Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 02:45 PM EDT

PDB ID	:	3OMN / pdb_00003omn
Title	:	Catalytic core subunits (I and II) of cytochrome C oxidase from Rhodobacter sphaeroides with D132A mutation in the reduced state
Authors	:	Liu, J.; Qin, L.; Ferguson-Miller, S.
Deposited on	:	2010-08-27
Resolution	:	2.15 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:

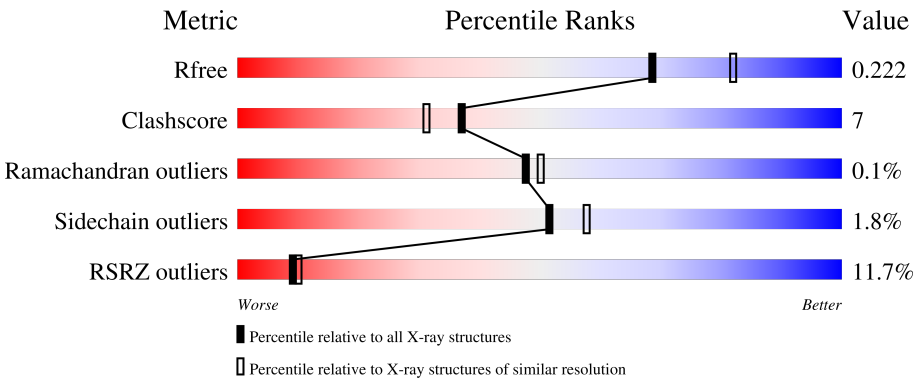
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	7% 88% 11% •
1	C	535	20% 85% 13% • •
2	B	256	4% 95% • •
2	D	256	10% 93% 6% •

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 13755 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, aa3 type, subunit I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	535	4274	2862	673	707	32	0	13	0
1	C	531	4219	2826	663	698	32	0	13	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	ALA	ASP	engineered mutation	UNP Q3J5A7
C	132	ALA	ASP	engineered mutation	UNP Q3J5A7

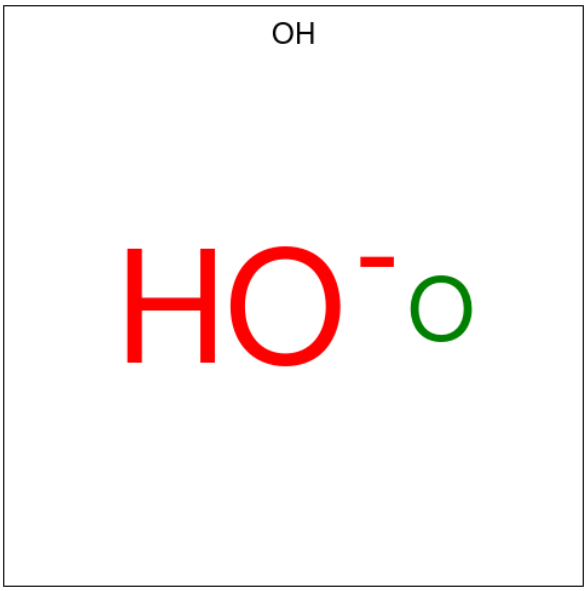
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	256	2021	1319	333	363	6	0	0	0
2	D	256	2015	1316	330	363	6	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

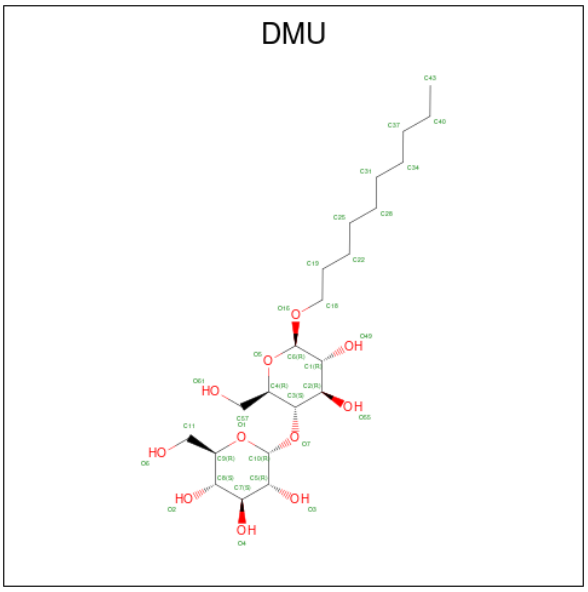
Chain	Residue	Modelled	Actual	Comment	Reference
B	282	HIS	-	expression tag	UNP Q3J5G0
B	283	HIS	-	expression tag	UNP Q3J5G0
B	284	HIS	-	expression tag	UNP Q3J5G0
B	285	HIS	-	expression tag	UNP Q3J5G0
D	282	HIS	-	expression tag	UNP Q3J5G0
D	283	HIS	-	expression tag	UNP Q3J5G0
D	284	HIS	-	expression tag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

- Molecule 3 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



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

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



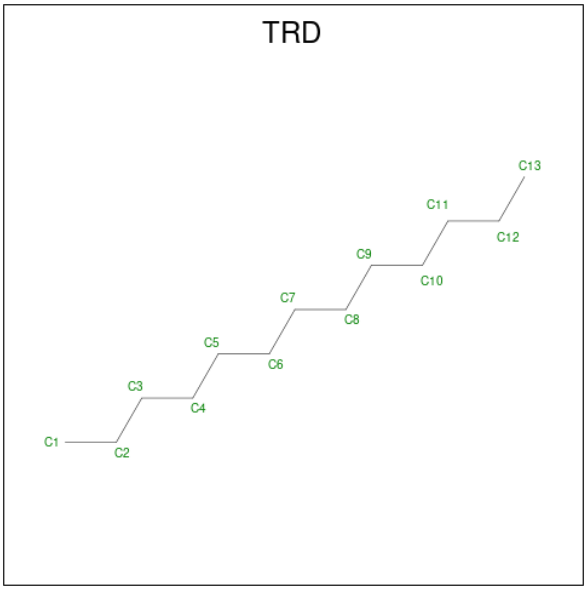
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 22 16 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 21 16 5	0	0
4	B	1	Total C O 33 22 11	0	0
4	B	1	Total C O 33 22 11	0	0
4	B	1	Total C O 33 22 11	0	0
4	B	1	Total C O 23 12 11	0	0
4	C	1	Total C O 23 12 11	0	0
4	C	1	Total C O 23 12 11	0	0
4	C	1	Total C O 33 22 11	0	0
4	D	1	Total C O 23 12 11	0	0
4	D	1	Total C O 23 12 11	0	0

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



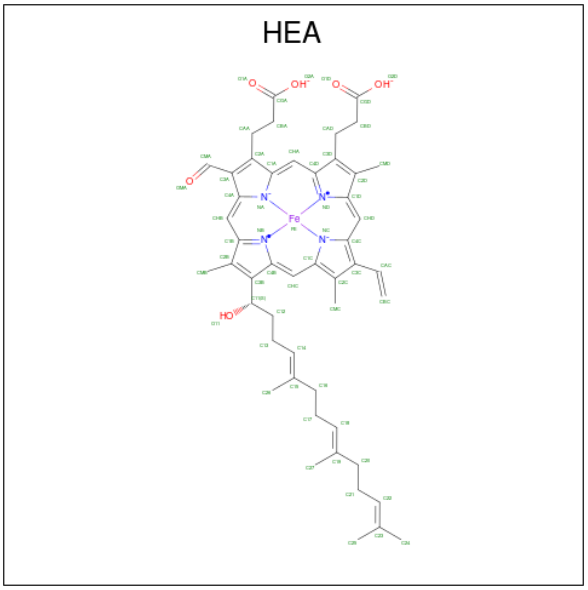
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 7 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
5	A	1	7	7	0	0
			Total	C		
5	A	1	6	6	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	8	8	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	7	7	0	0

- Molecule 6 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		
6	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
6	A	1	120	98	2	8	12	0	1
			Total	C	Fe	N	O		
6	C	1	60	49	1	4	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
6	C	1	120	98	2	8	12	0	1

- Molecule 7 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

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

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

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

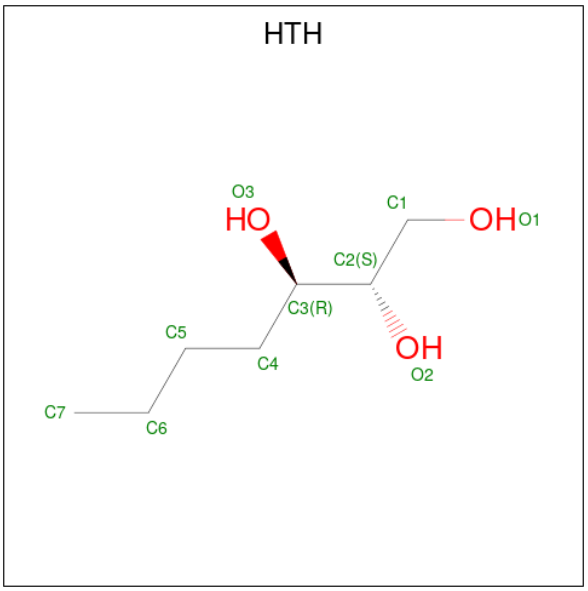
- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 12 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 13 is water.

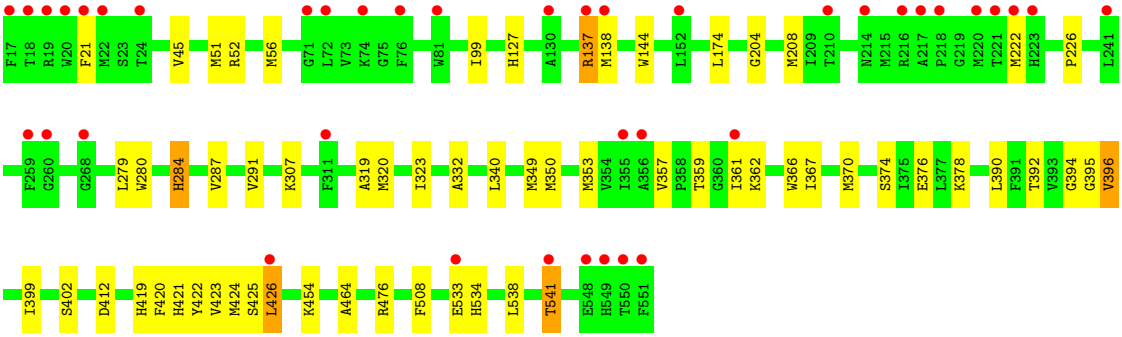
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	132	Total O 133 133	0	1
13	B	128	Total O 128 128	0	0
13	C	88	Total O 88 88	0	0
13	D	112	Total O 112 112	0	0

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.

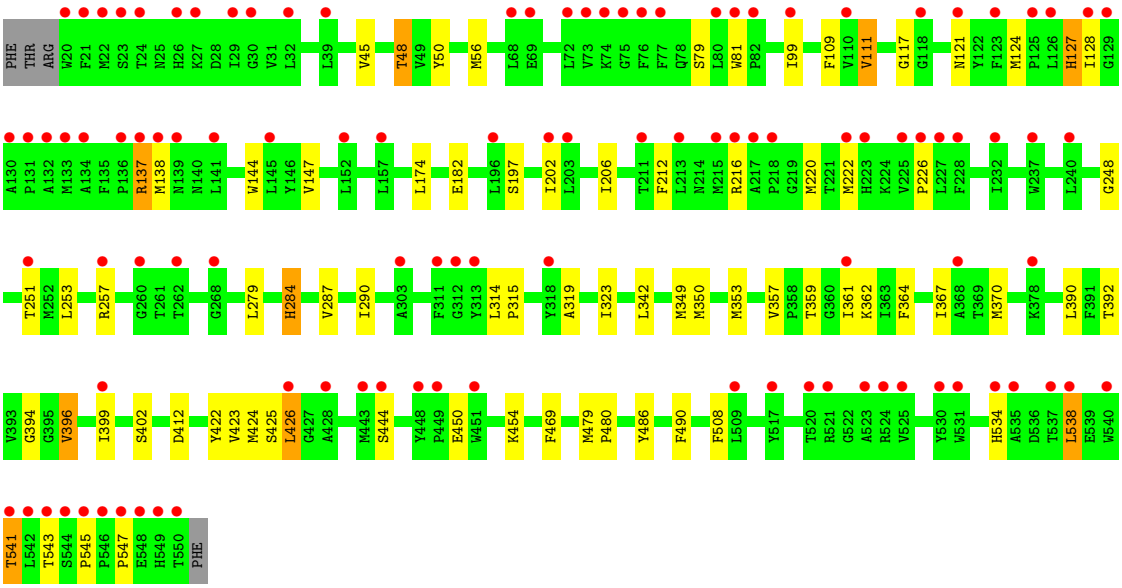
• Molecule 1: Cytochrome c oxidase, aa3 type, subunit I

Chain A:



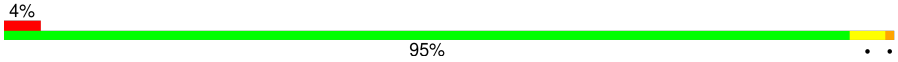
• Molecule 1: Cytochrome c oxidase, aa3 type, subunit I

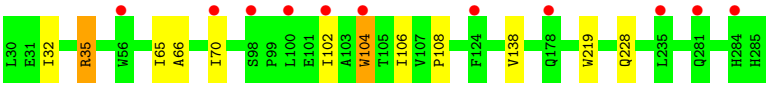
Chain C:



• Molecule 2: Cytochrome c oxidase subunit 2

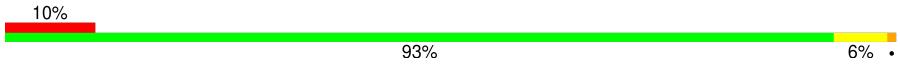
Chain B:

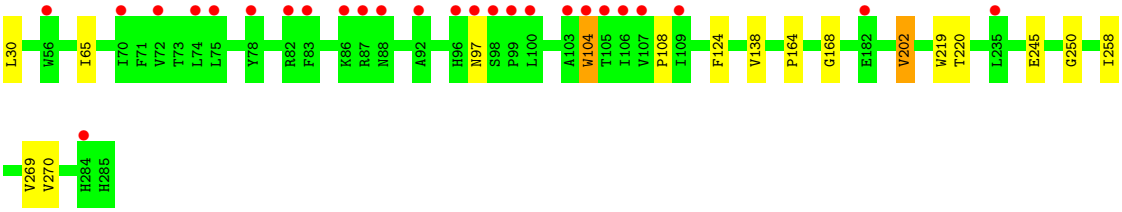




• Molecule 2: Cytochrome c oxidase subunit 2

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	124.67Å 132.03Å 176.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.70 – 2.15 42.70 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.2 (42.70-2.15) 97.2 (42.70-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.16Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.219 0.200 , 0.222	Depositor DCC
R_{free} test set	4627 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13755	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: DMU, CL, CA, HTH, OH, CU1, HEA, CD, MG, TRD

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	0.66	1/4430 (0.0%)	0.88	3/6048 (0.0%)
1	C	0.57	1/4373 (0.0%)	0.90	4/5973 (0.1%)
2	B	0.62	0/2083	0.78	0/2852
2	D	0.57	0/2077	0.79	1/2845 (0.0%)
All	All	0.61	2/12963 (0.0%)	0.86	8/17718 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	534	HIS	ND1-CE1	5.35	1.37	1.32
1	C	127	HIS	ND1-CE1	5.29	1.37	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	284	HIS	N-CA-CB	7.32	117.35	110.39
1	C	127	HIS	CB-CG-CD2	-6.64	122.56	131.20
1	A	534	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	C	127	HIS	CB-CG-ND1	5.70	131.25	122.70
1	A	534	HIS	CB-CG-ND1	5.64	131.16	122.70
2	D	258	ILE	N-CA-C	5.57	116.30	110.62
1	A	284	HIS	N-CA-CB	5.32	117.78	110.11
1	C	538	LEU	N-CA-C	5.24	117.74	111.71

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	4274	0	4182	71	0
1	C	4219	0	4120	88	0
2	B	2021	0	1978	11	0
2	D	2015	0	1967	15	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	43	0	61	2	0
4	B	122	0	147	0	0
4	C	79	0	84	2	0
4	D	46	0	42	1	0
5	A	46	0	90	2	0
5	B	8	0	12	0	0
5	C	13	0	28	1	0
5	D	20	0	41	0	0
6	A	180	0	162	20	0
6	C	180	0	162	21	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	1	0	0	0	0
10	C	1	0	0	0	0
11	B	10	0	16	0	0
12	B	2	0	0	0	0
12	D	2	0	0	0	0
13	A	133	0	0	1	0
13	B	128	0	0	2	0
13	C	88	0	0	1	0
13	D	112	0	0	1	0
All	All	13755	0	13092	186	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 7.

