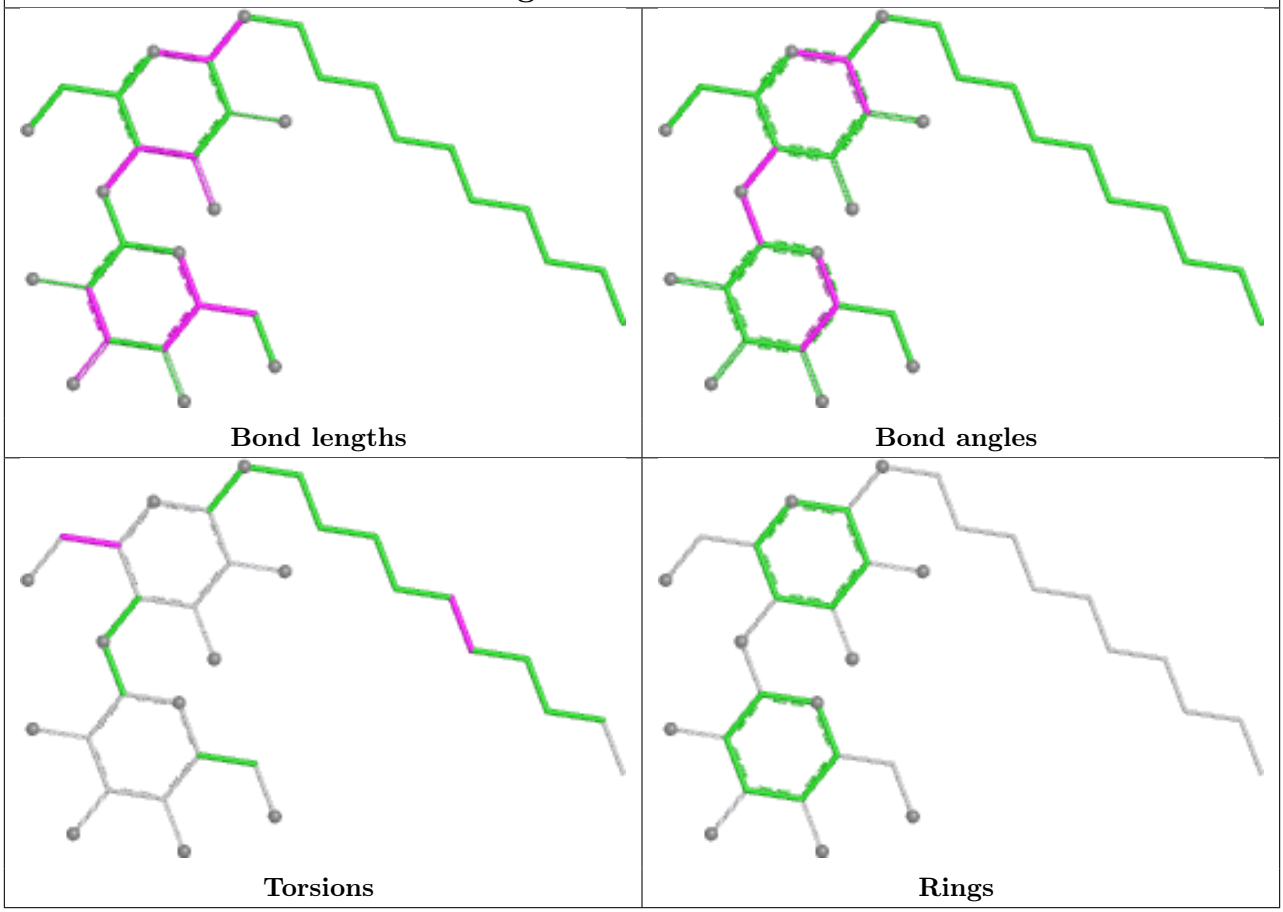
There are no ring outliers.

13 monomers are involved in 28 short contacts:

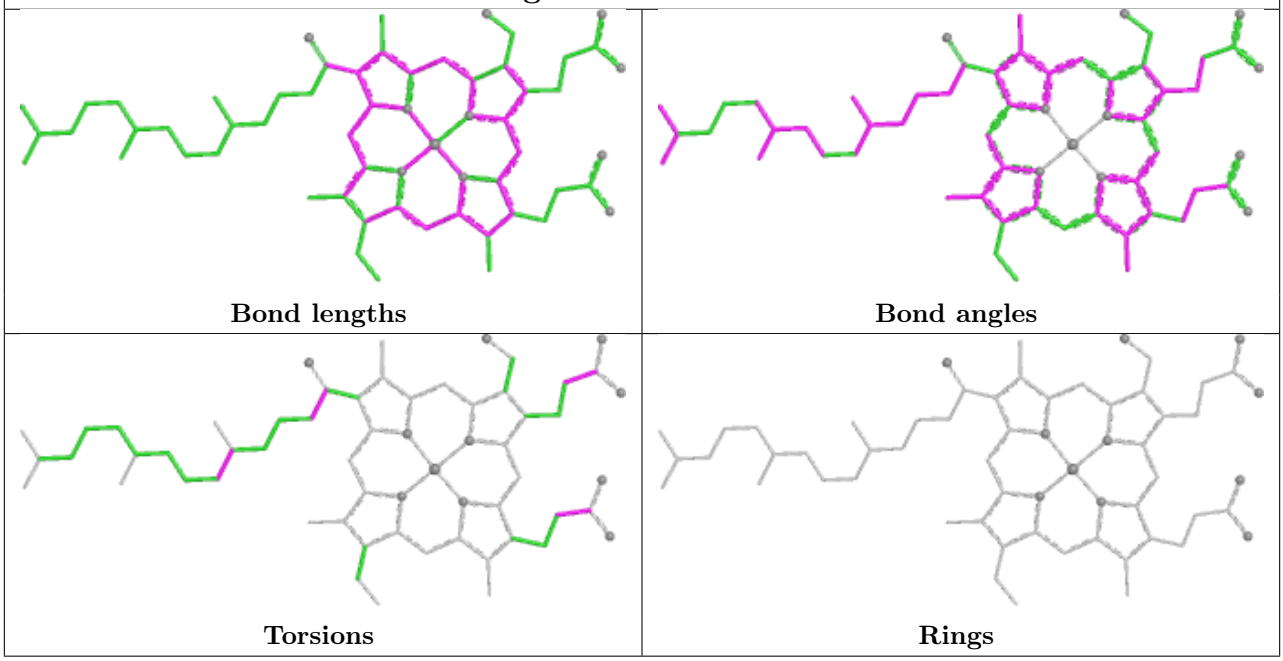
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	606	TRD	1	0
5	A	607	TRD	1	0
5	B	302	TRD	3	0
9	C	606	HEA	4	0
9	A	618	HEA	6	0
9	C	605	HEA	3	0
4	D	301	DMU	2	0
11	B	310	HTH	1	0
4	A	604	DMU	3	0
5	D	303	TRD	1	0
9	A	617	HEA	2	0
4	A	601	DMU	1	0
5	A	612	TRD	2	0

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 then 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.