All (186) 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:137:ARG:HG3	1:A:137:ARG:HH11	1.03	1.17
1:A:357:VAL:O	1:A:361[B]:ILE:HG12	1.52	1.07
1:C:422[A]:TYR:HA	1:C:426[A]:LEU:HG	1.41	1.00
1:C:422[A]:TYR:CD2	1:C:426[A]:LEU:HD12	1.97	0.99
1:C:137:ARG:HH11	1:C:137:ARG:HG3	1.30	0.93
1:C:48:THR:HG23	6:C:1:HEA:HMB2	1.49	0.93
1:A:390:LEU:HD13	1:A:426[A]:LEU:HB3	1.50	0.92
1:C:390:LEU:HD13	1:C:426[A]:LEU:HB3	1.52	0.91
1:A:137:ARG:HG3	1:A:137:ARG:NH1	1.83	0.91
1:A:137:ARG:HH11	1:A:137:ARG:CG	1.85	0.90
1:C:357:VAL:O	1:C:361[B]:ILE:HG12	1.74	0.88
1:C:422[A]:TYR:CE2	1:C:426[A]:LEU:HD12	2.11	0.84
1:A:21:PHE:HB3	1:A:144:TRP:HZ2	1.41	0.83
2:B:228:GLN:NE2	13:B:777:HOH:O	2.12	0.82
1:C:137:ARG:HH11	1:C:137:ARG:CG	1.95	0.80
1:A:426[A]:LEU:CD2	1:A:464:ALA:HB1	2.13	0.78
1:C:422[A]:TYR:O	1:C:426[A]:LEU:HB2	1.82	0.78
1:A:137:ARG:HD2	1:A:138:MET:H	1.47	0.78
1:A:425[A]:SER:C	1:A:426[A]:LEU:HD23	2.09	0.78
2:B:66:ALA:O	2:B:70:ILE:HG12	1.86	0.74
1:C:48:THR:HG21	6:C:1:HEA:O11	1.86	0.74
1:C:182:GLU:O	1:C:257:ARG:NH1	2.22	0.73
1:C:422[A]:TYR:HA	1:C:426[A]:LEU:CG	2.20	0.72
1:A:422[A]:TYR:CD2	1:A:426[A]:LEU:HD12	2.26	0.71
1:C:56:MET:HE1	4:C:10:DMU:H6	1.73	0.70
6:C:1:HEA:HBC1	6:C:1:HEA:HMC3	1.72	0.70
2:B:32:ILE:HG22	2:B:35:ARG:HD3	1.72	0.70
1:C:287:VAL:HB	6:C:2[B]:HEA:HAC	1.75	0.69
6:A:1:HEA:HBC1	6:A:1:HEA:HMC3	1.75	0.68
1:A:426[A]:LEU:HD21	1:A:464:ALA:HB1	1.76	0.68
1:A:287:VAL:HB	6:A:2[B]:HEA:HAC	1.75	0.67
1:C:144:TRP:CE3	1:C:147:VAL:HG11	2.30	0.67
1:C:534:HIS:HD2	13:C:629:HOH:O	1.78	0.66
1:C:48:THR:CG2	6:C:1:HEA:HMB2	2.25	0.66
1:A:426[A]:LEU:HD22	1:A:464:ALA:HB1	1.78	0.66
6:C:2[B]:HEA:HMD1	6:C:2[B]:HEA:HBD2	1.77	0.65
1:A:402:SER:HA	6:A:2[B]:HEA:OMA	1.96	0.65
1:C:425[A]:SER:C	1:C:426[A]:LEU:HD23	2.22	0.65
1:A:21:PHE:HB3	1:A:144:TRP:CZ2	2.30	0.65
1:A:396:VAL:HG13	2:B:65:ILE:HB	1.78	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:MET:HG3	1:A:362[B]:LYS:HE3	1.81	0.63
1:C:137:ARG:HG3	1:C:137:ARG:NH1	2.09	0.63
1:C:350:MET:HA	1:C:353:MET:HE3	1.81	0.63
1:C:137:ARG:HD2	1:C:138:MET:H	1.64	0.62
1:A:399:ILE:HD13	6:A:2[B]:HEA:HMB2	1.82	0.61
1:C:222:MET:HE3	1:C:222:MET:HA	1.83	0.61
2:D:202:VAL:HG23	2:D:270:VAL:O	2.01	0.61
1:C:144:TRP:HE3	1:C:147:VAL:HG11	1.66	0.61
1:C:359[A]:THR:HG21	6:C:2[A]:HEA:C14	2.30	0.61
1:C:424[A]:MET:HG2	6:C:2[A]:HEA:CBC	2.30	0.61
1:C:396:VAL:HG13	2:D:65:ILE:HB	1.83	0.61
1:A:422[A]:TYR:HA	1:A:426[A]:LEU:HG	1.83	0.60
1:C:248:GLY:O	1:C:251:THR:HG22	2.01	0.60
1:A:137:ARG:HD2	1:A:138:MET:N	2.15	0.60
1:A:424[A]:MET:HG2	6:A:2[A]:HEA:CBC	2.31	0.60
4:D:8:DMU:H35	4:D:8:DMU:H29	1.82	0.59
1:C:424[A]:MET:HG2	6:C:2[A]:HEA:HBC2	1.84	0.59
1:A:350:MET:HA	1:A:353:MET:HE3	1.84	0.58
1:C:319:ALA:HB3	1:C:362[B]:LYS:HE2	1.85	0.58
2:D:202:VAL:CG2	2:D:245:GLU:HG2	2.33	0.58
1:C:349:MET:HG2	1:C:353:MET:HE2	1.84	0.58
1:C:394:GLY:HA3	1:C:423[A]:VAL:HG13	1.86	0.58
1:A:361[B]:ILE:HD11	2:B:108:PRO:HG2	1.86	0.57
1:C:137:ARG:CG	1:C:137:ARG:NH1	2.64	0.56
1:C:392:THR:HG23	6:C:2[B]:HEA:H171	1.87	0.56
1:C:394:GLY:C	1:C:423[B]:VAL:HG13	2.29	0.56
1:C:284:HIS:O	1:C:287:VAL:HG22	2.03	0.56
1:C:253:LEU:O	1:C:257:ARG:HG3	2.06	0.56
1:A:425[A]:SER:O	1:A:426[A]:LEU:HD23	2.05	0.55
1:A:422[A]:TYR:CE2	1:A:426[A]:LEU:HD12	2.42	0.55
1:A:424[A]:MET:HG2	6:A:2[A]:HEA:HBC2	1.89	0.55
1:C:543:THR:HG23	1:C:545:PRO:O	2.07	0.55
1:A:538:LEU:O	1:A:541:THR:HB	2.06	0.55
6:C:1:HEA:HBC1	6:C:1:HEA:CMC	2.37	0.55
1:C:50:TYR:OH	1:C:79:SER:HB2	2.06	0.54
1:A:56:MET:HE1	4:A:1005:DMU:H6	1.87	0.54
1:A:399:ILE:HD13	6:A:2[B]:HEA:CMB	2.37	0.54
1:C:284:HIS:CD2	1:C:284:HIS:C	2.85	0.54
1:C:422[A]:TYR:HA	1:C:426[A]:LEU:HB2	1.88	0.54
1:A:307:LYS:HE2	1:A:374:SER:HB3	1.90	0.53
1:C:399:ILE:HD13	6:C:2[B]:HEA:HMB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:ILE:HG13	6:C:2[A]:HEA:H242	1.89	0.53
1:C:111:VAL:HG11	1:C:290:ILE:HG23	1.89	0.53
1:A:284:HIS:C	1:A:284:HIS:CD2	2.87	0.53
1:A:396:VAL:CG1	2:B:65:ILE:HB	2.38	0.53
1:A:454:LYS:HE3	13:A:758:HOH:O	2.07	0.53
1:C:394:GLY:CA	1:C:422[B]:TYR:HB3	2.39	0.52
1:C:396:VAL:CG1	2:D:65:ILE:HB	2.39	0.52
1:C:124:MET:CE	1:C:212:PHE:HD2	2.22	0.52
2:B:35:ARG:HD2	13:B:743:HOH:O	2.10	0.52
1:A:419[B]:HIS:CE1	1:A:423[B]:VAL:HG21	2.45	0.52
1:A:51:MET:HE3	1:A:99:ILE:HG22	1.92	0.52
1:A:350:MET:HA	1:A:353:MET:CE	2.39	0.51
1:A:392:THR:HG23	6:A:2[B]:HEA:H171	1.93	0.51
1:A:533:GLU:H	1:A:533:GLU:CD	2.19	0.51
1:C:361[B]:ILE:HD11	2:D:108:PRO:HG2	1.92	0.51
1:C:128:ILE:HA	1:C:220:MET:HE2	1.92	0.50
1:C:422[A]:TYR:CA	1:C:426[A]:LEU:HB2	2.41	0.50
1:C:127:HIS:HB3	1:C:226:PRO:HG2	1.94	0.50
1:C:444:SER:HA	4:C:9:DMU:H5	1.94	0.50
1:A:476:ARG:HH21	5:A:3:TRD:H31	1.77	0.49
1:A:399:ILE:HG13	6:A:2[A]:HEA:H242	1.93	0.49
1:A:394:GLY:HA3	1:A:423[A]:VAL:HG13	1.94	0.49
1:C:402:SER:HA	6:C:2[B]:HEA:OMA	2.12	0.49
1:A:359[A]:THR:HG21	6:A:2[A]:HEA:H14	1.93	0.49
1:C:367:ILE:HA	1:C:370:MET:CE	2.42	0.49
1:A:45:VAL:HG21	6:A:1:HEA:H171	1.95	0.49
1:A:137:ARG:NH1	1:A:137:ARG:CG	2.55	0.49
1:C:422[A]:TYR:HA	1:C:426[A]:LEU:CB	2.43	0.49
1:C:202:ILE:O	1:C:206:ILE:HG12	2.13	0.48
1:C:350:MET:HA	1:C:353:MET:CE	2.42	0.48
1:C:538:LEU:O	1:C:541:THR:HB	2.14	0.48
2:D:202:VAL:HG21	2:D:245:GLU:HG2	1.93	0.48
1:A:395:GLY:O	6:A:2[B]:HEA:H121	2.12	0.48
1:C:124:MET:HE2	1:C:212:PHE:HD2	1.79	0.48
1:A:279:LEU:C	1:A:279:LEU:HD13	2.39	0.47
2:B:102:ILE:O	2:B:106:ILE:HG12	2.13	0.47
1:C:422[A]:TYR:C	1:C:426[A]:LEU:HB2	2.39	0.47
1:C:508:PHE:HB2	6:C:1:HEA:H261	1.97	0.47
2:D:30:LEU:N	13:D:728:HOH:O	2.47	0.47
1:C:128:ILE:HB	1:C:216:ARG:HB3	1.95	0.47
1:A:127:HIS:HB3	1:A:226:PRO:HG2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:THR:HG22	1:C:547:PRO:HD3	1.97	0.47
1:A:508:PHE:HB2	6:A:1:HEA:H261	1.97	0.47
1:C:45:VAL:HG21	6:C:1:HEA:H171	1.96	0.47
6:A:2[B]:HEA:HMD1	6:A:2[B]:HEA:HBD2	1.97	0.47
1:A:332:ALA:HB1	1:A:340:LEU:HD11	1.97	0.46
1:C:422[A]:TYR:O	1:C:426[A]:LEU:C	2.58	0.46
1:C:359[A]:THR:HG22	6:C:2[A]:HEA:H172	1.98	0.46
1:C:117:GLY:O	1:C:121:ASN:HB2	2.15	0.46
1:C:361[B]:ILE:O	1:C:364:PHE:N	2.46	0.46
1:A:204:GLY:O	1:A:208:MET:HG2	2.16	0.46
1:C:396:VAL:HG13	2:D:65:ILE:HD12	1.98	0.46
2:B:138:VAL:HG11	2:B:219:TRP:CD1	2.51	0.45
1:C:144:TRP:O	1:C:147:VAL:HG12	2.17	0.45
1:A:395:GLY:N	1:A:423[B]:VAL:HG13	2.31	0.45
1:A:319:ALA:HB3	1:A:362[B]:LYS:HE2	1.97	0.45
4:A:1005:DMU:H8	5:A:553:TRD:H71	1.99	0.45
1:A:396:VAL:HG13	2:B:65:ILE:HD12	1.98	0.44
1:C:422[A]:TYR:O	1:C:426[A]:LEU:CB	2.61	0.44
1:A:349:MET:HG2	1:A:353:MET:HE2	1.98	0.44
1:C:342:LEU:HD21	2:D:124:PHE:CD2	2.52	0.44
1:A:426[A]:LEU:HD22	1:A:464:ALA:CB	2.47	0.44
1:A:287:VAL:HB	6:A:2[A]:HEA:CAC	2.47	0.44
6:C:2[B]:HEA:HBD2	6:C:2[B]:HEA:CMD	2.46	0.44
1:C:81:TRP:CZ2	5:C:552:TRD:H92	2.54	0.43
1:C:422[A]:TYR:OH	1:C:469:PHE:HB2	2.19	0.43
1:C:314:LEU:HB3	1:C:315:PRO:HD3	2.00	0.43
2:D:202:VAL:HG21	2:D:245:GLU:CG	2.48	0.43
1:A:362[A]:LYS:HD3	1:A:366:TRP:CH2	2.54	0.43
6:A:2[B]:HEA:H18	6:A:2[B]:HEA:H212	1.78	0.43
1:A:280:TRP:CH2	6:A:2[A]:HEA:HBD1	2.54	0.43
1:C:367:ILE:HA	1:C:370:MET:HE3	2.00	0.43
2:D:104:TRP:CD1	2:D:104:TRP:C	2.96	0.43
1:A:420:PHE:HA	1:A:423[A]:VAL:HG22	2.00	0.43
1:C:349:MET:O	1:C:353:MET:HG3	2.18	0.43
1:A:349:MET:O	1:A:353:MET:HG3	2.19	0.43
2:D:138:VAL:HG11	2:D:219:TRP:CD1	2.54	0.43
1:A:280:TRP:HH2	6:A:2[A]:HEA:HBD1	1.83	0.42
1:A:320:MET:CG	1:A:362[B]:LYS:HE3	2.49	0.42
1:A:394:GLY:CA	1:A:422[B]:TYR:HB3	2.50	0.42
1:C:392:THR:O	1:C:396:VAL:HB	2.19	0.42
1:A:376:GLU:HG2	1:A:378:LYS:HG2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1:HEA:HBC1	6:A:1:HEA:CMC	2.46	0.42
1:C:399:ILE:HD13	6:C:2[B]:HEA:CMB	2.50	0.42
2:D:164:PRO:HA	2:D:168:GLY:O	2.20	0.42
2:D:202:VAL:HG22	2:D:269:VAL:HG12	2.02	0.42
1:A:426[A]:LEU:HD23	1:A:426[A]:LEU:N	2.35	0.42
1:C:323:ILE:HD11	1:C:359[B]:THR:HA	2.02	0.42
1:C:450:GLU:HG3	1:C:454:LYS:HE2	2.02	0.42
2:B:104:TRP:CD1	2:B:104:TRP:C	2.98	0.42
2:D:220:THR:O	2:D:250:GLY:HA3	2.20	0.42
1:C:144:TRP:HA	1:C:147:VAL:HG12	2.01	0.42
1:C:424[A]:MET:HE2	6:C:2[A]:HEA:HMD2	2.02	0.41
1:C:399:ILE:HG13	6:C:2[A]:HEA:C24	2.50	0.41
1:A:421:HIS:HA	1:A:425[B]:SER:HB2	2.02	0.41
1:C:109:PHE:CE1	1:C:197:SER:HB2	2.55	0.41
1:A:323:ILE:HD11	1:A:359[B]:THR:HA	2.03	0.41
1:A:350:MET:HG2	1:A:353:MET:CE	2.51	0.41
1:A:422[A]:TYR:O	1:A:426[A]:LEU:HB2	2.21	0.41
1:C:350:MET:HG2	1:C:353:MET:CE	2.50	0.41
1:C:479:MET:HA	1:C:480:PRO:HD3	1.95	0.41
1:C:486:TYR:CD2	1:C:490:PHE:HB2	2.56	0.41
1:A:367:ILE:HA	1:A:370:MET:HE2	2.02	0.40
1:C:426[A]:LEU:HD23	1:C:426[A]:LEU:N	2.36	0.40
1:A:399:ILE:HA	6:A:2[B]:HEA:HMB2	2.03	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	546/535 (102%)	533 (98%)	13 (2%)	0	100 100
1	C	542/535 (101%)	526 (97%)	16 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	254/256 (99%)	246 (97%)	8 (3%)	0	100	100
2	D	254/256 (99%)	248 (98%)	5 (2%)	1 (0%)	30	26
All	All	1596/1582 (101%)	1553 (97%)	42 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	97	ASN

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	437/434 (101%)	427 (98%)	10 (2%)	44	49
1	C	430/434 (99%)	419 (97%)	11 (3%)	40	43
2	B	214/215 (100%)	212 (99%)	2 (1%)	70	77
2	D	213/215 (99%)	211 (99%)	2 (1%)	70	77
All	All	1294/1298 (100%)	1269 (98%)	25 (2%)	51	56

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	137	ARG
1	A	174	LEU
1	A	222	MET
1	A	291	VAL
1	A	396	VAL
1	A	412	ASP
1	A	426[A]	LEU
1	A	426[B]	LEU
1	A	541	THR
2	B	35	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	104	TRP
1	C	48	THR
1	C	99	ILE
1	C	111	VAL
1	C	137	ARG
1	C	174	LEU
1	C	279	LEU
1	C	396	VAL
1	C	412	ASP
1	C	426[A]	LEU
1	C	426[B]	LEU
1	C	541	THR
2	D	104	TRP
2	D	202	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	139	ASN
2	B	53	GLN
2	B	96	HIS
2	B	125	ASN
2	B	170	ASN
2	B	203	ASN
2	B	251	GLN
1	C	25	ASN
1	C	78	GLN
1	C	91	ASN
1	C	163	ASN
1	C	165	GLN
1	C	214	ASN
2	D	96	HIS
2	D	170	ASN
2	D	251	GLN