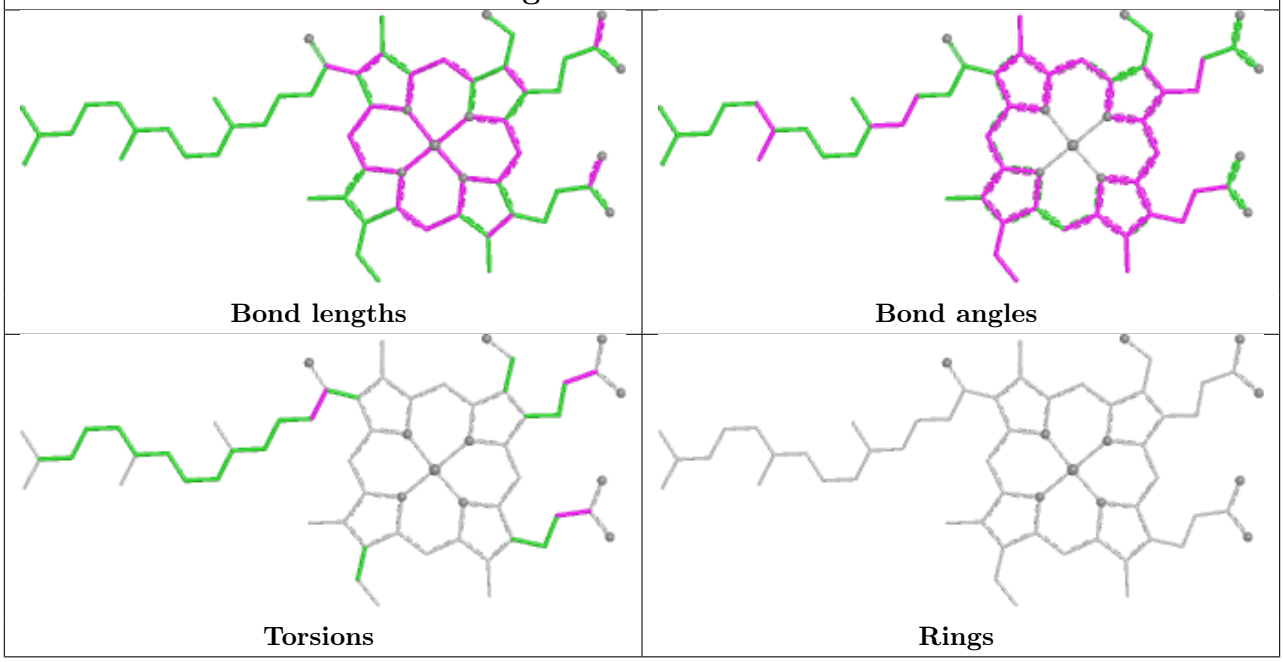
Ligand DMU A 602



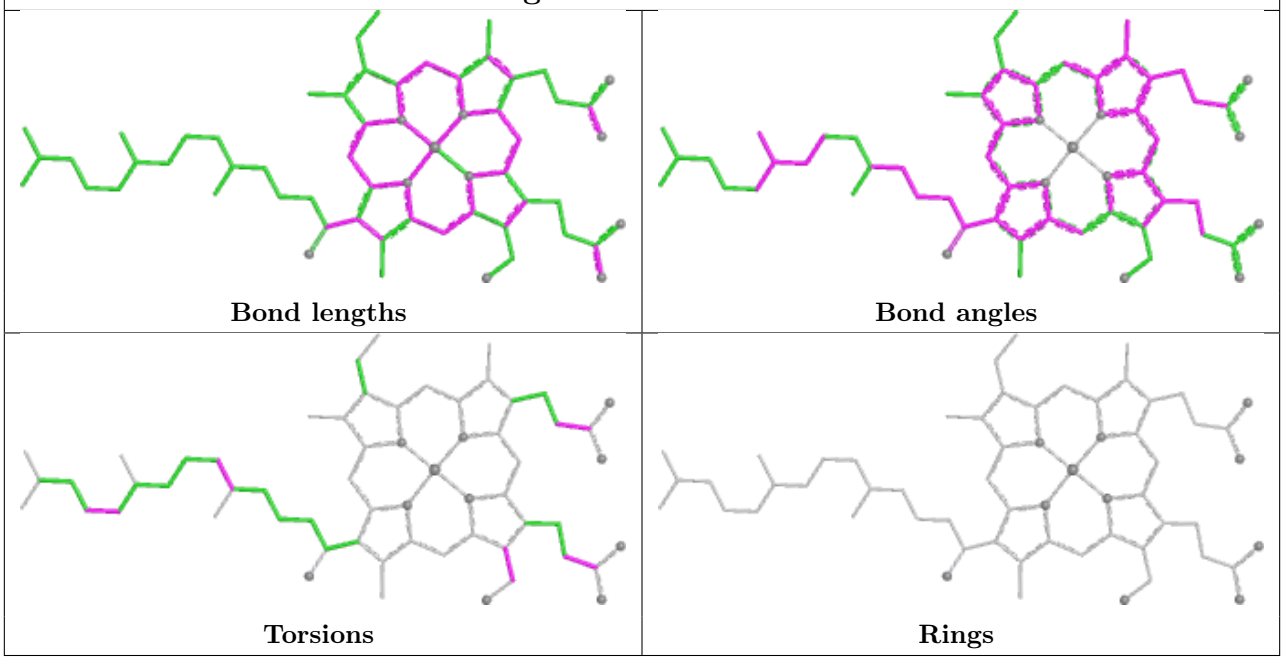
Ligand HEA C 606



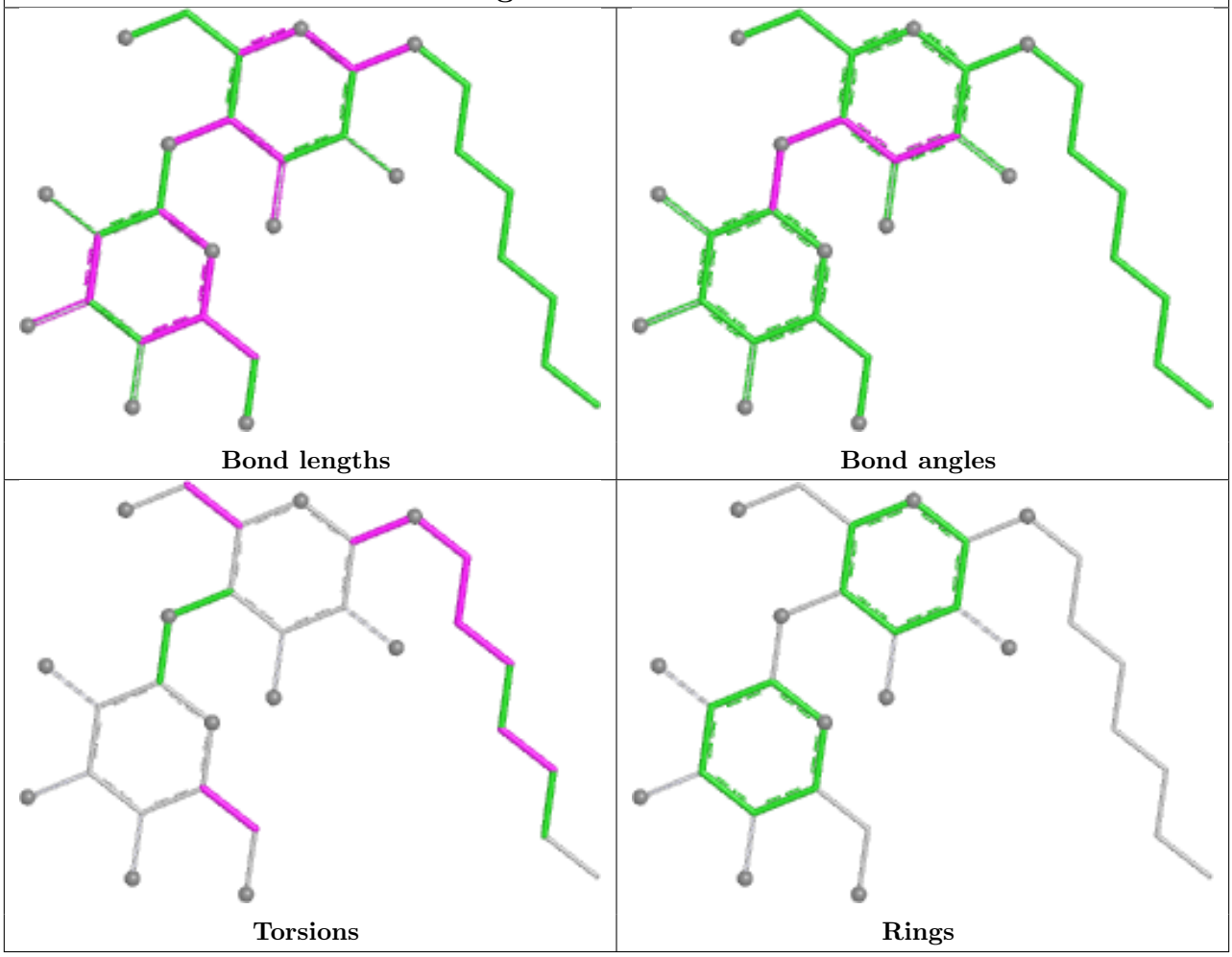
Ligand HEA A 618



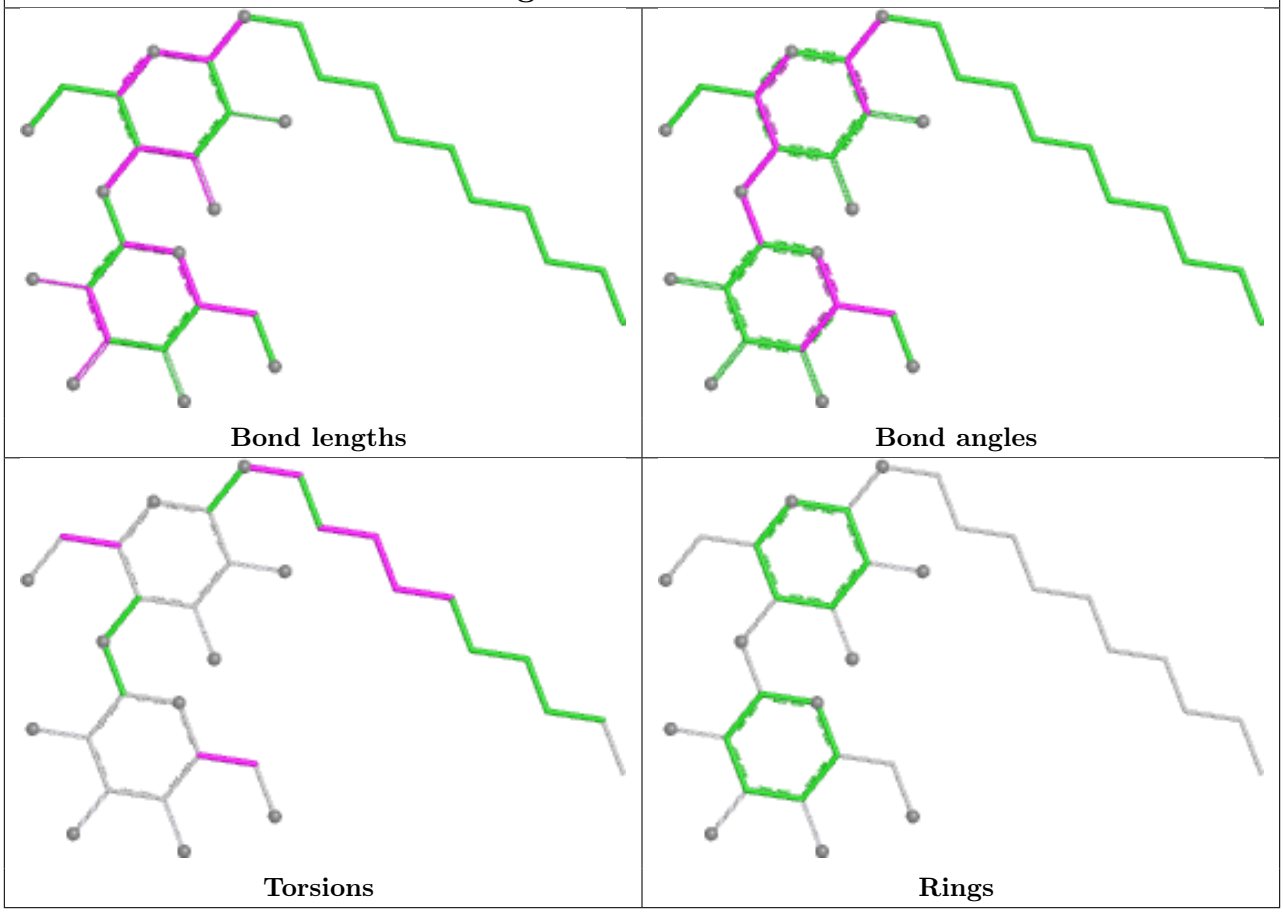
Ligand HEA C 605



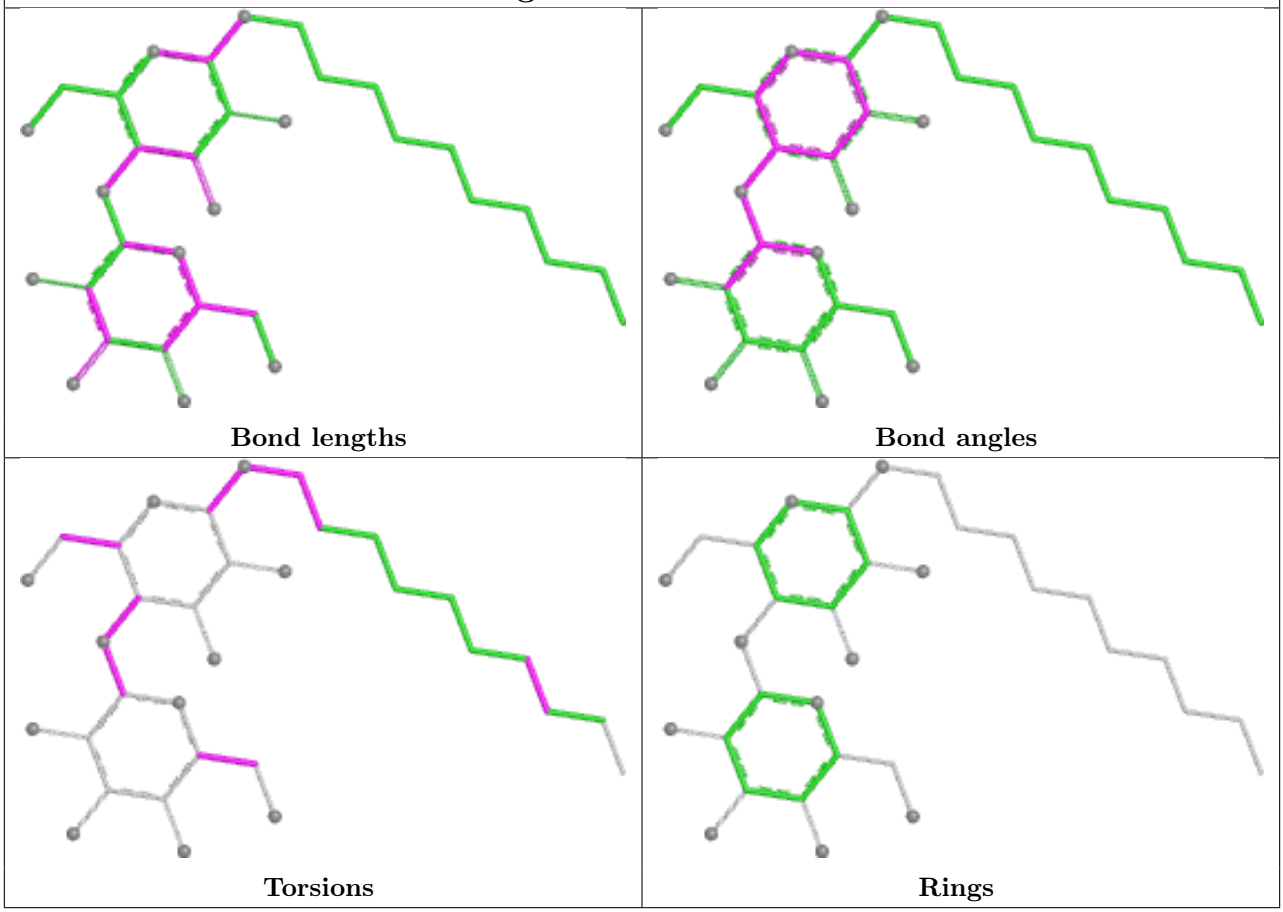
Ligand DMU D 301



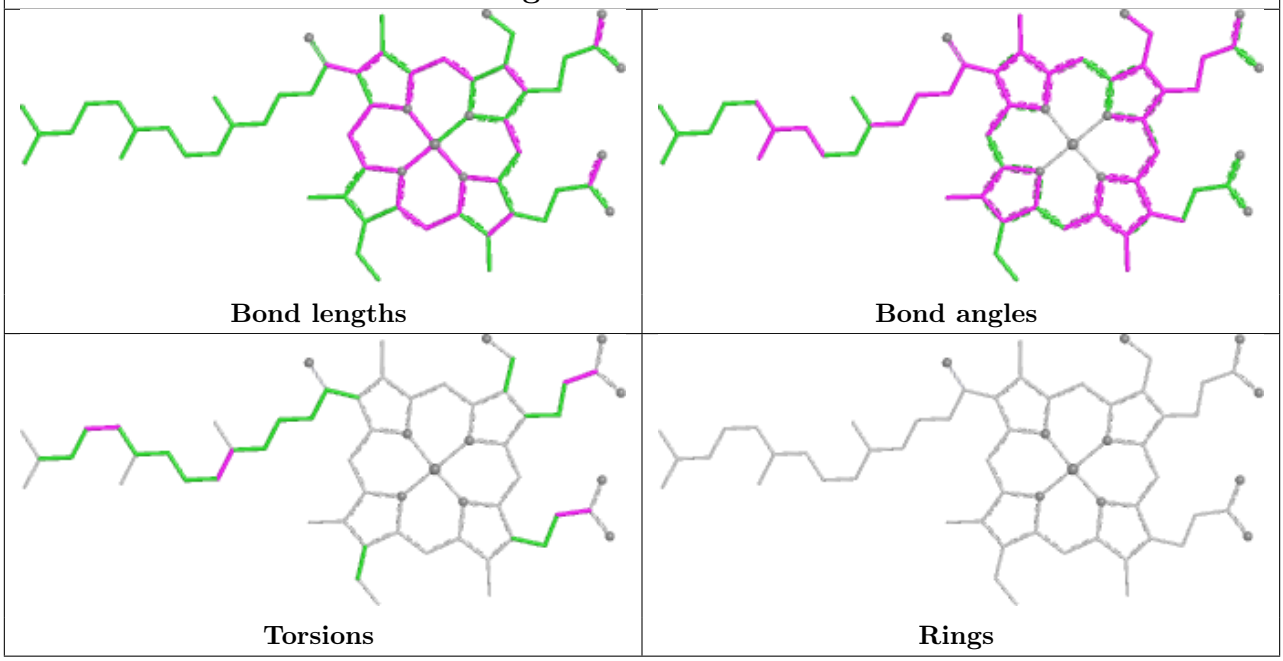
Ligand DMU A 603



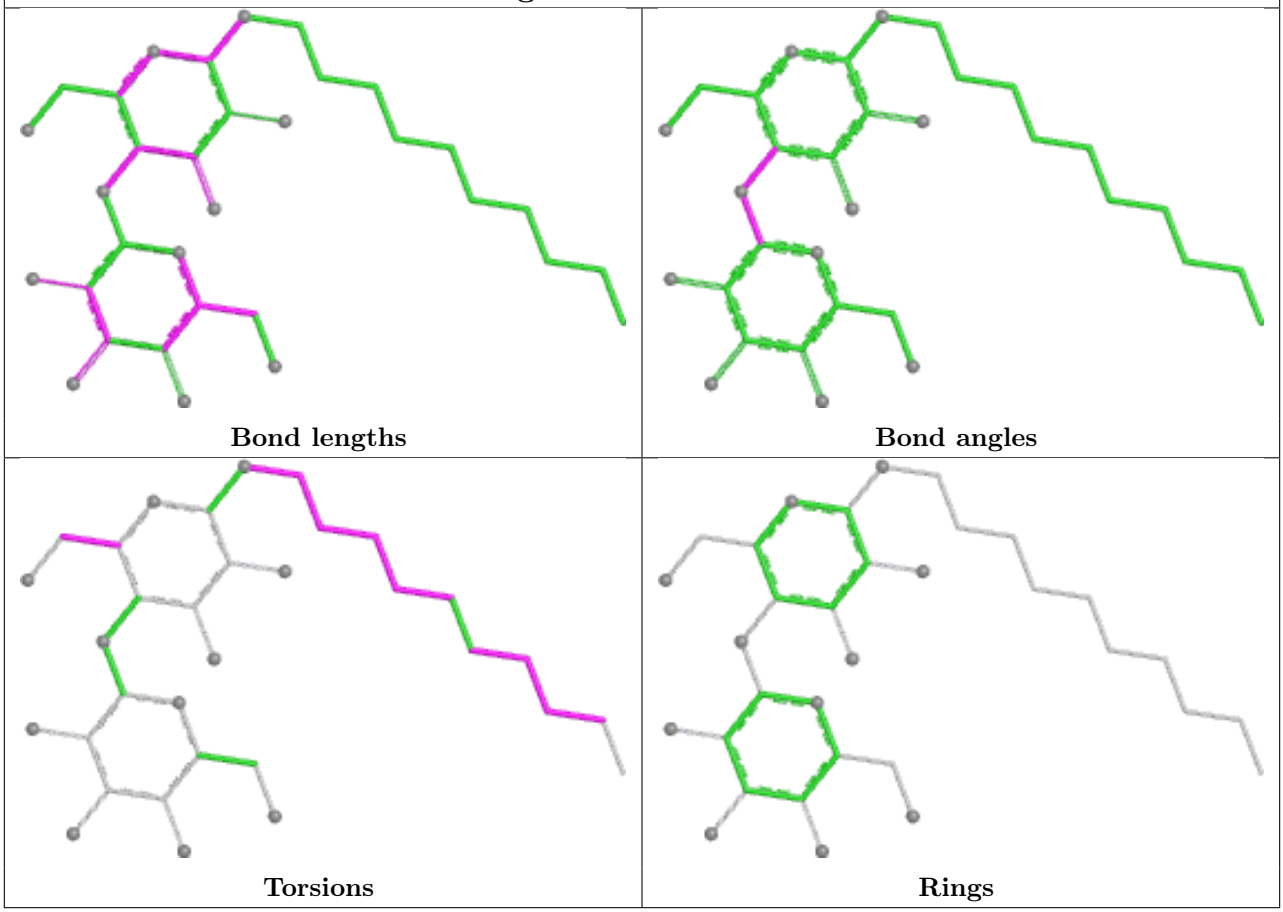
Ligand DMU A 604

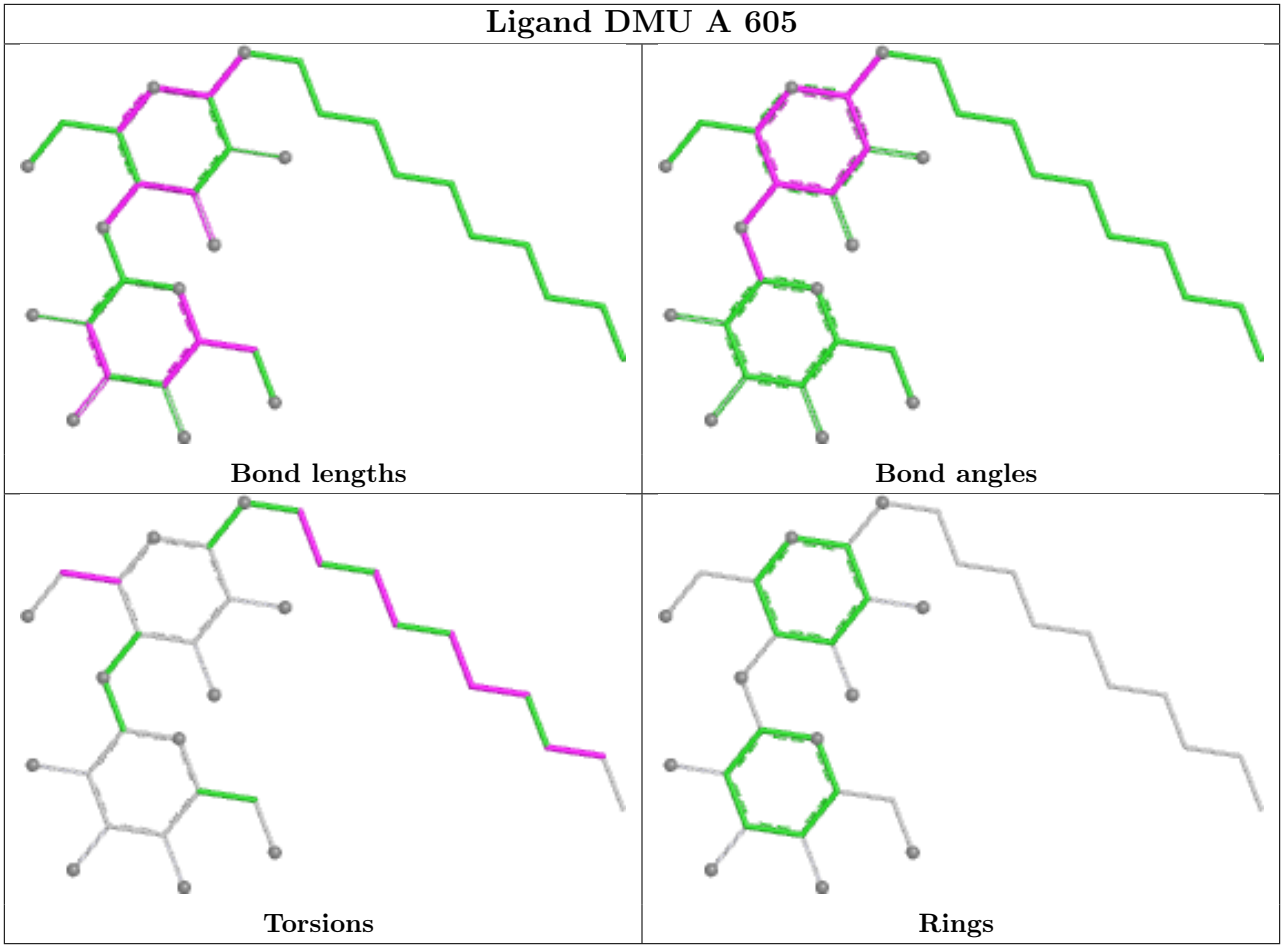


Ligand HEA A 617



Ligand DMU A 601





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	535/535 (100%)	0.32	18 (3%) 48 44	37, 54, 83, 115	0
1	C	531/535 (99%)	1.24	110 (20%) 2 2	51, 77, 108, 130	0
2	B	256/257 (99%)	0.33	12 (4%) 36 32	38, 58, 81, 89	0
2	D	257/257 (100%)	0.62	19 (7%) 20 17	45, 66, 96, 116	0
All	All	1579/1584 (99%)	0.68	159 (10%) 12 9	37, 64, 99, 130	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	TRP	6.4
1	C	548	GLU	6.0
1	C	549	HIS	5.3
1	C	517	TYR	4.8
1	C	69	GLU	4.6
1	A	20	TRP	4.6
1	C	550	THR	4.6
1	A	550	THR	4.6
2	D	29	SER	4.5
1	C	81	TRP	4.2
1	C	77	PHE	4.2
1	C	207	ASN	4.2
1	C	184	GLY	4.1
1	C	23	SER	4.1
1	C	129	GLY	4.0
1	C	145	LEU	4.0
2	D	56	TRP	3.8
1	C	217	ALA	3.8
1	A	25	ASN	3.8
1	C	534	HIS	3.7
1	A	551	PHE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	222	MET	3.6
1	A	81	TRP	3.6
1	C	533	GLU	3.5
2	B	104	TRP	3.5
2	D	102	ILE	3.5
1	C	74	LYS	3.5
1	C	72	LEU	3.4
1	A	373	GLY	3.4
2	D	96	HIS	3.4
1	C	75	GLY	3.4
1	A	548	GLU	3.4
1	C	224	LYS	3.3
2	D	85	GLU	3.3
1	A	549	HIS	3.3
2	D	131	GLU	3.3
2	D	86	LYS	3.3
2	D	101	ALA	3.2
2	B	117	ALA	3.2
1	C	80	LEU	3.2
1	C	540	TRP	3.1
1	C	547	PRO	3.1
1	A	18	THR	3.1
1	C	530	TYR	3.1
1	C	509	LEU	3.1
1	C	543	THR	3.0
1	C	223	HIS	3.0
1	C	83	SER	3.0
1	C	268	GLY	3.0
1	C	22	MET	2.9
1	C	73	VAL	2.9
1	C	221	THR	2.9
2	B	56	TRP	2.9
1	C	70	SER	2.9
1	C	128	ILE	2.9
2	D	97	ASN	2.9