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)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 45 ligands modelled in this entry, 2 are modelled with single atom and 16 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	$\#\|Z\| > 2$
5	TRD	A	3	-	12,12,12	0.28	0	11,11,11	0.51	0
4	DMU	C	9	-	24,24,34	0.57	0	35,35,45	0.88	2 (5%)
6	HEA	C	2[B]	13,1	67,67,67	1.67	8 (11%)	81,103,103	1.48	15 (18%)
6	HEA	C	1	1	67,67,67	1.42	8 (11%)	81,103,103	1.45	14 (17%)
6	HEA	C	2[A]	13,1	67,67,67	1.50	8 (11%)	81,103,103	1.36	11 (13%)
5	TRD	A	1013	-	6,6,12	0.25	0	5,5,11	0.47	0
5	TRD	A	1009	-	6,6,12	0.26	0	5,5,11	0.39	0
4	DMU	D	8	-	24,24,34	0.53	0	35,35,45	0.61	0
11	HTH	B	286	-	9,9,9	0.41	0	10,10,10	0.84	0
4	DMU	B	1	-	34,34,34	0.49	0	45,45,45	0.89	2 (4%)
4	DMU	C	10	-	34,34,34	0.59	0	45,45,45	0.80	1 (2%)
4	DMU	D	4	-	24,24,34	0.51	0	35,35,45	0.63	0
4	DMU	B	3	-	34,34,34	0.56	0	45,45,45	0.59	0
6	HEA	A	2[B]	13,1	67,67,67	1.72	8 (11%)	81,103,103	1.51	16 (19%)
4	DMU	B	2	-	34,34,34	0.53	0	45,45,45	0.77	1 (2%)
5	TRD	A	552	-	5,5,12	0.33	0	4,4,11	0.33	0
5	TRD	A	553	-	12,12,12	0.23	0	11,11,11	0.52	0
6	HEA	A	2[A]	13,1	67,67,67	1.56	7 (10%)	81,103,103	1.39	11 (13%)
5	TRD	B	4	-	7,7,12	0.25	0	6,6,11	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	TRD	D	14	-	6,6,12	0.25	0	5,5,11	0.37	0
4	DMU	C	5	-	24,24,34	0.51	0	35,35,45	0.61	0
5	TRD	C	552	-	12,12,12	0.23	0	11,11,11	0.56	0
5	TRD	D	3	-	12,12,12	0.18	0	11,11,11	0.66	0
4	DMU	B	6	-	24,24,34	0.54	0	35,35,45	0.68	0
6	HEA	A	1	1	67,67,67	1.42	8 (11%)	81,103,103	1.53	18 (22%)
4	DMU	A	7	-	21,21,34	0.60	0	24,25,45	1.09	2 (8%)
4	DMU	A	1005	-	22,22,34	0.56	0	27,27,45	0.93	1 (3%)

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	3	-	-	2/10/10/10	-
4	DMU	C	9	-	-	4/8/48/59	0/2/2/2
6	HEA	C	2[B]	13,1	-	12/36/76/76	-
6	HEA	C	1	1	-	5/36/76/76	-
6	HEA	C	2[A]	13,1	-	5/36/76/76	-
5	TRD	A	1013	-	-	1/4/4/10	-
5	TRD	A	1009	-	-	1/4/4/10	-
4	DMU	D	8	-	-	2/8/48/59	0/2/2/2
11	HTH	B	286	-	-	5/10/10/10	-
4	DMU	B	1	-	-	1/19/59/59	0/2/2/2
4	DMU	C	10	-	-	10/19/59/59	0/2/2/2
4	DMU	D	4	-	-	0/8/48/59	0/2/2/2
4	DMU	B	3	-	-	6/19/59/59	0/2/2/2
6	HEA	A	2[B]	13,1	-	12/36/76/76	-
4	DMU	B	2	-	-	8/19/59/59	0/2/2/2
5	TRD	A	552	-	-	0/3/3/10	-
5	TRD	A	553	-	-	6/10/10/10	-
6	HEA	A	2[A]	13,1	-	11/36/76/76	-
5	TRD	B	4	-	-	4/5/5/10	-
5	TRD	D	14	-	-	1/4/4/10	-
4	DMU	C	5	-	-	2/8/48/59	0/2/2/2
5	TRD	C	552	-	-	4/10/10/10	-
5	TRD	D	3	-	-	9/10/10/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMU	B	6	-	-	2/8/48/59	0/2/2/2
6	HEA	A	1	1	-	7/36/76/76	-
4	DMU	A	7	-	-	6/13/29/59	0/1/1/2
4	DMU	A	1005	-	-	3/13/33/59	0/1/1/2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2[B]	HEA	FE-ND	8.70	2.21	1.94
6	A	2[A]	HEA	FE-NB	6.99	2.16	1.94
6	C	2[B]	HEA	FE-NB	6.61	2.15	1.94
6	C	1	HEA	FE-NA	6.55	2.16	1.95
6	A	2[B]	HEA	FE-NA	5.47	2.13	1.95
6	C	2[A]	HEA	FE-NC	5.47	2.13	1.95
6	A	2[A]	HEA	FE-NC	5.27	2.12	1.95
6	C	2[B]	HEA	FE-ND	5.25	2.11	1.94
6	A	1	HEA	FE-NA	5.24	2.12	1.95
6	C	2[B]	HEA	FE-NC	5.15	2.12	1.95
6	A	2[A]	HEA	C11-C3B	4.50	1.56	1.51
6	C	2[A]	HEA	FE-ND	4.47	2.08	1.94
6	C	2[A]	HEA	C11-C3B	4.39	1.56	1.51
6	C	2[A]	HEA	FE-NB	4.36	2.08	1.94
6	C	1	HEA	FE-NC	4.33	2.09	1.95
6	A	2[B]	HEA	FE-NC	4.20	2.09	1.95
6	A	1	HEA	FE-NC	4.17	2.08	1.95
6	C	2[B]	HEA	C11-C3B	4.13	1.56	1.51
6	C	2[B]	HEA	FE-NA	4.06	2.08	1.95
6	A	1	HEA	FE-NB	3.76	2.06	1.94
6	A	1	HEA	FE-ND	3.72	2.06	1.94
6	A	2[B]	HEA	C11-C3B	3.67	1.55	1.51
6	C	1	HEA	C11-C3B	3.00	1.55	1.51
6	A	2[A]	HEA	CMA-C3A	2.83	1.51	1.45
6	C	2[A]	HEA	CMA-C3A	2.78	1.51	1.45
6	A	2[A]	HEA	CAC-C3C	2.69	1.54	1.47
6	A	2[A]	HEA	FE-NA	2.64	2.03	1.95
6	A	1	HEA	CAC-C3C	2.63	1.54	1.47
6	C	2[A]	HEA	FE-NA	2.63	2.03	1.95
6	C	2[A]	HEA	CAC-C3C	2.59	1.54	1.47
6	C	2[B]	HEA	CAC-C3C	2.59	1.54	1.47
6	A	2[B]	HEA	CMA-C3A	2.58	1.51	1.45
6	C	2[B]	HEA	CMA-C3A	2.57	1.51	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1	HEA	FE-ND	2.54	2.02	1.94
6	A	2[B]	HEA	FE-NB	2.49	2.02	1.94
6	A	1	HEA	C11-C3B	2.45	1.54	1.51
6	A	1	HEA	CMA-C3A	2.45	1.50	1.45
6	A	2[B]	HEA	CAC-C3C	2.42	1.53	1.47
6	C	1	HEA	CMA-C3A	2.38	1.50	1.45
6	C	1	HEA	CAC-C3C	2.32	1.53	1.47
6	A	1	HEA	CMD-C2D	2.30	1.55	1.50
6	A	2[B]	HEA	CMD-C2D	2.28	1.55	1.50
6	C	2[B]	HEA	CMD-C2D	2.20	1.55	1.50
6	C	1	HEA	CMD-C2D	2.19	1.55	1.50
6	A	2[A]	HEA	CMD-C2D	2.18	1.55	1.50
6	C	2[A]	HEA	CMD-C2D	2.13	1.55	1.50
6	C	1	HEA	CMC-C2C	2.04	1.54	1.50

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2[B]	HEA	C3C-C4C-NC	-4.41	106.08	109.80
6	C	1	HEA	C2A-C1A-NA	-4.18	106.29	110.32
6	C	2[B]	HEA	C3C-C4C-NC	-3.64	106.73	109.80
6	A	2[A]	HEA	CAD-CBD-CGD	-3.61	104.10	113.67
6	A	1	HEA	C4B-NB-C1B	3.51	109.36	105.21
6	C	2[B]	HEA	C4B-NB-C1B	3.41	109.25	105.21
6	C	2[A]	HEA	C2A-C1A-NA	-3.41	107.03	110.32
4	A	7	DMU	O16-C6-C1	3.37	113.38	108.27
6	A	1	HEA	C3D-C4D-ND	-3.26	107.20	110.35
6	A	2[B]	HEA	C1D-ND-C4D	3.21	109.00	105.21
6	C	2[B]	HEA	C1D-ND-C4D	3.19	108.98	105.21
6	A	2[A]	HEA	C4B-NB-C1B	3.16	108.95	105.21
6	A	1	HEA	C1D-ND-C4D	3.12	108.91	105.21
6	A	2[B]	HEA	C4B-NB-C1B	3.03	108.80	105.21
6	C	2[A]	HEA	C27-C19-C20	3.01	120.45	115.23
6	A	1	HEA	C2A-C1A-NA	-2.96	107.46	110.32
6	C	2[A]	HEA	CAD-CBD-CGD	-2.96	105.83	113.67
6	A	1	HEA	C17-C18-C19	-2.94	120.89	127.62
6	A	1	HEA	C27-C19-C20	2.90	120.26	115.23
6	A	2[A]	HEA	C2A-C1A-NA	-2.87	107.55	110.32
6	C	1	HEA	C3D-C4D-ND	-2.87	107.58	110.35
6	A	2[A]	HEA	C27-C19-C20	2.85	120.18	115.23
6	C	1	HEA	C13-C14-C15	-2.85	121.11	127.62
6	C	2[A]	HEA	C1D-ND-C4D	2.80	108.52	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2[B]	HEA	C2A-C1A-NA	-2.79	107.63	110.32
6	C	2[B]	HEA	C2A-C1A-NA	-2.79	107.63	110.32
6	C	2[A]	HEA	C3D-C4D-ND	-2.78	107.66	110.35
6	A	2[B]	HEA	C2D-C1D-ND	-2.76	106.67	109.84
6	A	2[A]	HEA	C1D-ND-C4D	2.75	108.47	105.21
6	C	2[B]	HEA	C17-C18-C19	-2.75	121.33	127.62
6	C	2[A]	HEA	C4B-NB-C1B	2.75	108.46	105.21
6	C	2[B]	HEA	C2B-C1B-NB	-2.73	106.75	109.90
6	A	1	HEA	C3C-C4C-NC	-2.73	107.50	109.80
6	A	2[B]	HEA	C26-C15-C16	2.70	119.92	115.23
6	C	2[B]	HEA	C26-C15-C16	2.68	119.88	115.23
6	A	2[A]	HEA	C3D-C4D-ND	-2.65	107.79	110.35
6	C	1	HEA	C4A-NA-C1A	2.65	110.15	105.82
4	B	2	DMU	O16-C6-C1	2.62	112.25	108.27
6	A	1	HEA	C3B-C4B-NB	-2.62	106.83	109.84
6	C	2[B]	HEA	CMB-C2B-C3B	-2.57	125.30	130.28
6	A	1	HEA	C13-C14-C15	-2.56	121.75	127.62
6	C	2[B]	HEA	C2D-C1D-ND	-2.56	106.89	109.84
6	A	2[A]	HEA	C2B-C1B-NB	-2.55	106.96	109.90
6	A	1	HEA	C12-C11-C3B	-2.52	108.19	112.12
4	A	7	DMU	C18-O16-C6	-2.50	109.40	113.68
6	A	1	HEA	CHC-C4B-NB	2.50	127.45	124.37
6	A	2[B]	HEA	CMB-C2B-C3B	-2.49	125.46	130.28
6	A	2[B]	HEA	C4C-NC-C1C	2.48	109.87	105.82
6	C	1	HEA	C3C-C4C-NC	-2.47	107.72	109.80
6	A	1	HEA	C2B-C1B-NB	-2.46	107.05	109.90
6	A	1	HEA	OMA-CMA-C3A	-2.45	120.09	125.62
6	C	1	HEA	C27-C19-C20	2.45	119.48	115.23
6	C	1	HEA	C1D-ND-C4D	2.41	108.06	105.21
4	B	1	DMU	C10-O7-C3	-2.37	112.36	117.98
6	C	2[B]	HEA	C4A-C3A-C2A	2.37	108.87	106.81
6	A	1	HEA	C4C-NC-C1C	2.36	109.66	105.82
6	A	2[B]	HEA	OMA-CMA-C3A	-2.35	120.32	125.62
6	C	2[A]	HEA	C3C-C4C-NC	-2.34	107.83	109.80
6	A	2[A]	HEA	OMA-CMA-C3A	-2.33	120.35	125.62
6	A	2[B]	HEA	C17-C18-C19	-2.33	122.28	127.62
6	A	2[B]	HEA	C4A-C3A-C2A	2.30	108.81	106.81
4	C	9	DMU	C10-O7-C3	-2.29	112.54	117.98
6	C	1	HEA	C4C-NC-C1C	2.28	109.55	105.82
6	A	2[B]	HEA	C2B-C1B-NB	-2.27	107.28	109.90
6	C	2[A]	HEA	C2B-C1B-NB	-2.26	107.29	109.90
6	A	2[A]	HEA	CMB-C2B-C3B	-2.25	125.92	130.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1	HEA	C4A-C3A-C2A	2.25	108.76	106.81
6	C	2[B]	HEA	OMA-CMA-C3A	-2.24	120.56	125.62
6	C	1	HEA	CHB-C1B-NB	2.19	126.78	124.42
6	C	2[A]	HEA	C13-C12-C11	-2.19	110.89	114.39
4	B	1	DMU	O2-C8-C9	2.17	114.66	109.32
6	C	1	HEA	C13-C12-C11	-2.17	110.93	114.39
6	C	2[A]	HEA	C26-C15-C16	2.16	118.98	115.23
6	C	2[A]	HEA	C4A-NA-C1A	2.16	109.33	105.82
6	C	2[B]	HEA	C4C-NC-C1C	2.15	109.32	105.82
6	A	2[B]	HEA	CBD-CAD-C3D	2.15	118.46	112.53
6	A	2[A]	HEA	CHA-C4D-ND	2.14	126.73	124.42
6	C	1	HEA	CHC-C4B-NB	2.12	126.99	124.37
6	C	1	HEA	C25-C23-C24	2.12	119.46	114.59
6	A	1	HEA	CHA-C4D-ND	2.11	126.69	124.42
6	A	1	HEA	C13-C12-C11	-2.10	111.04	114.39
6	C	2[B]	HEA	C3D-C4D-ND	-2.09	108.34	110.35
4	A	1005	DMU	C18-O16-C6	-2.08	110.12	113.68
6	A	2[B]	HEA	C25-C23-C24	2.08	119.37	114.59
6	A	1	HEA	C2D-C1D-ND	-2.06	107.47	109.84
6	A	2[B]	HEA	C3D-C4D-ND	-2.06	108.36	110.35
4	C	9	DMU	C8-C7-C5	2.05	114.43	110.83
6	C	1	HEA	O2D-CGD-CBD	2.05	120.48	114.00
6	A	2[A]	HEA	C3C-C4C-NC	-2.04	108.08	109.80
6	C	2[B]	HEA	C25-C23-C24	2.02	119.24	114.59
4	C	10	DMU	C10-O1-C9	2.02	117.67	113.72
6	C	1	HEA	C3A-C2A-C1A	2.01	108.95	107.05
6	A	2[B]	HEA	C13-C14-C15	-2.01	123.02	127.62
6	C	2[B]	HEA	C1B-C2B-C3B	2.00	109.11	106.80

There are no chirality outliers.

All (129) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	7	DMU	C1-C6-O16-C18
4	B	2	DMU	C19-C18-O16-C6
6	A	2[A]	HEA	C2A-C3A-CMA-OMA
6	A	2[B]	HEA	C2D-C3D-CAD-CBD
6	A	2[B]	HEA	C19-C20-C21-C22
6	C	2[B]	HEA	C2A-C3A-CMA-OMA
6	C	2[B]	HEA	C2D-C3D-CAD-CBD
11	B	286	HTH	O1-C1-C2-C3
4	C	9	DMU	O5-C4-C57-O61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	10	DMU	O1-C10-O7-C3
11	B	286	HTH	O1-C1-C2-O2
6	A	2[B]	HEA	C4D-C3D-CAD-CBD
6	C	2[B]	HEA	C4D-C3D-CAD-CBD
4	C	9	DMU	C3-C4-C57-O61
6	C	2[B]	HEA	C19-C20-C21-C22
4	C	5	DMU	O5-C4-C57-O61
4	B	2	DMU	O5-C6-O16-C18
4	C	9	DMU	O6-C11-C9-O1
4	D	8	DMU	O6-C11-C9-O1
4	C	9	DMU	O6-C11-C9-C8
4	D	8	DMU	O6-C11-C9-C8
4	B	2	DMU	C1-C6-O16-C18
4	C	5	DMU	C3-C4-C57-O61
4	A	7	DMU	O5-C6-O16-C18
4	B	6	DMU	O6-C11-C9-C8
4	B	6	DMU	O6-C11-C9-O1
11	B	286	HTH	O3-C3-C4-C5
4	A	7	DMU	C19-C22-C25-C28
5	C	552	TRD	C9-C10-C11-C12
4	C	10	DMU	C18-C19-C22-C25
5	B	4	TRD	C3-C4-C5-C6
4	B	3	DMU	C25-C28-C31-C34
4	C	10	DMU	C25-C28-C31-C34
5	B	4	TRD	C5-C6-C7-C8
5	C	552	TRD	C3-C4-C5-C6
4	B	3	DMU	C28-C31-C34-C37
4	A	7	DMU	C28-C31-C34-C37
4	B	1	DMU	C31-C34-C37-C40
5	A	553	TRD	C2-C3-C4-C5
4	A	7	DMU	O16-C18-C19-C22
5	D	3	TRD	C2-C3-C4-C5
4	B	2	DMU	C25-C28-C31-C34
4	C	10	DMU	C31-C34-C37-C40
4	B	2	DMU	C18-C19-C22-C25
5	C	552	TRD	C2-C3-C4-C5
5	D	3	TRD	C4-C5-C6-C7
5	A	553	TRD	C3-C4-C5-C6
6	C	2[B]	HEA	C18-C19-C20-C21
5	D	3	TRD	C6-C7-C8-C9
4	B	3	DMU	C22-C25-C28-C31
5	A	3	TRD	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	B	286	HTH	C2-C3-C4-C5
5	D	3	TRD	C5-C6-C7-C8
6	C	2[B]	HEA	C27-C19-C20-C21
5	D	14	TRD	C3-C4-C5-C6
5	A	553	TRD	C10-C11-C12-C13
5	A	553	TRD	C1-C2-C3-C4
6	A	2[A]	HEA	C3B-C11-C12-C13
5	C	552	TRD	C10-C11-C12-C13
5	A	3	TRD	C4-C5-C6-C7
6	A	2[B]	HEA	C27-C19-C20-C21
5	D	3	TRD	C10-C11-C12-C13
6	A	2[B]	HEA	C18-C19-C20-C21
4	A	1005	DMU	C34-C37-C40-C43
4	C	10	DMU	C34-C37-C40-C43
5	A	1009	TRD	C4-C5-C6-C7
4	A	7	DMU	C18-C19-C22-C25
4	B	2	DMU	C34-C37-C40-C43
5	A	553	TRD	C4-C5-C6-C7
5	D	3	TRD	C11-C10-C9-C8
4	A	1005	DMU	C1-C6-O16-C18
6	C	1	HEA	C26-C15-C16-C17
5	A	553	TRD	C9-C10-C11-C12
6	A	2[A]	HEA	C4A-C3A-CMA-OMA
6	C	2[B]	HEA	C4A-C3A-CMA-OMA
6	A	2[A]	HEA	C4D-C3D-CAD-CBD
6	C	2[A]	HEA	C3B-C11-C12-C13
5	B	4	TRD	C2-C3-C4-C5
6	A	2[B]	HEA	C4C-C3C-CAC-CBC
6	A	2[A]	HEA	C2D-C3D-CAD-CBD
6	C	1	HEA	CAD-CBD-CGD-O2D
6	C	1	HEA	C14-C15-C16-C17
6	A	2[A]	HEA	CAD-CBD-CGD-O2D
4	C	10	DMU	C28-C31-C34-C37
6	C	1	HEA	CAD-CBD-CGD-O1D
6	A	2[A]	HEA	CAD-CBD-CGD-O1D
6	C	2[B]	HEA	CAA-CBA-CGA-O1A
6	A	2[B]	HEA	C2C-C3C-CAC-CBC
6	C	2[A]	HEA	CAA-CBA-CGA-O1A
6	A	2[A]	HEA	O11-C11-C12-C13
6	A	2[A]	HEA	CAA-CBA-CGA-O1A
6	A	2[B]	HEA	CAA-CBA-CGA-O1A
6	A	1	HEA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	1	HEA	C26-C15-C16-C17
6	A	2[A]	HEA	C26-C15-C16-C17
6	C	2[B]	HEA	CAA-CBA-CGA-O2A
6	A	2[B]	HEA	CAA-CBA-CGA-O2A
6	A	2[A]	HEA	CAA-CBA-CGA-O2A
6	C	2[B]	HEA	C4C-C3C-CAC-CBC
6	C	2[A]	HEA	CAA-CBA-CGA-O2A
6	A	2[B]	HEA	C11-C12-C13-C14
6	C	2[B]	HEA	C11-C12-C13-C14
6	A	1	HEA	CAD-CBD-CGD-O1D
4	A	1005	DMU	O5-C6-O16-C18
4	C	10	DMU	C2-C3-O7-C10
5	D	3	TRD	C3-C4-C5-C6
6	C	2[A]	HEA	CAD-CBD-CGD-O2D
6	A	2[B]	HEA	CAD-CBD-CGD-O2D
6	C	2[A]	HEA	CAD-CBD-CGD-O1D
4	B	3	DMU	C34-C37-C40-C43
4	C	10	DMU	O5-C6-O16-C18
4	C	10	DMU	O16-C18-C19-C22
6	A	2[B]	HEA	CAD-CBD-CGD-O1D
5	A	1013	TRD	C1-C2-C3-C4
4	B	3	DMU	C3-C4-C57-O61
4	B	3	DMU	O6-C11-C9-O1
6	A	1	HEA	C2C-C3C-CAC-CBC
6	C	2[B]	HEA	C2C-C3C-CAC-CBC
5	D	3	TRD	C9-C10-C11-C12
11	B	286	HTH	C1-C2-C3-O3
4	C	10	DMU	C4-C3-O7-C10
4	B	2	DMU	O16-C18-C19-C22
6	A	1	HEA	CAA-CBA-CGA-O1A
5	D	3	TRD	C7-C8-C9-C10
6	A	1	HEA	C14-C15-C16-C17
5	B	4	TRD	C4-C5-C6-C7
4	B	2	DMU	C28-C31-C34-C37
6	C	1	HEA	CAA-CBA-CGA-O1A
6	A	1	HEA	CAA-CBA-CGA-O2A

There are no ring outliers.

13 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3	TRD	1	0

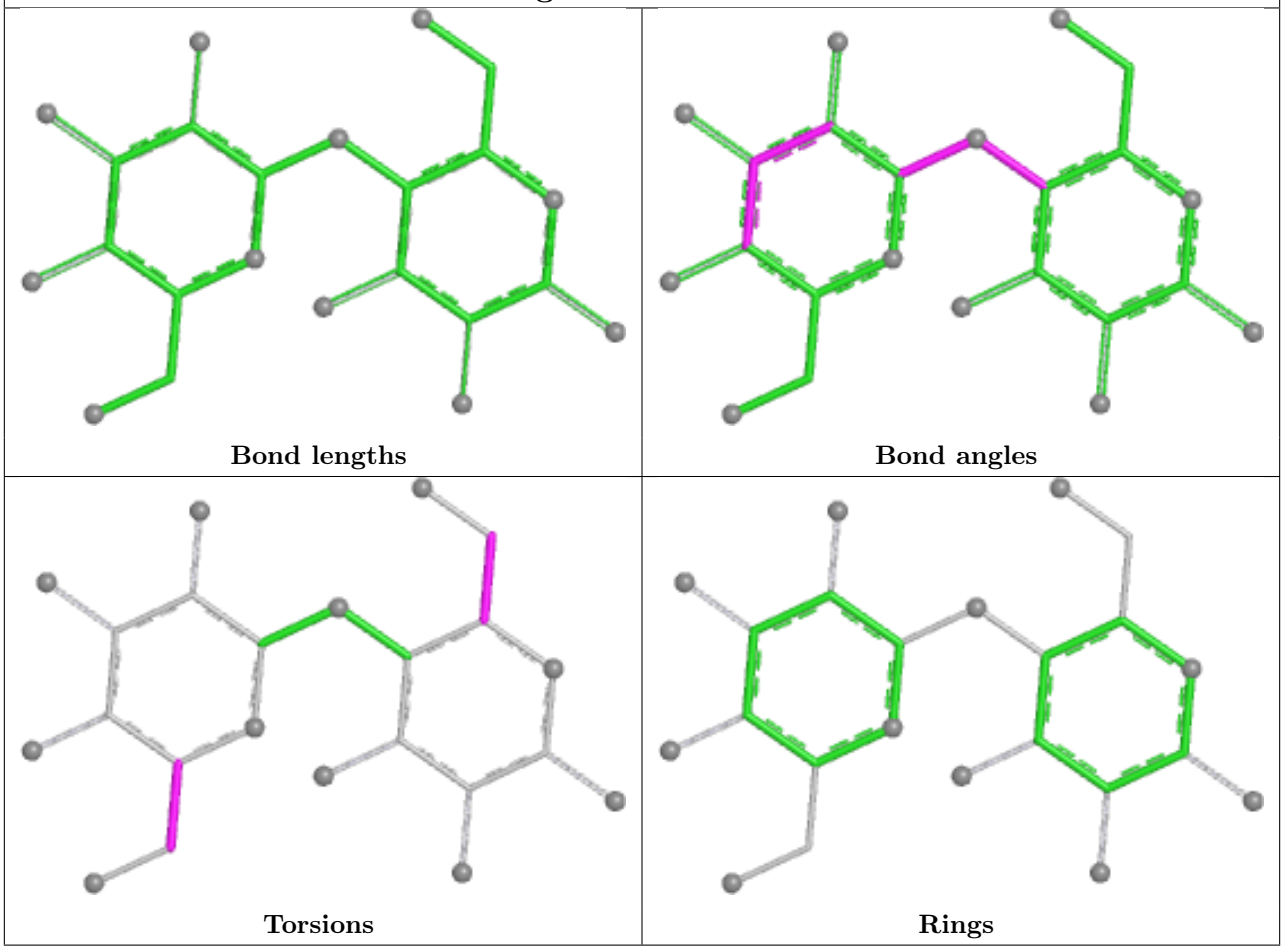
Continued on next page...

Continued from previous page...

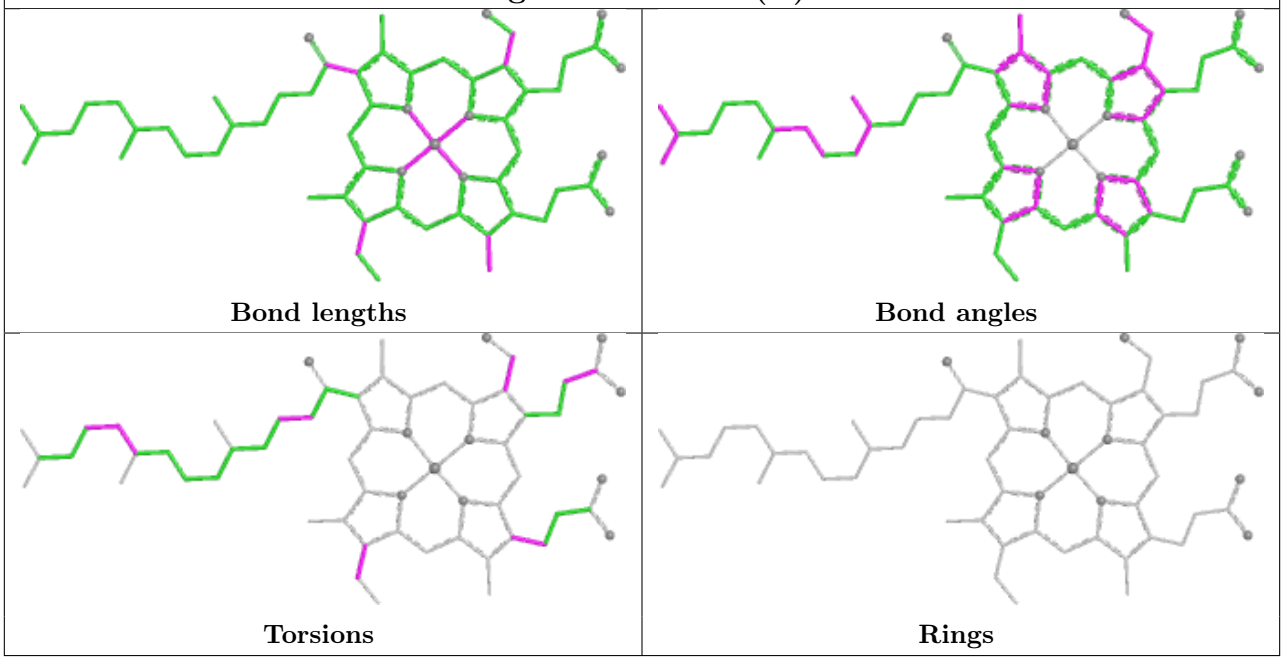
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	9	DMU	1	0
6	C	2[B]	HEA	7	0
6	C	1	HEA	7	0
6	C	2[A]	HEA	7	0
4	D	8	DMU	1	0
4	C	10	DMU	1	0
6	A	2[B]	HEA	9	0
5	A	553	TRD	1	0
6	A	2[A]	HEA	7	0
5	C	552	TRD	1	0
6	A	1	HEA	4	0
4	A	1005	DMU	2	0

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.

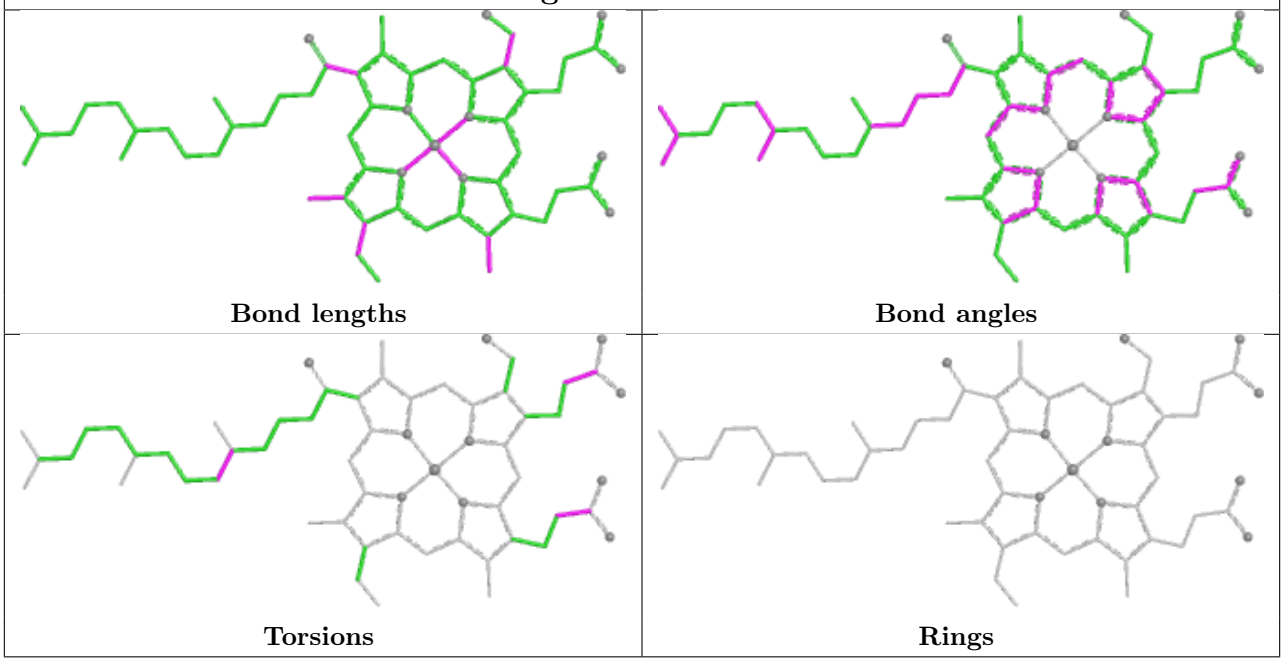
Ligand DMU C 9



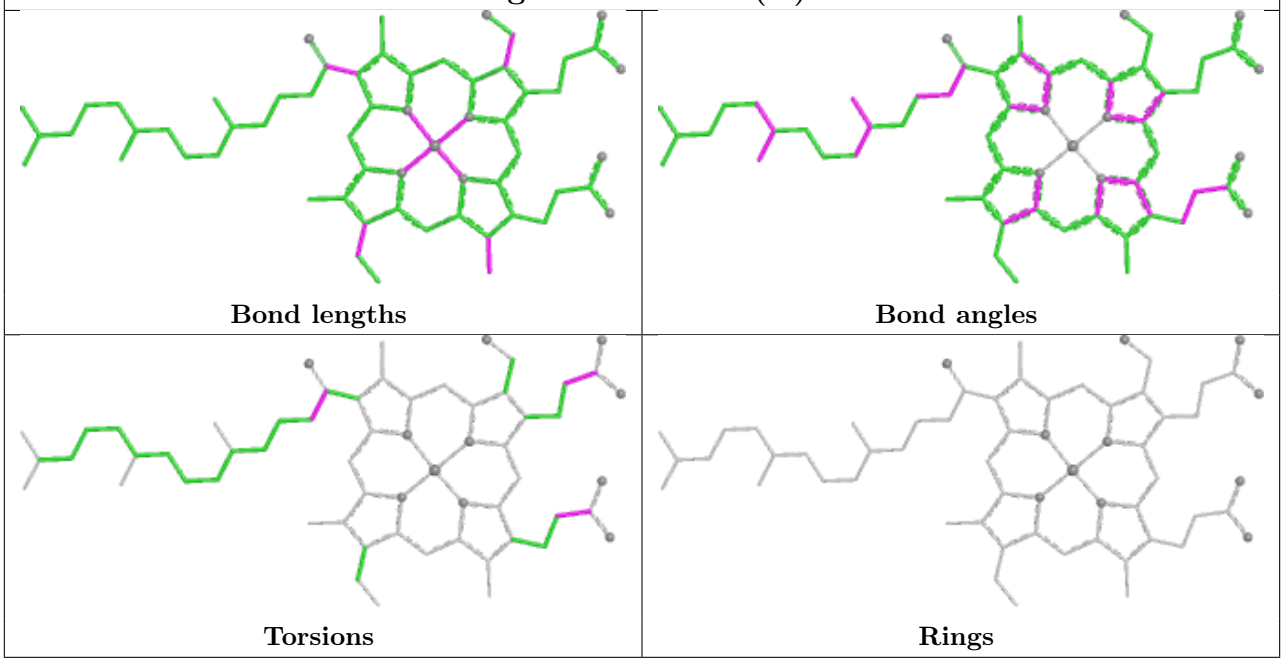
Ligand HEA C 2 (B)