1	C	524	ARG	2.9
1	C	215	MET	2.9
1	C	139	ASN	2.8
1	C	520	THR	2.8
2	D	284	HIS	2.8
2	B	95	THR	2.7
1	C	135	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	82	PRO	2.7
1	A	318	TYR	2.7
1	C	544	SER	2.7
1	C	131	PRO	2.7
1	C	26	HIS	2.7
1	C	88	CYS	2.6
2	B	98	SER	2.6
1	C	30	GLY	2.6
1	C	440	ILE	2.6
1	C	516	PHE	2.6
1	C	367	ILE	2.6
1	C	196	LEU	2.6
1	C	340	LEU	2.6
1	A	221	THR	2.6
2	D	103	ALA	2.6
1	C	230	TRP	2.6
1	C	34	LEU	2.6
1	C	134	ALA	2.6
1	C	210	THR	2.6
1	C	216	ARG	2.5
1	C	185	TYR	2.5
1	C	451	TRP	2.5
1	C	531	TRP	2.5
1	C	211	THR	2.5
1	C	539	GLU	2.5
2	B	102	ILE	2.5
1	C	137	ARG	2.5
1	C	78	GLN	2.5
1	C	521	ARG	2.5
1	C	168	SER	2.5
1	C	152	LEU	2.4
1	C	76	PHE	2.4
1	C	144	TRP	2.4
1	C	130	ALA	2.4
2	D	74	LEU	2.4
1	C	469	PHE	2.4
2	D	40	GLY	2.4
1	C	536	ASP	2.4
1	C	466	LEU	2.4
1	C	542	LEU	2.4
1	C	318	TYR	2.4
1	C	56	MET	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	81	TRP	2.4
1	C	149	GLY	2.4
1	A	130	ALA	2.4