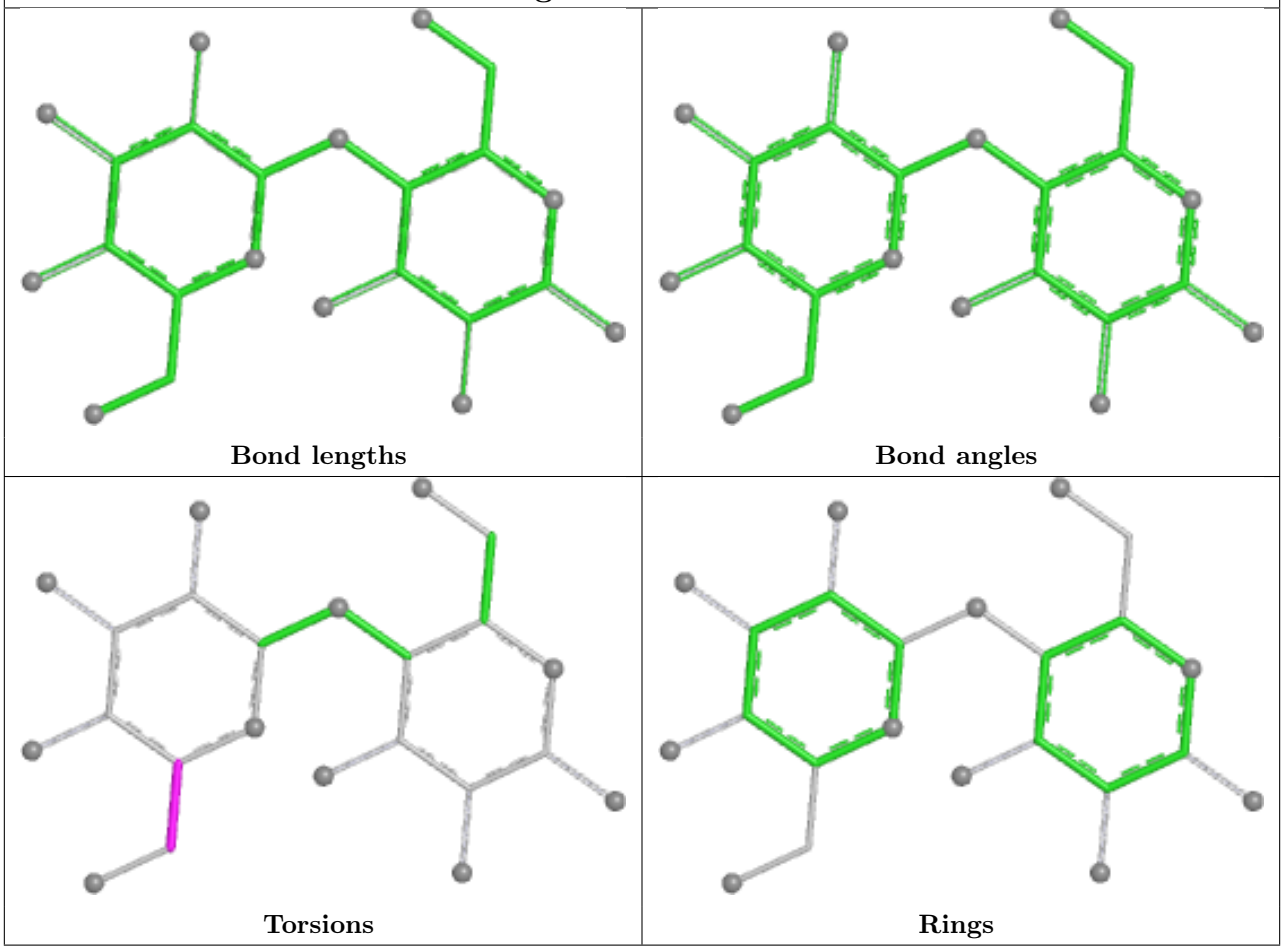
Ligand HEA C 1

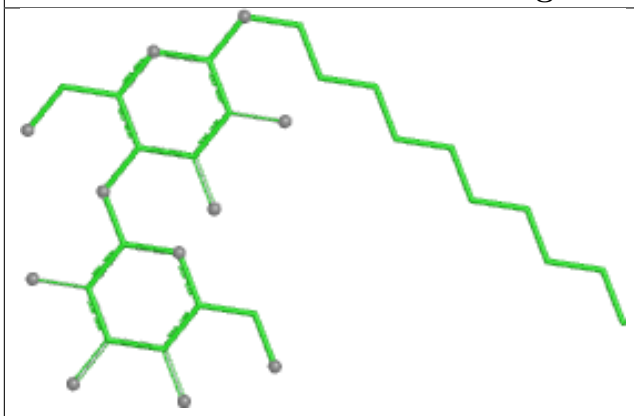
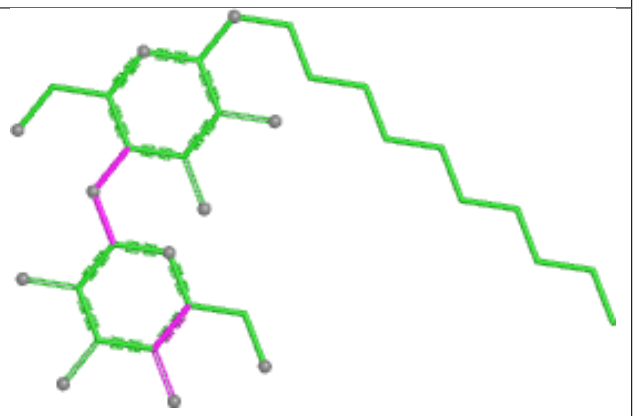
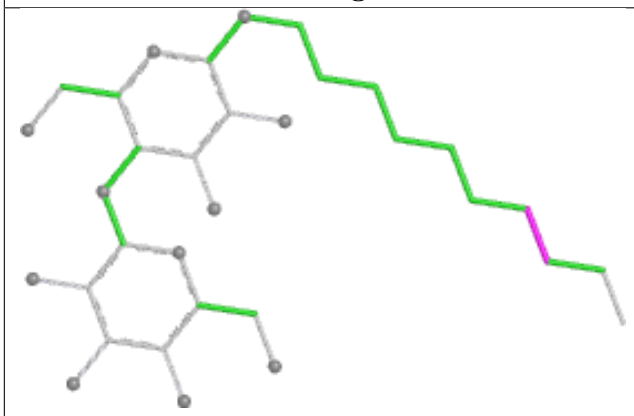
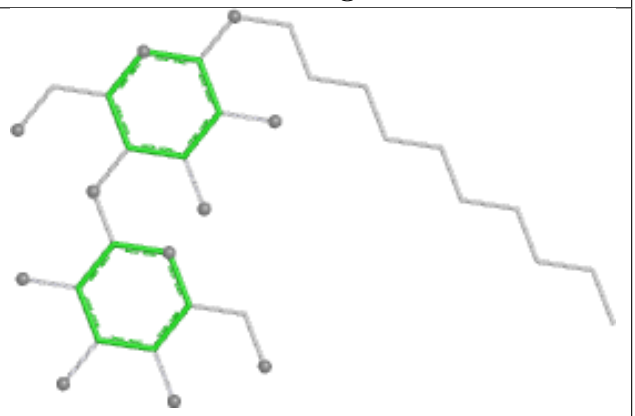


Ligand HEA C 2 (A)

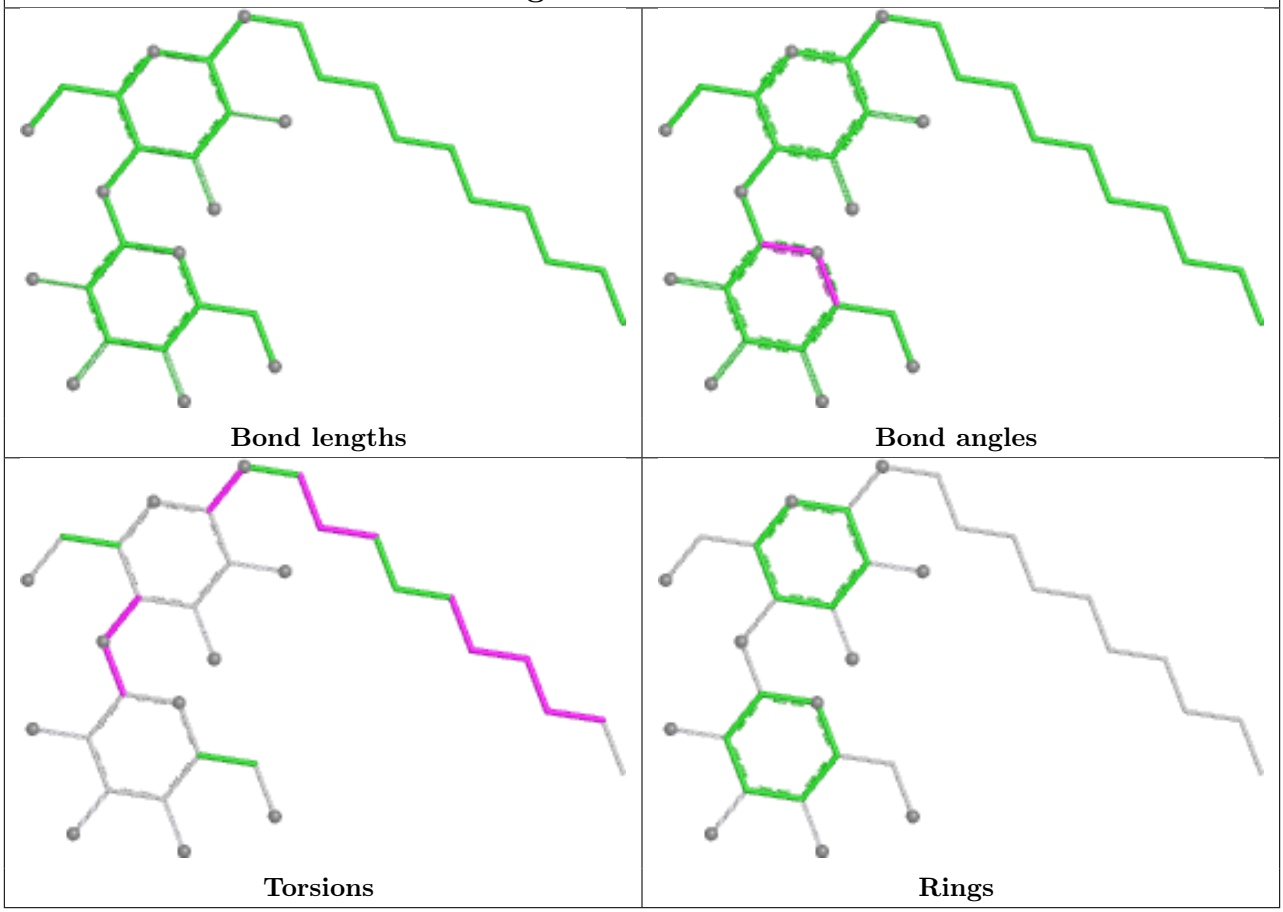


Ligand DMU D 8

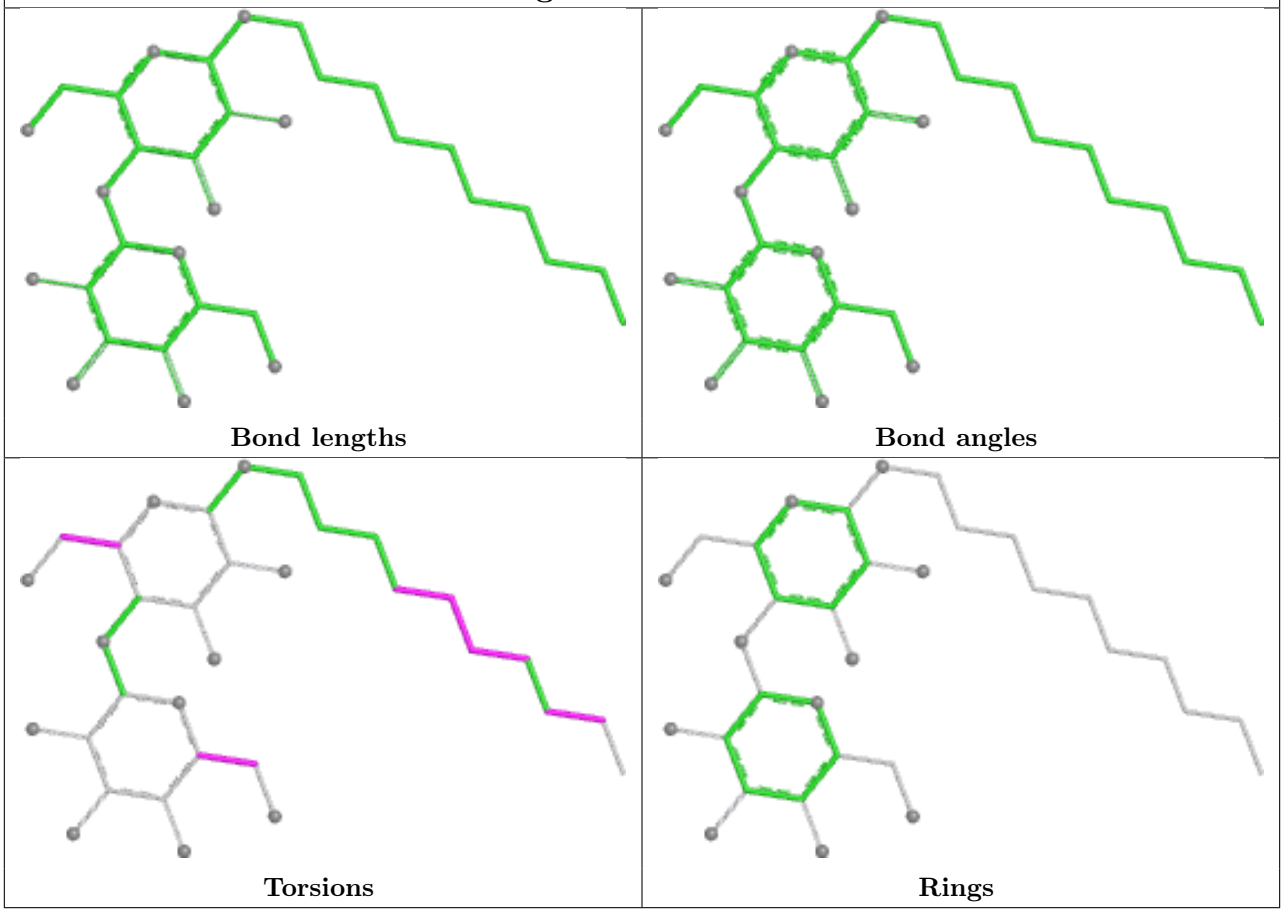


Ligand DMU B 1	
 Bond lengths	 Bond angles
 Torsions	 Rings

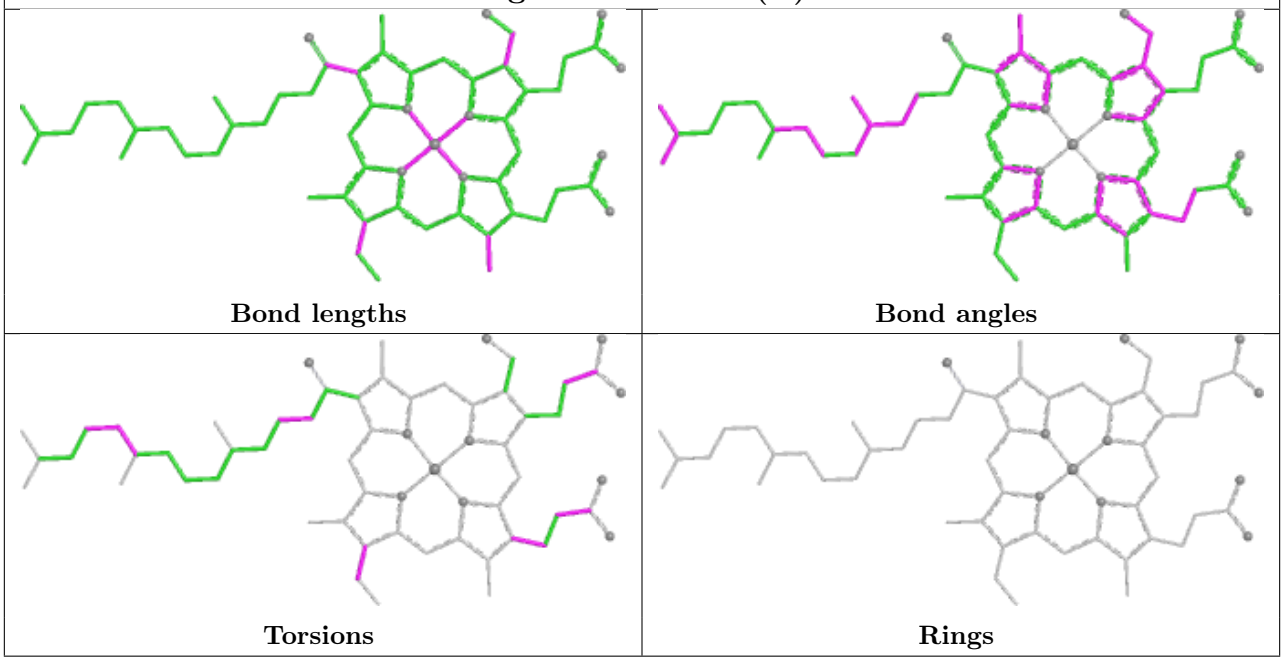
Ligand DMU C 10



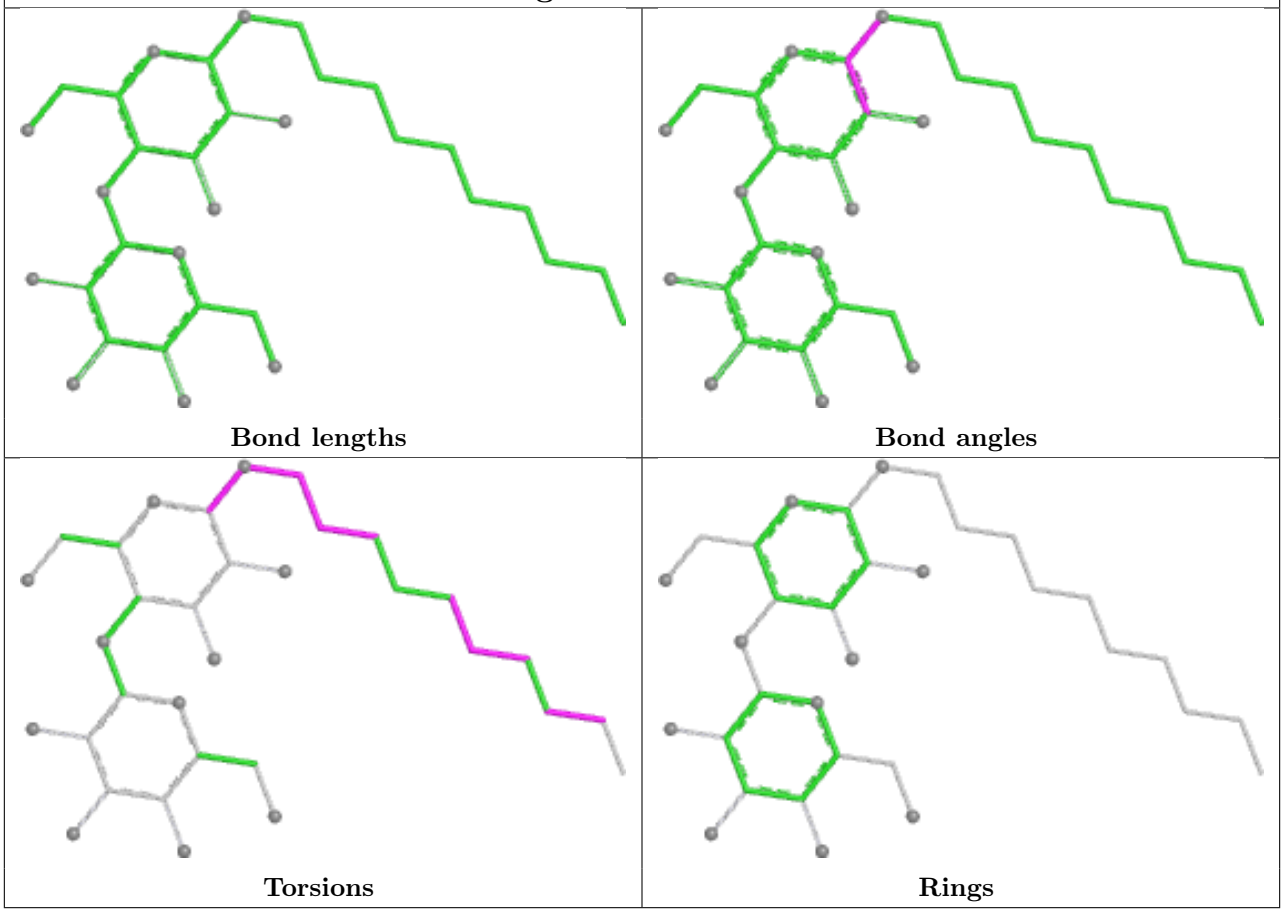
Ligand DMU B 3



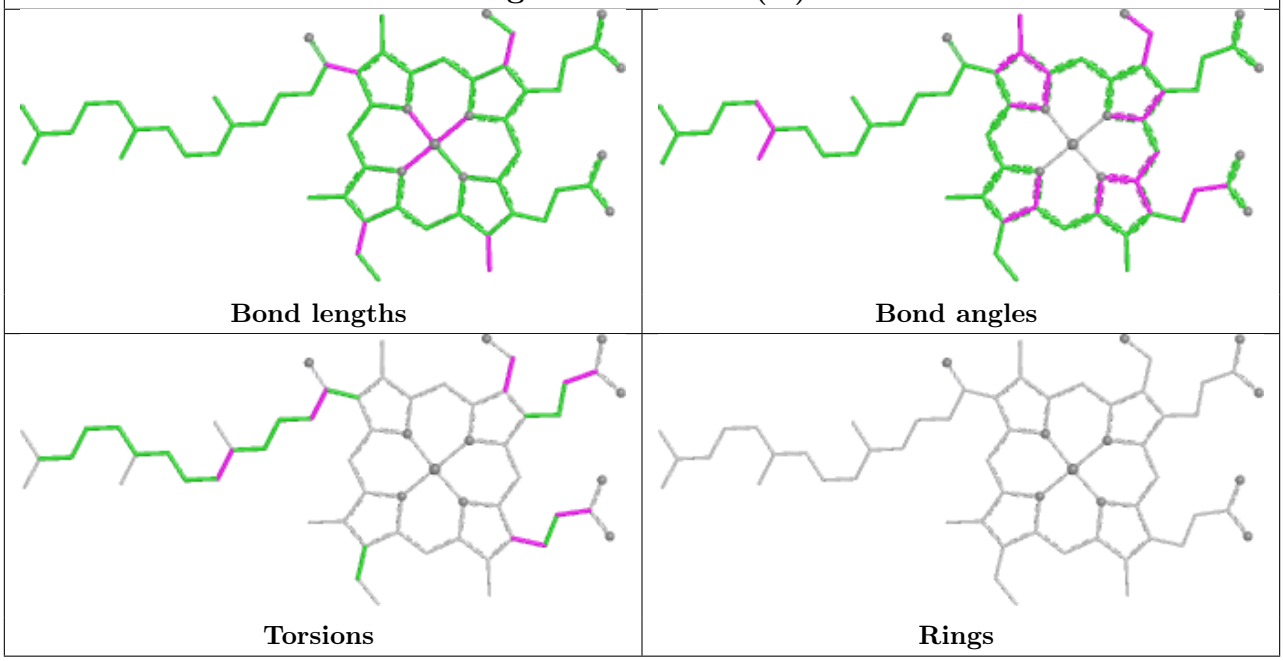
Ligand HEA A 2 (B)



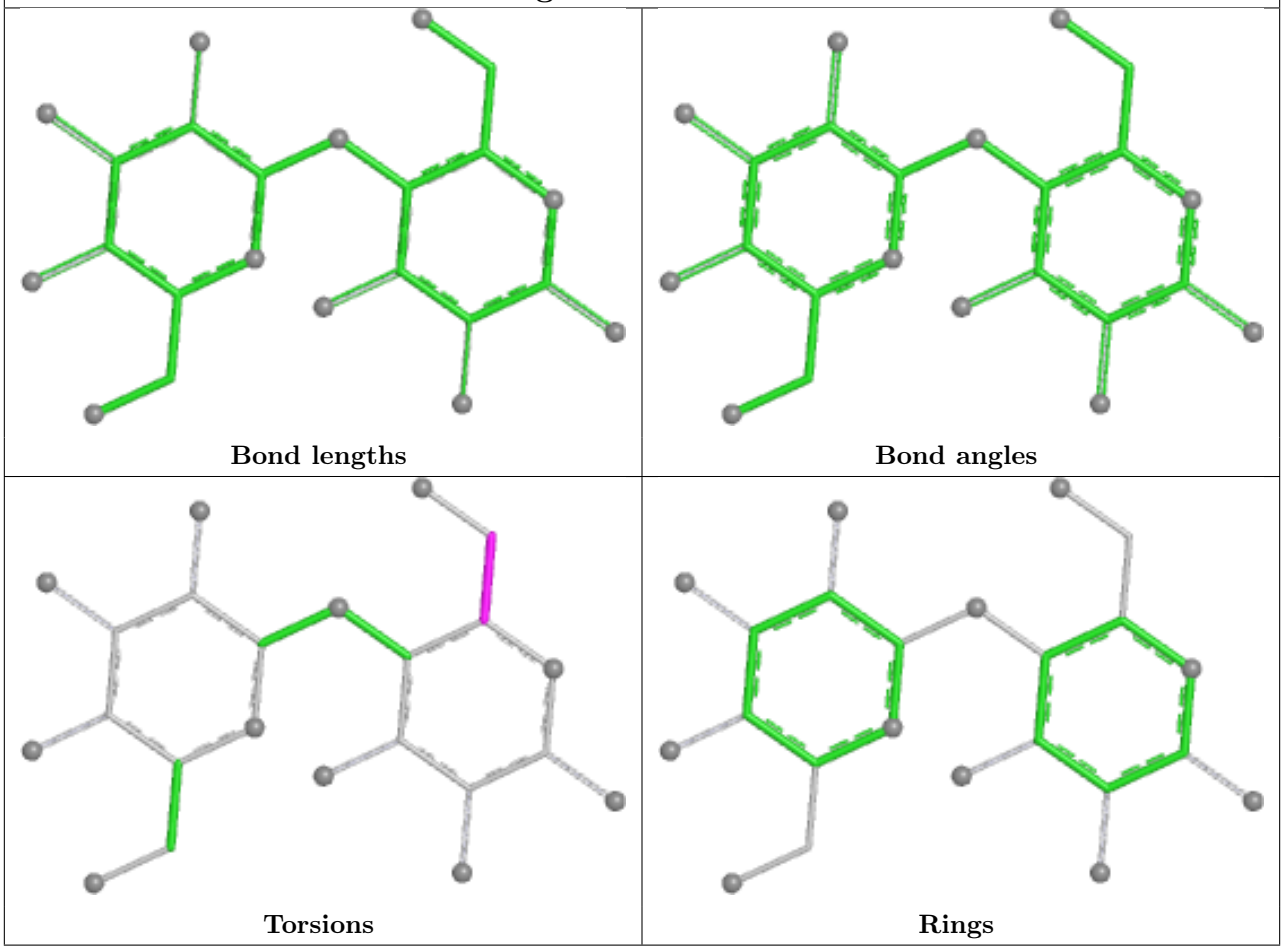
Ligand DMU B 2



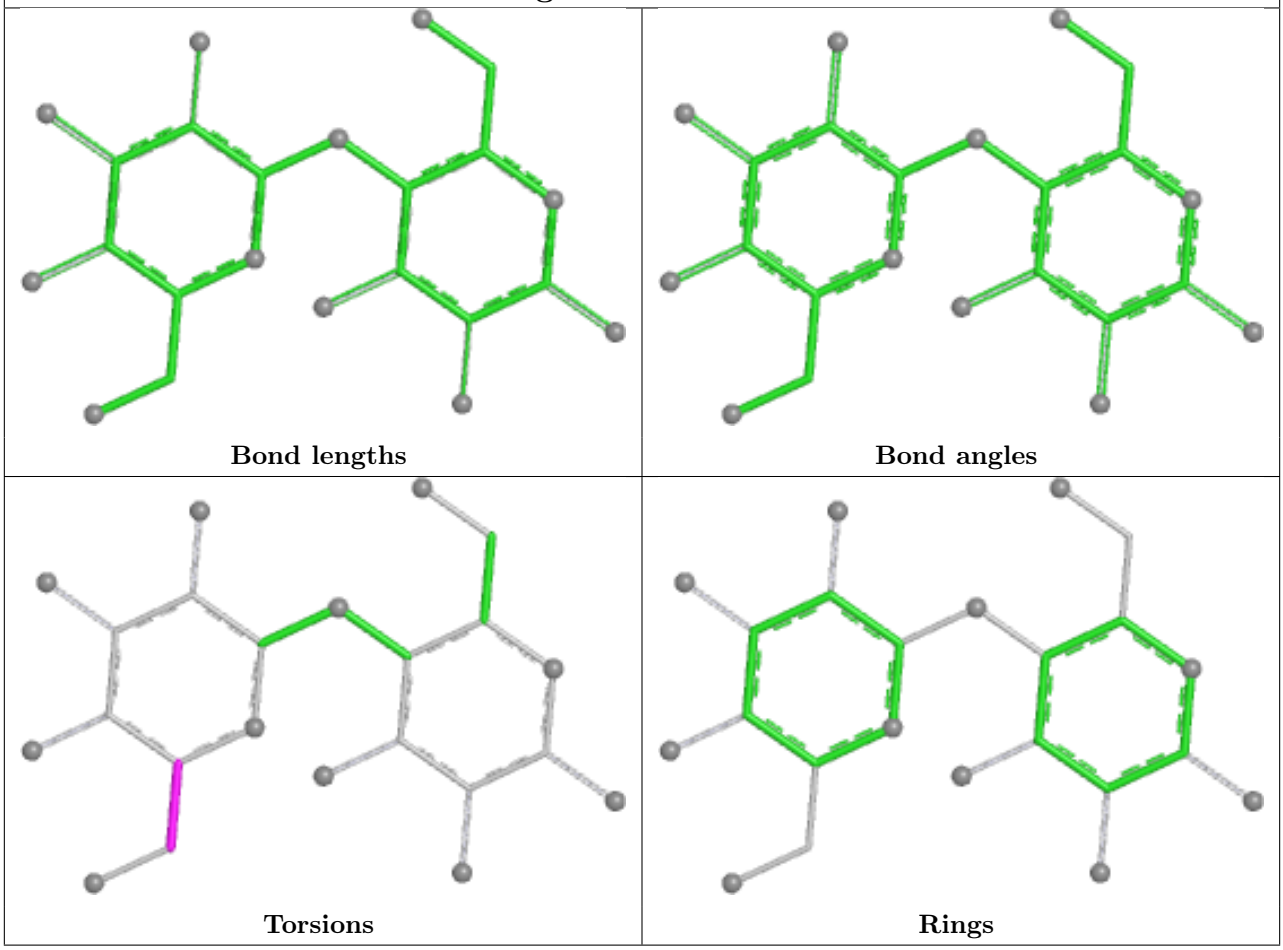
Ligand HEA A 2 (A)



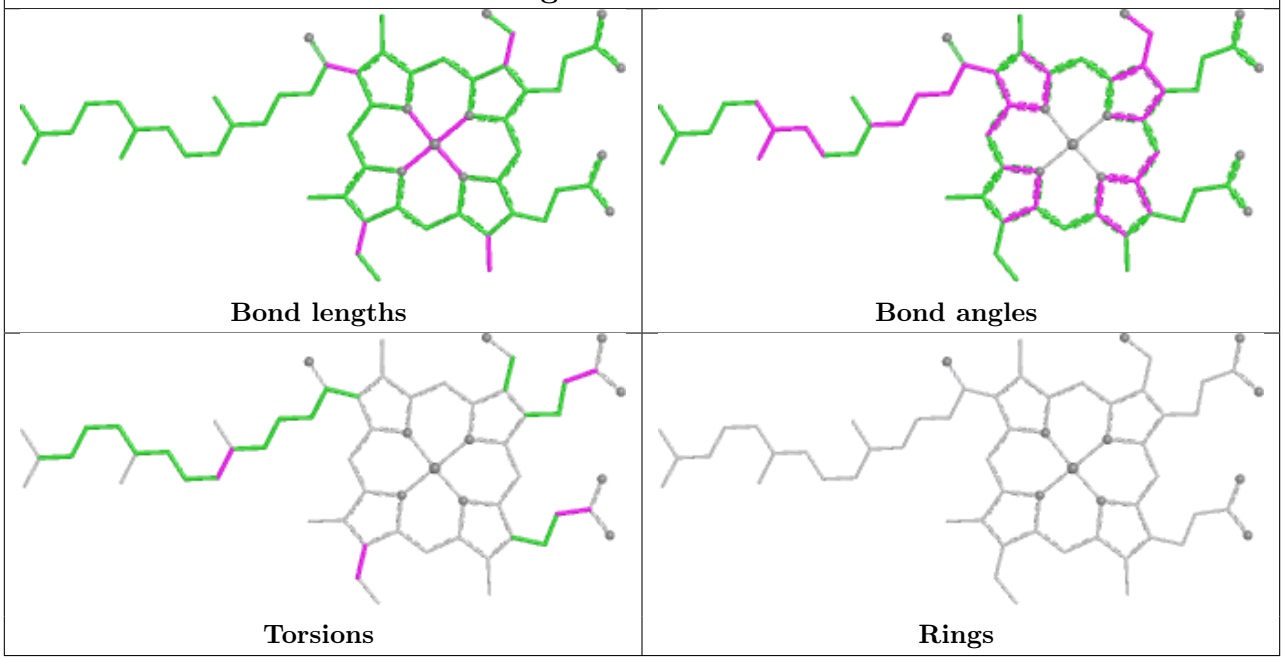
Ligand DMU C 5



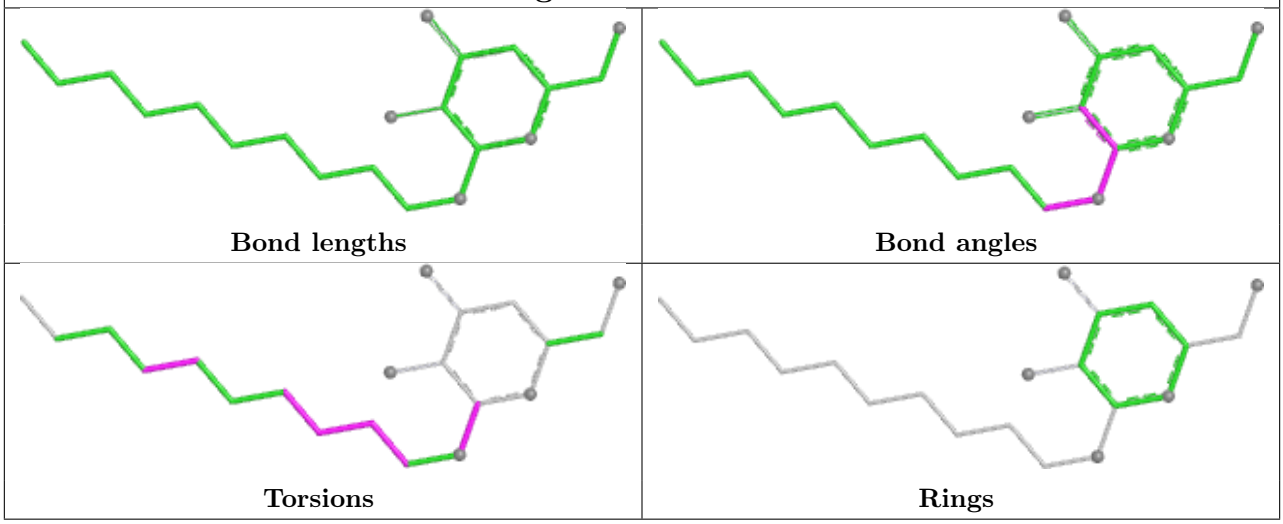
Ligand DMU B 6



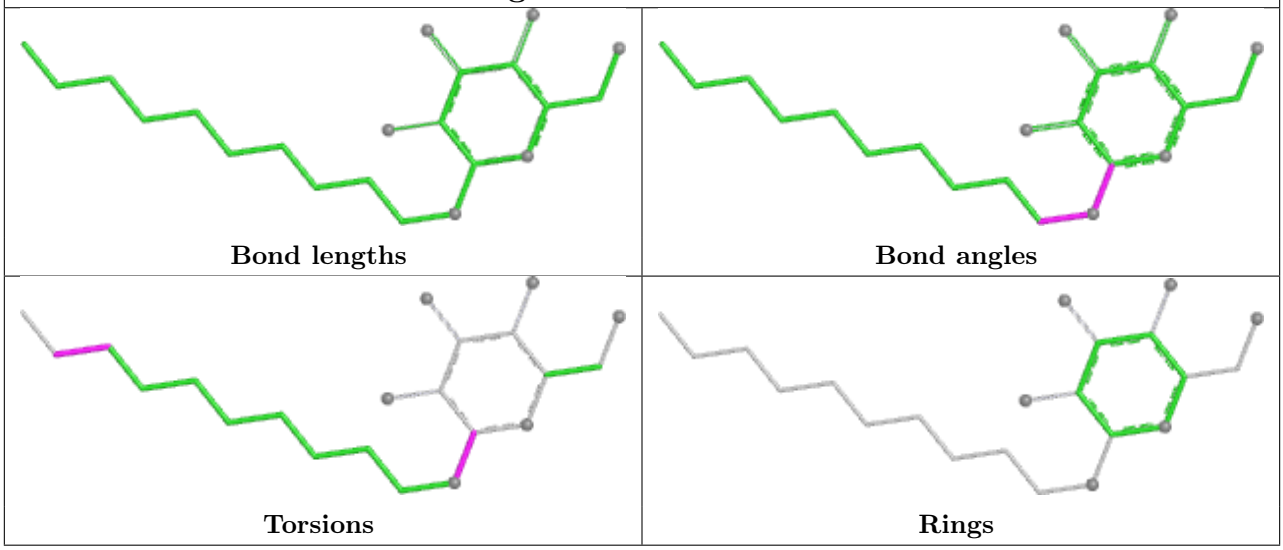
Ligand HEA A 1



Ligand DMU A 7



Ligand DMU A 1005



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%)	0.36	40 (7%) 20 23	13, 35, 57, 81	13 (2%)
1	C	531/535 (99%)	1.29	107 (20%) 3 3	16, 52, 76, 88	13 (2%)
2	B	256/256 (100%)	0.34	11 (4%) 40 45	23, 39, 55, 59	0
2	D	256/256 (100%)	0.68	26 (10%) 12 13	30, 44, 64, 72	0
All	All	1578/1582 (99%)	0.72	184 (11%) 9 10	13, 42, 67, 88	26 (1%)