1	C	535	ALA	2.4
2	D	109	ILE	2.3
1	A	209	ILE	2.3
1	C	33	TYR	2.3
1	C	160	PRO	2.3
1	C	218	PRO	2.3
1	A	210	THR	2.3
1	C	209	ILE	2.3
1	C	259	PHE	2.3
1	C	452	ALA	2.2
1	A	223	HIS	2.2
1	C	447	GLN	2.2
1	C	27	LYS	2.2
1	C	132	ASP	2.2
1	C	21	PHE	2.2
1	C	389	PHE	2.2
1	A	19	ARG	2.2
1	C	525	VAL	2.2
1	C	528	ASN	2.2
2	B	88	ASN	2.2
1	C	39	LEU	2.2
1	C	519	LEU	2.2
1	C	279	LEU	2.2
1	C	427	GLY	2.2
1	C	29	ILE	2.2
1	C	237	TRP	2.2
2	D	107	VAL	2.2
1	C	243	LEU	2.2
1	C	212	PHE	2.2
2	D	106	ILE	2.1
1	A	17	PHE	2.1
1	C	457	PHE	2.1
2	D	83	PHE	2.1
2	B	126	GLN	2.1
1	C	232	ILE	2.1
1	C	142	SER	2.1
1	C	133	MET	2.1
2	B	124	PHE	2.1
1	A	152	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	446	ARG	2.1
2	B	273	GLU	2.1
1	C	220	MET	2.1
2	B	94	PHE	2.0
1	C	32	LEU	2.0
1	C	117	GLY	2.0
1	C	439	TRP	2.0
2	B	115	ILE	2.0
1	C	65	ALA	2.0
2	D	88	ASN	2.0
1	C	28	ASP	2.0
1	C	460	MET	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)