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	361[A]	ILE	15.3
1	A	361[A]	ILE	13.2
1	C	20	TRP	7.8
2	B	56	TRP	7.2
2	D	284	HIS	5.6
1	A	20	TRP	5.3
1	C	134	ALA	5.0
1	C	138	MET	4.9
1	C	222	MET	4.9
1	C	23	SER	4.8
1	A	551	PHE	4.7
1	C	550	THR	4.7
1	C	72	LEU	4.6
1	A	81	TRP	4.5
1	C	136	PRO	4.4
1	C	139	ASN	4.2
1	C	217	ALA	4.1
1	C	525	VAL	3.9
2	D	109	ILE	3.9
1	C	22	MET	3.8
1	C	21	PHE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	74	LEU	3.6
1	A	220	MET	3.6
1	A	426[A]	LEU	3.6
1	C	76	PHE	3.6
1	A	221	THR	3.6
1	C	426[A]	LEU	3.6
1	A	17	PHE	3.6
1	C	24	THR	3.6
1	A	72	LEU	3.6
1	A	217	ALA	3.5
1	C	81	TRP	3.5
1	C	130	ALA	3.5
1	C	399	ILE	3.4
1	C	524	ARG	3.4
1	C	530	TYR	3.4
1	C	543	THR	3.4
2	D	56	TRP	3.4
1	C	137	ARG	3.4
1	C	69	GLU	3.3
1	A	223	HIS	3.3
1	C	80	LEU	3.3
1	C	196	LEU	3.2
1	C	318	TYR	3.2
2	D	83	PHE	3.2
1	A	549	HIS	3.2
2	B	281	GLN	3.2
1	C	451	TRP	3.1
1	A	19	ARG	3.1
1	C	213	LEU	3.1
1	C	77	PHE	3.1
1	A	18	THR	3.1
1	C	549	HIS	3.1
1	C	141	LEU	3.1
1	C	133	MET	3.1
1	C	262	THR	3.0
2	D	107	VAL	3.0
1	C	520	THR	3.0
1	C	129	GLY	3.0
1	A	259	PHE	3.0
1	C	132	ALA	3.0
1	C	32	LEU	3.0
1	C	268	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	106	ILE	3.0
1	A	22	MET	3.0
1	C	223	HIS	2.9
2	B	98	SER	2.9
1	C	30	GLY	2.9
1	C	215	MET	2.9
1	C	548	GLU	2.9
1	A	130	ALA	2.9
1	A	21	PHE	2.9
2	D	75	LEU	2.8
1	C	541	THR	2.8
2	D	98	SER	2.8
1	C	534	HIS	2.8
2	D	235	LEU	2.8
1	A	550	THR	2.8
1	C	121	ASN	2.7
2	D	96	HIS	2.7
1	C	311	PHE	2.7
2	D	70	ILE	2.7
1	C	26	HIS	2.7
1	C	237	TRP	2.7
1	C	312	GLY	2.7
1	C	126	LEU	2.7
1	A	222	MET	2.7
1	C	216	ARG	2.7
1	C	523	ALA	2.6
1	A	214	ASN	2.6
1	C	538	LEU	2.6
1	C	313	TYR	2.6
2	D	72	VAL	2.6
2	B	284	HIS	2.6
1	A	241	LEU	2.6
1	A	216	ARG	2.6
1	C	540	TRP	2.6
1	C	542	LEU	2.6
1	C	521	ARG	2.6
1	C	157	LEU	2.6
1	A	355	ILE	2.5
1	C	211	THR	2.5
1	C	203	LEU	2.5
1	A	533	GLU	2.5
1	C	123	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	443	MET	2.5
2	D	86	LYS	2.5
1	C	251	THR	2.5
1	C	82	PRO	2.5
1	C	531	TRP	2.5
1	A	74	LYS	2.5
2	D	87	ARG	2.5
1	C	448	TYR	2.5
1	A	548	GLU	2.5
1	C	537	THR	2.5
1	C	546	PRO	2.5
2	B	235	LEU	2.5
1	A	311	PHE	2.4
1	C	228	PHE	2.4
1	C	128	ILE	2.4
1	C	218	PRO	2.4
1	C	547	PRO	2.4
1	C	74	LYS	2.4
1	C	68	LEU	2.4
2	B	100	LEU	2.4
2	B	124	PHE	2.4
1	C	225	VAL	2.4
2	B	102	ILE	2.4
1	A	152	LEU	2.4
1	A	268	GLY	2.4
1	C	145	LEU	2.3
1	C	509	LEU	2.3
2	D	100	LEU	2.3
2	D	105	THR	2.3
1	C	517	TYR	2.3
2	B	70	ILE	2.3
1	C	545	PRO	2.3
1	A	71	GLY	2.3
1	C	39	LEU	2.3
1	C	75	GLY	2.3
1	C	240	LEU	2.3
1	A	210	THR	2.3
1	C	131	PRO	2.3
2	D	103	ALA	2.3
1	A	138	MET	2.2
1	A	541	THR	2.2
1	C	227	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	76	PHE	2.2
2	D	99	PRO	2.2
1	C	73	VAL	2.2
1	A	260	GLY	2.2
1	C	118	GLY	2.2
2	D	92	ALA	2.2
1	A	137	ARG	2.2
1	C	27	LYS	2.2
1	A	356	ALA	2.1
2	B	104	TRP	2.1
1	C	368	ALA	2.1
1	C	152	LEU	2.1
2	D	97	ASN	2.1
1	C	202	ILE	2.1
1	C	232	ILE	2.1
1	C	257	ARG	2.1
1	C	110	VAL	2.1
1	C	378	LYS	2.1
1	A	24	THR	2.1
1	C	226	PRO	2.1
2	D	82	ARG	2.1
1	C	260	GLY	2.1
1	C	29	ILE	2.1
1	C	303	ALA	2.1
1	C	535	ALA	2.1
1	C	544	SER	2.1
2	D	182	GLU	2.0
2	D	88	ASN	2.0
2	B	178	GLN	2.0
1	A	218	PRO	2.0
1	C	99	ILE	2.0
1	C	444	SER	2.0
1	C	428[A]	ALA	2.0
2	D	104	TRP	2.0
1	C	125	PRO	2.0
1	C	449	PRO	2.0
2	D	78	TYR	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)

There are no oligosaccharides in this entry.

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	DMU	C	9	23/33	0.63	0.22	85,86,89,89	23
4	DMU	C	5	23/33	0.67	0.23	97,98,98,99	23
4	DMU	D	8	23/33	0.72	0.23	89,90,93,93	23
5	TRD	A	1013	7/13	0.72	0.31	54,56,57,57	0
5	TRD	A	552	6/13	0.77	0.28	62,63,63,63	0
4	DMU	D	4	23/33	0.78	0.29	91,91,91,91	23
5	TRD	A	553	13/13	0.81	0.26	71,71,73,73	0
4	DMU	B	2	33/33	0.82	0.23	49,54,56,57	33
5	TRD	C	552	13/13	0.82	0.31	80,82,83,84	0
5	TRD	B	4	8/13	0.83	0.20	35,36,37,37	0
4	DMU	A	7	21/33	0.83	0.18	43,59,70,72	0
4	DMU	B	6	23/33	0.84	0.20	76,77,78,78	23
5	TRD	A	3	13/13	0.84	0.22	46,49,53,54	0
5	TRD	D	3	13/13	0.85	0.25	55,58,61,61	0
10	CL	C	554	1/1	0.85	0.21	68,68,68,68	0
4	DMU	A	1005	22/33	0.87	0.17	44,49,53,54	22
4	DMU	C	10	33/33	0.87	0.15	73,74,76,76	0
5	TRD	D	14	7/13	0.87	0.22	65,65,65,65	0
4	DMU	B	3	33/33	0.87	0.15	73,78,82,83	0
5	TRD	A	1009	7/13	0.89	0.19	57,58,58,58	0
11	HTH	B	286	10/10	0.90	0.19	56,60,61,61	0
4	DMU	B	1	33/33	0.94	0.09	26,35,46,48	0
6	HEA	C	2[B]	60/60	0.95	0.10	35,40,48,48	60
3	OH	C	802	1/1	0.95	0.34	21,21,21,21	1
6	HEA	C	2[A]	60/60	0.95	0.10	25,28,33,34	60
6	HEA	A	2[A]	60/60	0.96	0.09	21,22,30,32	60
6	HEA	A	2[B]	60/60	0.96	0.09	30,33,41,41	60
10	CL	A	10	1/1	0.97	0.06	41,41,41,41	0
3	OH	A	802	1/1	0.97	0.08	8,8,8,8	1
6	HEA	C	1	60/60	0.97	0.08	31,34,47,47	0
12	CD	D	9	1/1	0.97	0.07	63,63,63,63	1
12	CD	B	9	1/1	0.98	0.11	39,39,39,39	1

Continued on next page...

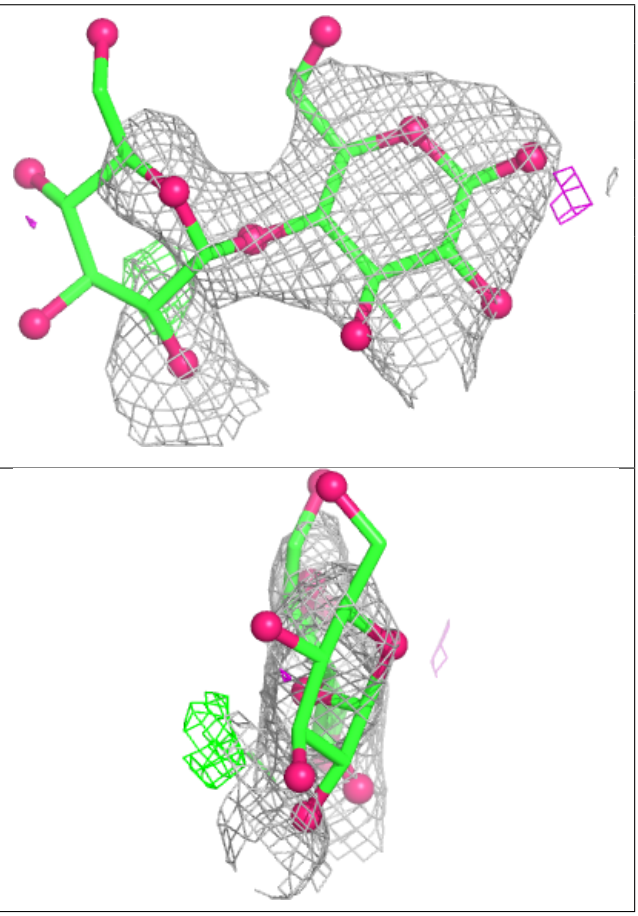
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	HEA	A	1	60/60	0.99	0.06	21,25,30,32	0
7	CU1	A	5	1/1	0.99	0.05	37,37,37,37	0
7	CU1	C	553	1/1	0.99	0.04	45,45,45,45	0
12	CD	B	8	1/1	0.99	0.02	41,41,41,41	0
8	MG	C	6	1/1	0.99	0.08	18,18,18,18	0
12	CD	D	288	1/1	0.99	0.02	40,40,40,40	0
9	CA	C	7	1/1	0.99	0.05	38,38,38,38	0
7	CU1	D	287	1/1	1.00	0.02	32,32,32,32	0
8	MG	A	6	1/1	1.00	0.08	13,13,13,13	0
7	CU1	B	288	1/1	1.00	0.02	26,26,26,26	0
9	CA	A	554	1/1	1.00	0.01	27,27,27,27	0
7	CU1	B	287	1/1	1.00	0.01	25,25,25,25	0
7	CU1	D	286	1/1	1.00	0.02	33,33,33,33	0

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

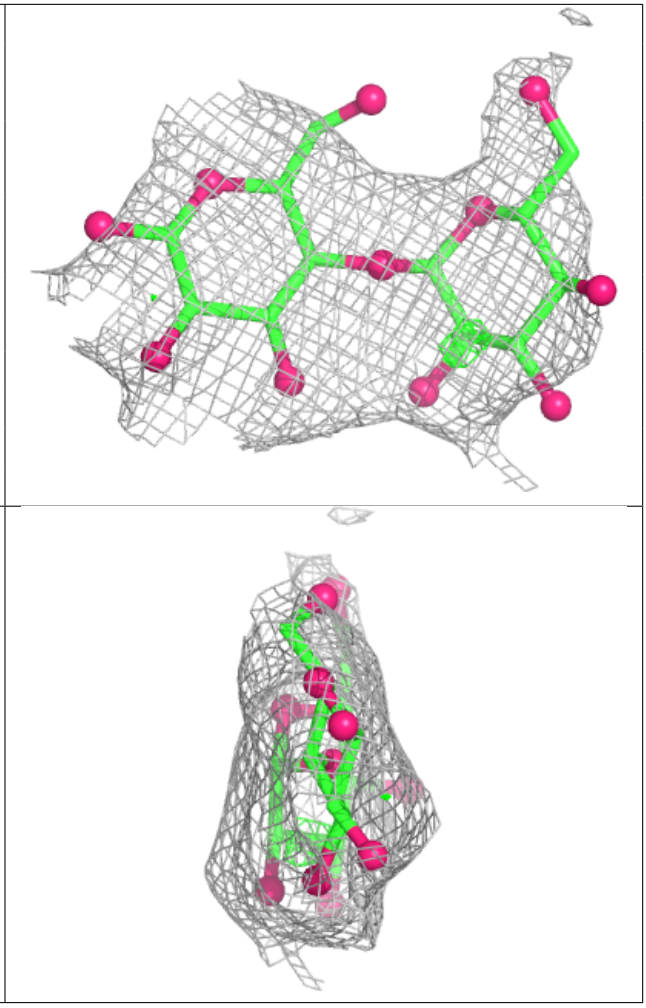
Electron density around DMU C 9:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



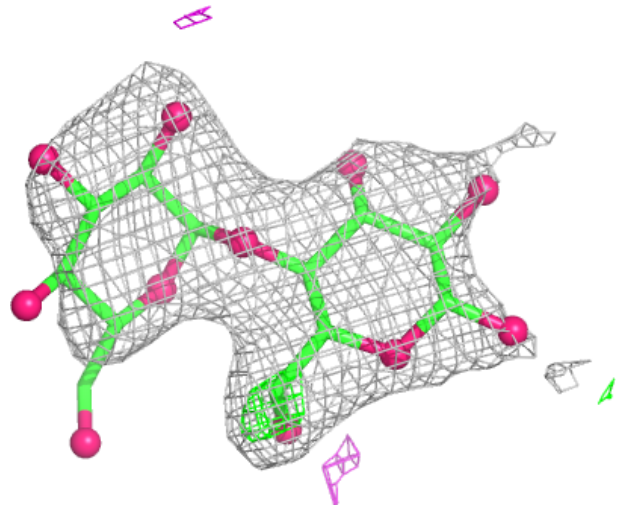
Electron density around DMU C 5:

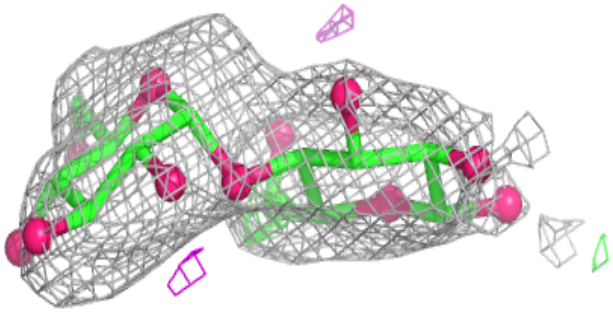
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

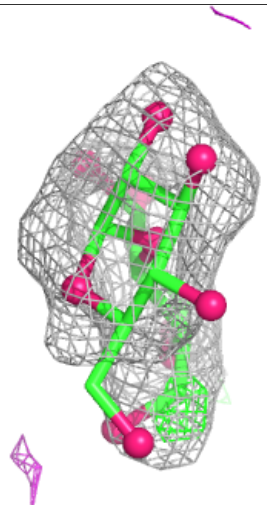


Electron density around DMU D 8:

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

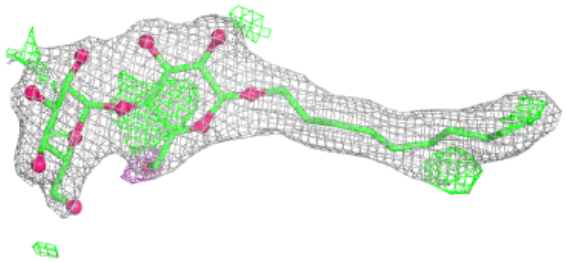


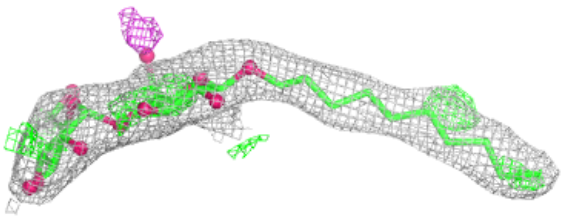


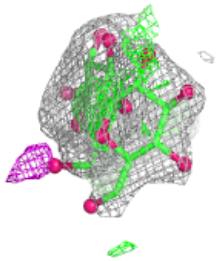


Electron density around DMU B 2:

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

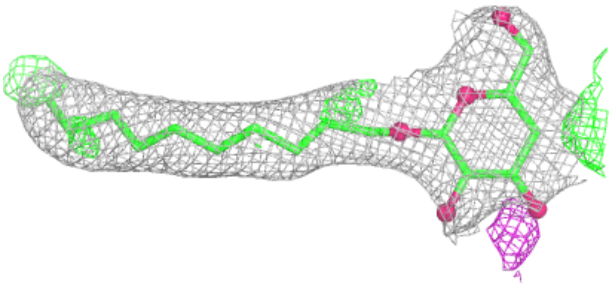


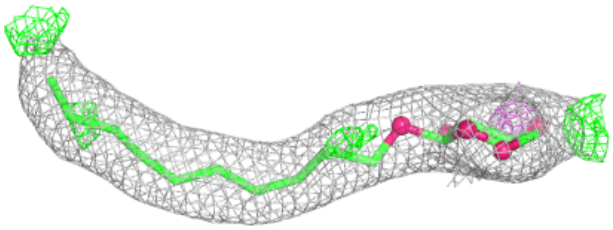


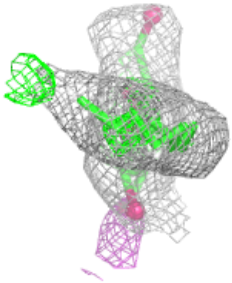


Electron density around DMU A 7:

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

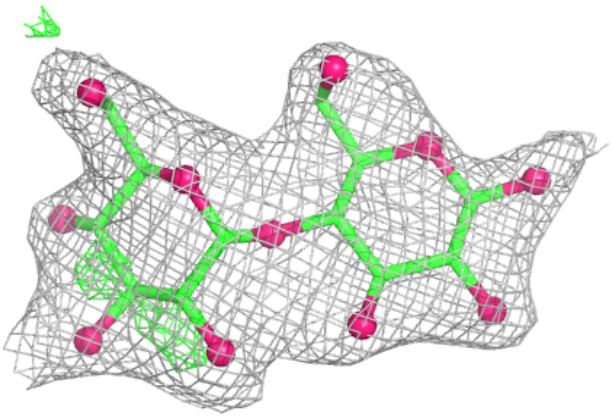


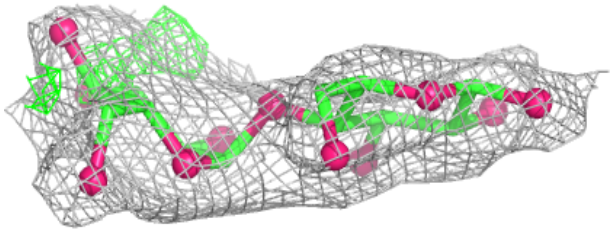


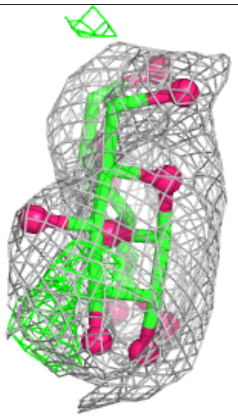


Electron density around DMU B 6:

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

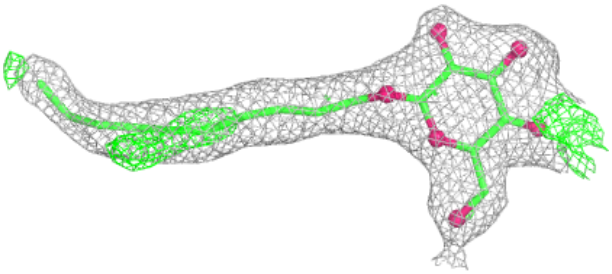


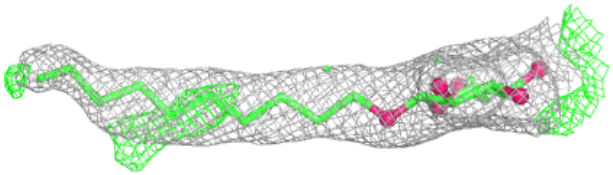


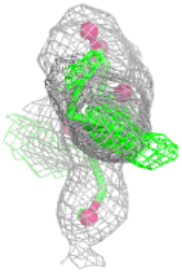


Electron density around DMU A 1005:

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

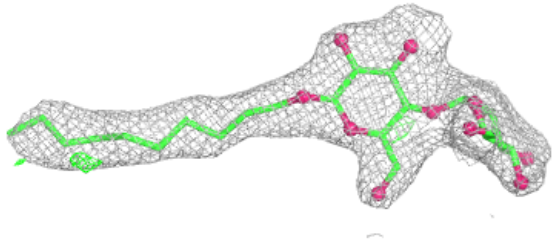


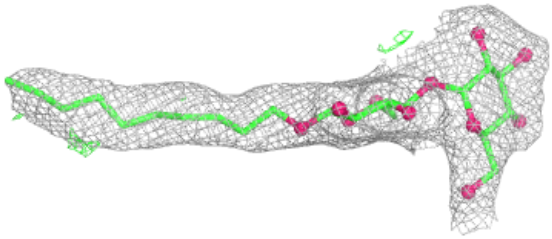


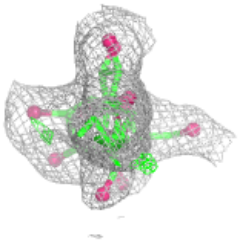


Electron density around DMU C 10:

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

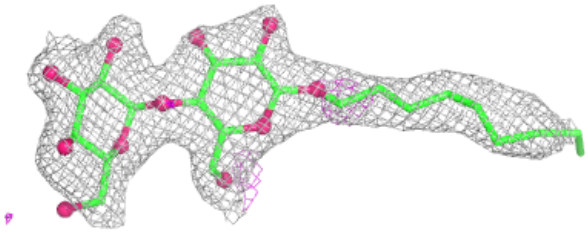


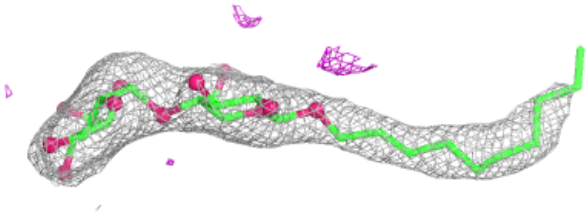


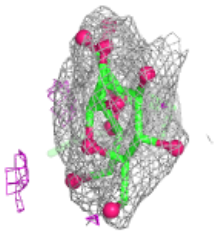


Electron density around DMU B 3:

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

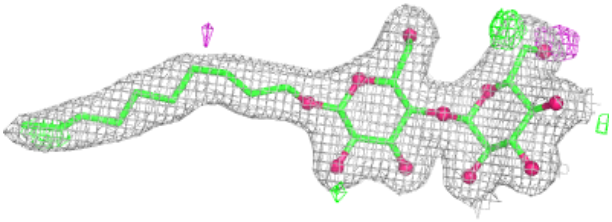


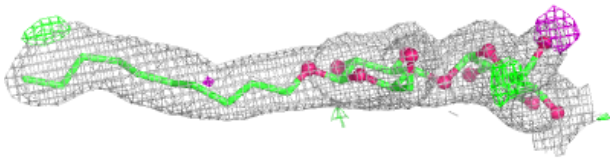




Electron density around DMU B 1:

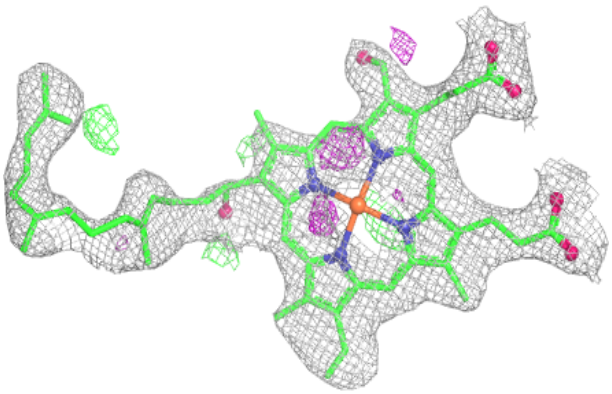
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

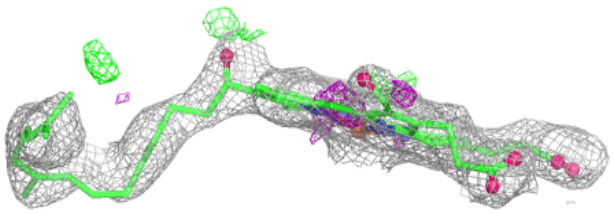


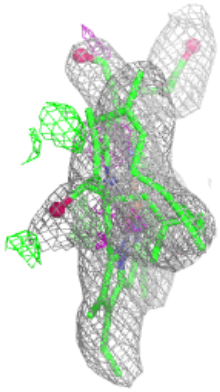


Electron density around HEA C 2 (B):

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

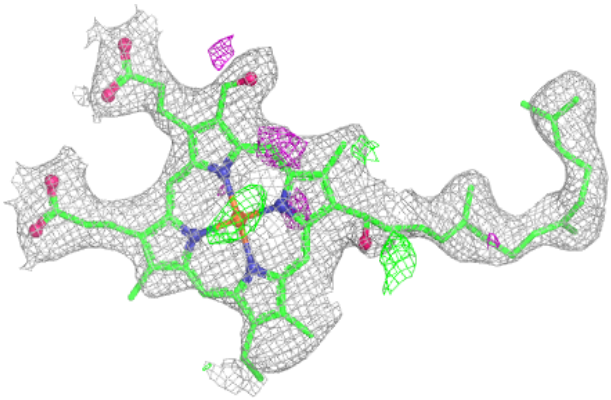


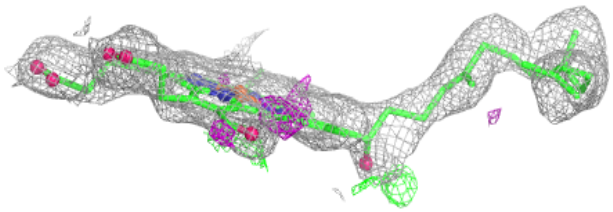


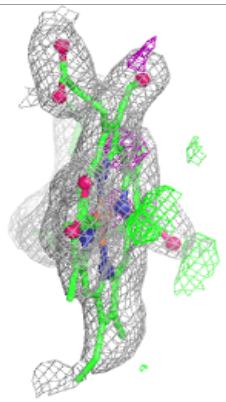


Electron density around HEA C 2 (A):

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

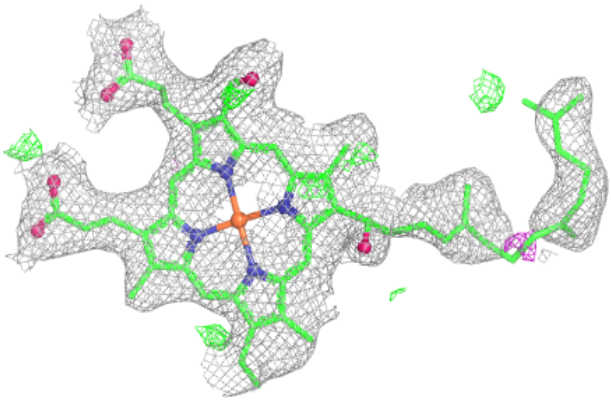


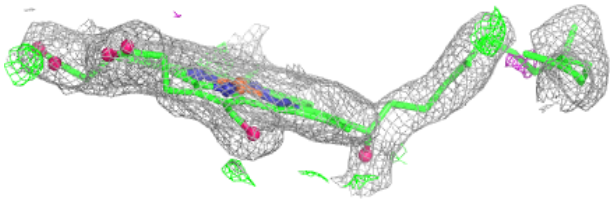


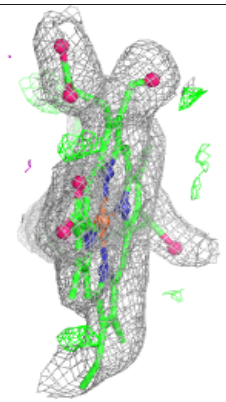


Electron density around HEA A 2 (A):

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

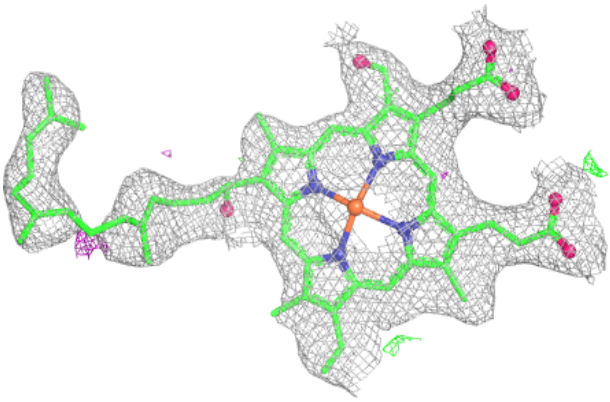


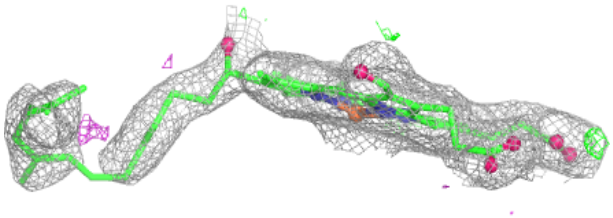


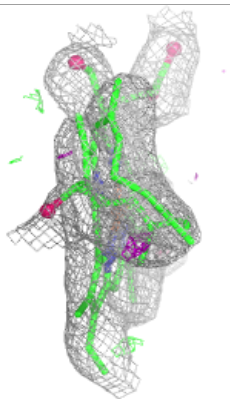


Electron density around HEA A 2 (B):

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

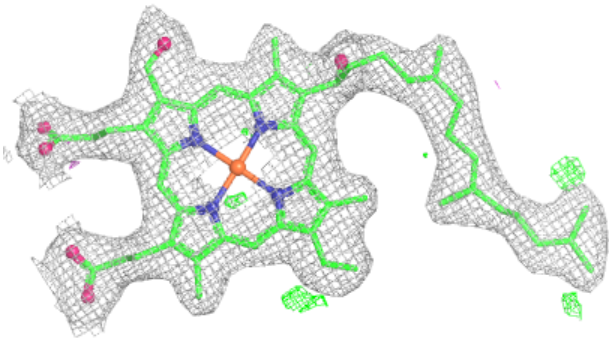


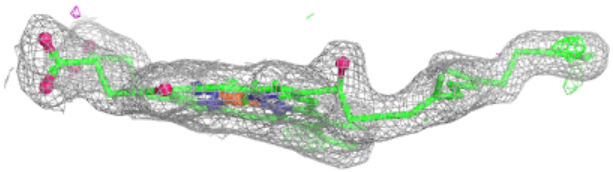


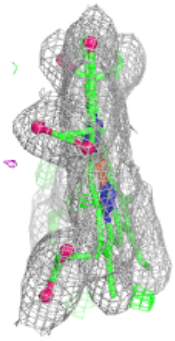


Electron density around HEA C 1:

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

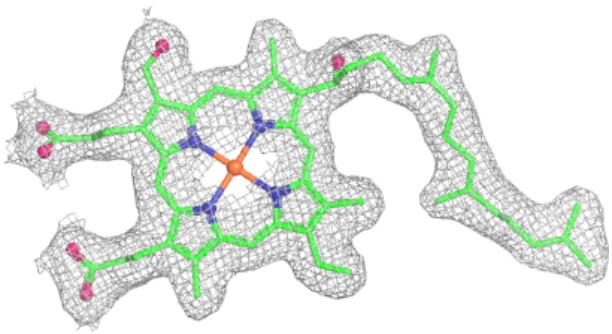


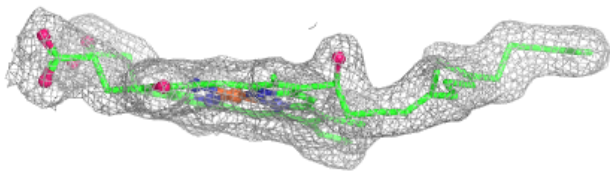


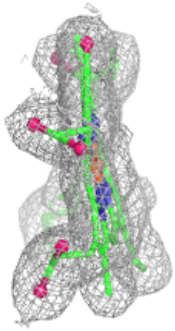


Electron density around HEA A 1:

$2mF_o$-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.