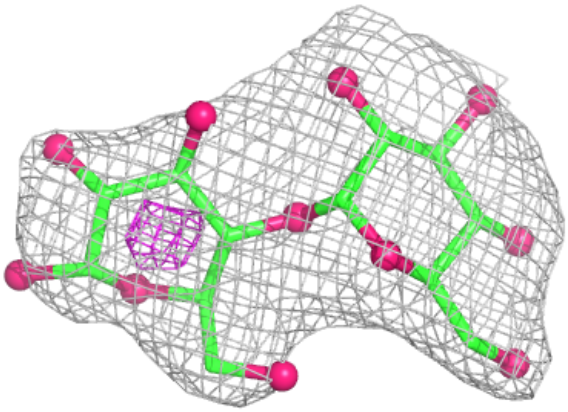
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

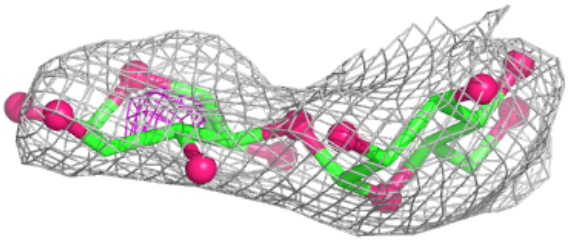
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	G	2	11/12	0.70	0.14	130,136,140,142	0
3	GLC	G	1	12/12	0.73	0.14	116,126,136,136	0
3	GLC	F	2	11/12	0.76	0.16	96,105,110,112	0
3	GLC	F	1	12/12	0.77	0.12	110,114,120,121	0
3	GLC	E	1	12/12	0.80	0.15	97,111,118,119	0
3	GLC	E	2	11/12	0.83	0.13	87,98,107,107	0

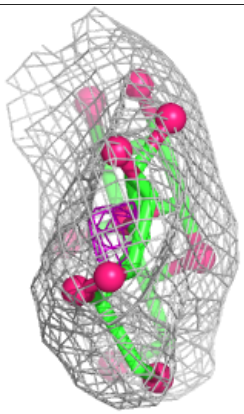
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

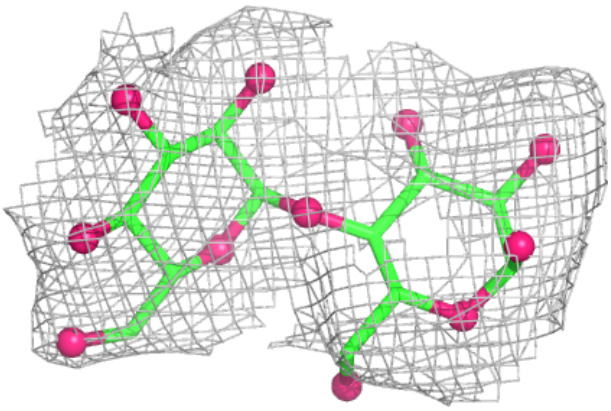


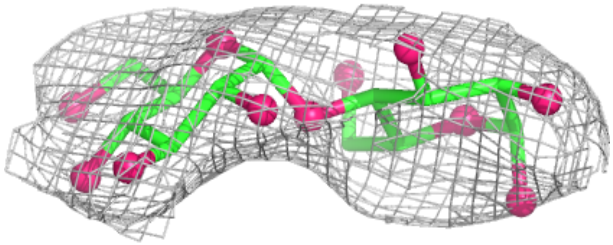


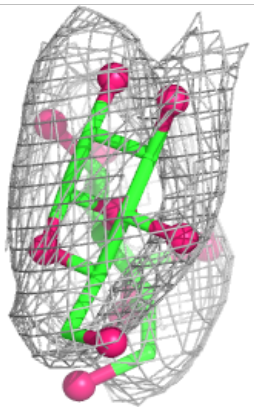


Electron density around Chain F:

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

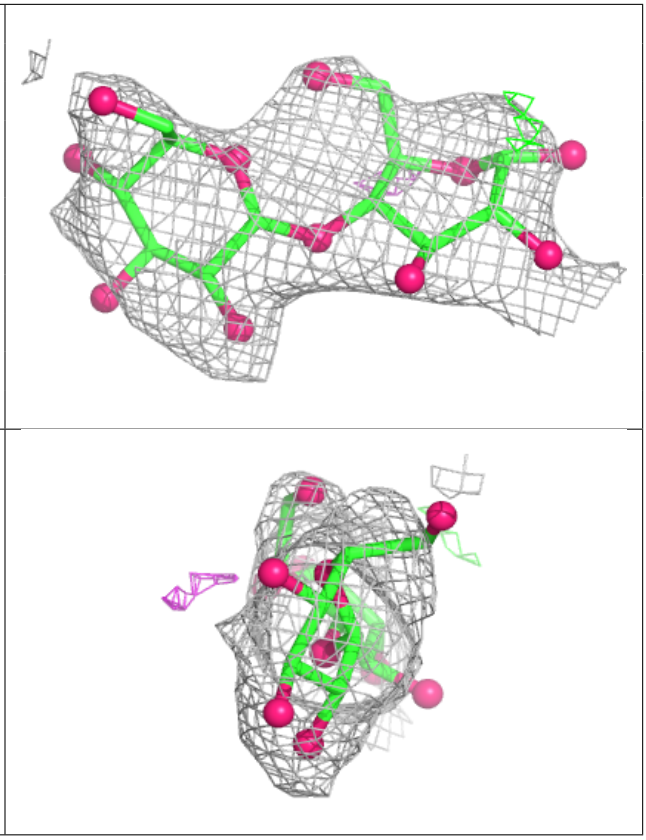






Electron density around Chain G:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	TRD	C	601	13/13	0.54	0.42	88,112,125,125	0
11	HTH	B	310	10/10	0.58	0.27	77,105,110,114	0
5	TRD	B	302	13/13	0.64	0.26	52,68,83,84	0
5	TRD	A	607	13/13	0.66	0.29	65,77,84,91	0
5	TRD	A	609	13/13	0.68	0.30	64,74,83,91	0
5	TRD	A	611	13/13	0.72	0.30	67,77,88,91	0
5	TRD	A	608	13/13	0.74	0.28	63,70,88,93	0
5	TRD	A	613	13/13	0.75	0.22	62,69,82,87	0
5	TRD	B	301	13/13	0.76	0.26	74,86,93,99	0
5	TRD	D	302	13/13	0.78	0.25	61,72,85,87	0
5	TRD	A	606	13/13	0.78	0.21	72,76,88,90	0
5	TRD	B	303	13/13	0.80	0.26	55,65,78,79	0
11	HTH	B	309	10/10	0.81	0.22	76,85,99,104	0
12	TRS	B	311	8/8	0.81	0.15	63,91,103,104	0

Continued on next page...

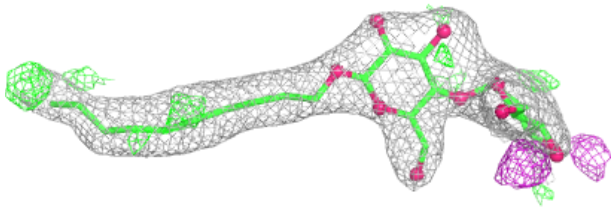
Continued from previous page...

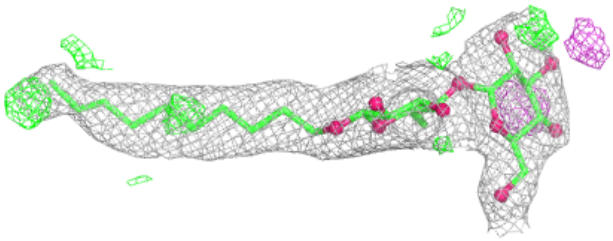
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DMU	A	604	33/33	0.82	0.17	46,68,79,83	33
5	TRD	A	610	7/13	0.82	0.26	58,69,74,78	0
4	DMU	A	601	33/33	0.83	0.15	53,88,122,126	0
5	TRD	A	612	13/13	0.84	0.22	68,80,93,97	0
4	DMU	A	605	33/33	0.84	0.20	56,67,74,79	33
13	K	B	312	1/1	0.84	0.15	123,123,123,123	0
4	DMU	D	301	30/33	0.85	0.14	67,100,113,115	0
4	DMU	A	603	33/33	0.87	0.13	58,73,86,96	0
5	TRD	D	303	9/13	0.90	0.20	83,84,84,88	0
11	HTH	B	308	10/10	0.91	0.22	56,66,77,78	10
4	DMU	A	602	33/33	0.95	0.09	41,54,69,71	0
9	HEA	C	606	60/60	0.96	0.12	50,63,75,81	0
9	HEA	A	618	60/60	0.97	0.08	38,47,61,65	0
9	HEA	C	605	60/60	0.97	0.11	47,63,80,92	0
9	HEA	A	617	60/60	0.98	0.08	34,42,56,73	0
10	CD	B	305	1/1	0.99	0.07	63,63,63,63	0
10	CD	D	306	1/1	0.99	0.06	62,62,62,62	0
8	CA	C	603	1/1	0.99	0.03	69,69,69,69	0
6	CU	A	614	1/1	0.99	0.05	51,51,51,51	0
6	CU	C	604	1/1	0.99	0.03	62,62,62,62	0
7	MG	A	615	1/1	0.99	0.09	37,37,37,37	0
8	CA	A	616	1/1	0.99	0.05	44,44,44,44	0
6	CU	B	307	1/1	1.00	0.02	41,41,41,41	0
7	MG	C	602	1/1	1.00	0.08	46,46,46,46	0
6	CU	B	306	1/1	1.00	0.02	42,42,42,42	0
6	CU	D	307	1/1	1.00	0.04	51,51,51,51	0
6	CU	D	308	1/1	1.00	0.03	53,53,53,53	0

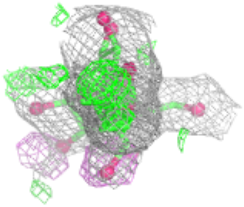
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

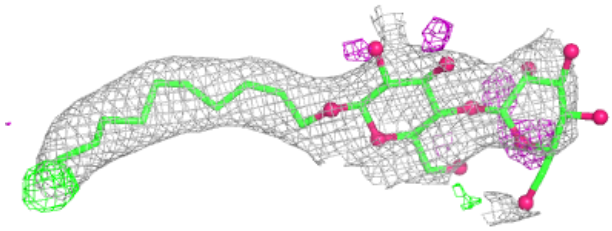


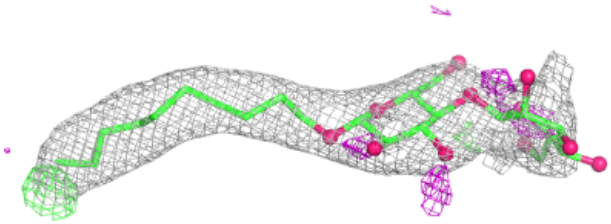


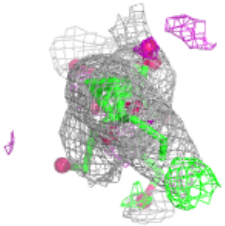


Electron density around DMU A 601:

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

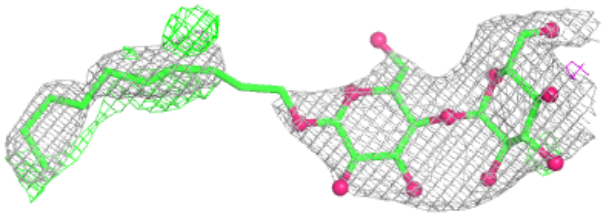


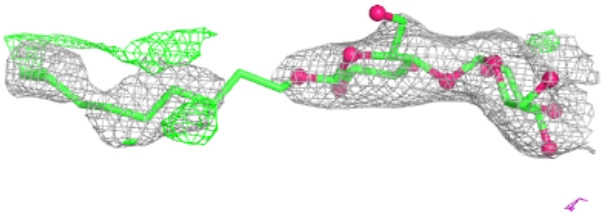


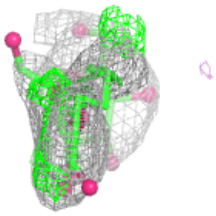


Electron density around DMU A 605:

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

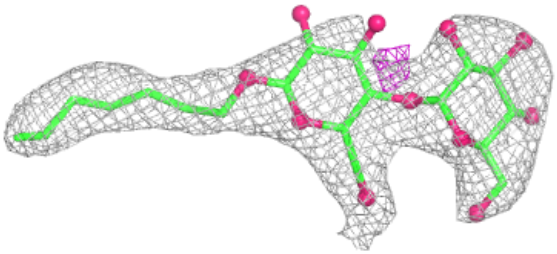


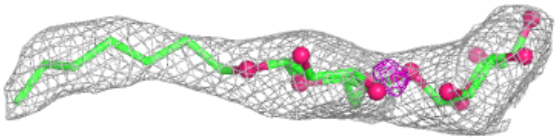


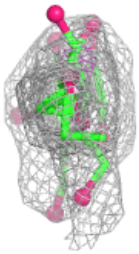


Electron density around DMU D 301:

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

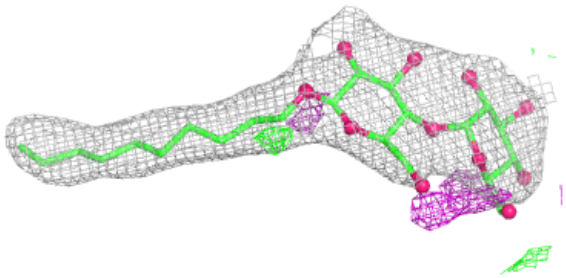


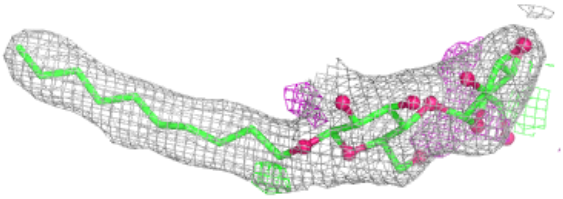


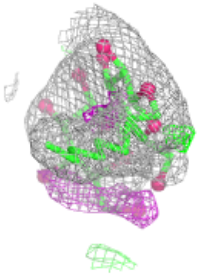


Electron density around DMU A 603:

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

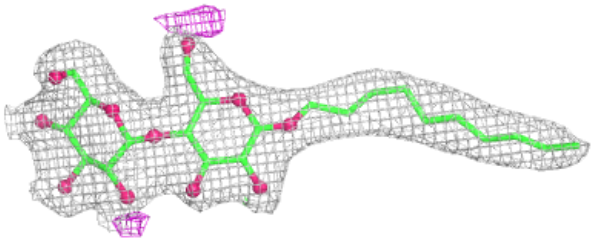


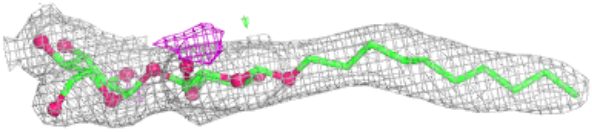




Electron density around DMU A 602:

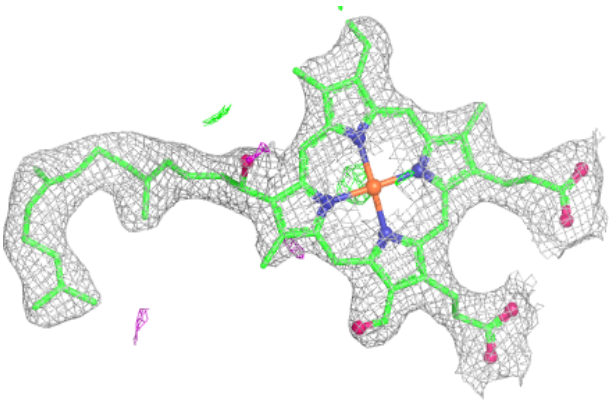
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

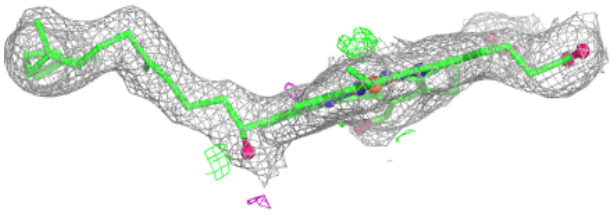


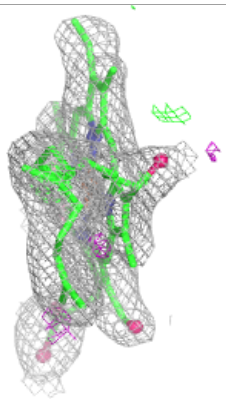


Electron density around HEA C 606:

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

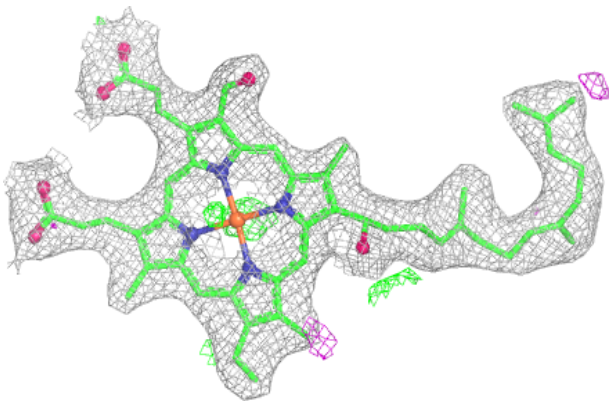


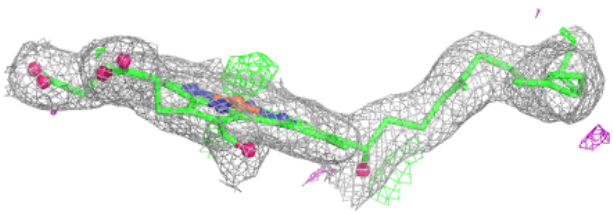




Electron density around HEA A 618:

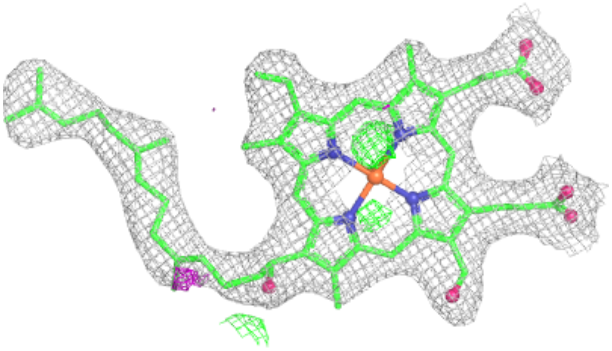
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

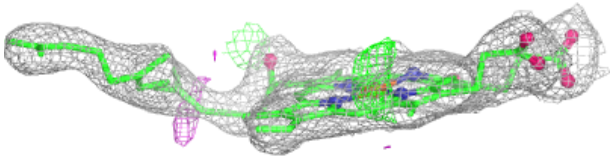


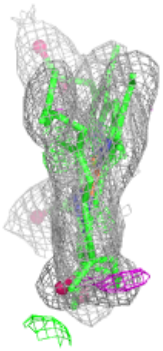


Electron density around HEA C 605:

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

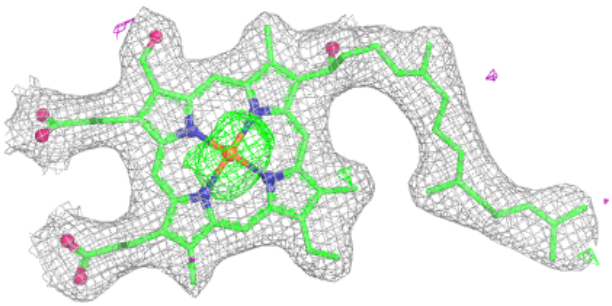


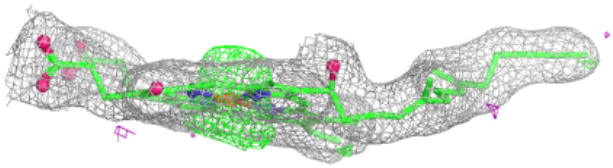




Electron density around HEA A 617:

$2mF_o$-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.