



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:13 AM UTC

PDB ID : 6TR1 / pdb_00006tr1
Title : Native cytochrome c6 from *Thermosynechococcus elongatus* in space group H3
Authors : Falke, S.; Feiler, C.G.; Sarrou, I.
Deposited on : 2019-12-17
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

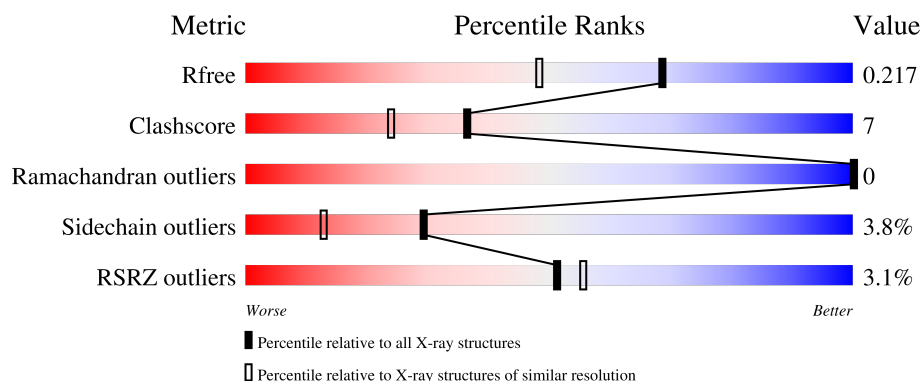
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	86	3% 74% 22% .
2	C	87	3% 56% 37% 7%
3	E	86	2% 67% 31% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2116 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 c6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	86	Total	C	N	O	S	0	0	0
			640	401	111	122	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	GLU	ASP	conflict	UNP P0A3X9
A	86	VAL	ALA	conflict	UNP P0A3X9

- Molecule 2 is a protein called Cytochrome c6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	87	Total	C	N	O	S	0	0	0
			643	402	113	122	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	45	GLU	ASP	conflict	UNP P0A3X9
C	72	MEN	ASP	conflict	UNP P0A3X9

- Molecule 3 is a protein called Cytochrome c6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	86	Total	C	N	O	S	0	1	0
			644	404	111	122	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	86	VAL	ALA	conflict	UNP P0A3X9

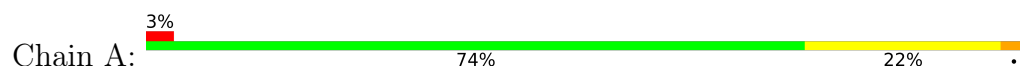
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- The chemical structure of HEC (Hydroxyethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure is labeled with various atoms and groups:
- Central Atom:** Iron (Fe) in purple.
 - Ring Nitrogens:** Four nitrogen atoms (N) in blue, labeled NA, NB, NC, and ND.
 - Ring Carbons:** Various carbon atoms in green, including C1A, C1B, C1C, C1D, C2A, C2B, C2C, C2D, C3A, C3B, C3C, C3D, C4A, C4B, C4C, and C4D.
 - Side Chains and Functional Groups:**
 - Top Left:** A carboxylic acid group with a carbonyl oxygen (O1A) and a hydroxyl group (OH) in red, attached to a carbon (CGA) which is also bonded to a methyl group (CAA) and a vinyl group (C2A).
 - Top Right:** A carboxylic acid group with a carbonyl oxygen (O1D) and a hydroxyl group (OH) in red, attached to a carbon (CGD) which is also bonded to a methyl group (CAD) and a vinyl group (C3D).
 - Bottom Left:** A vinyl group (C3B) and a methyl group (CAB) attached to a carbon (C4B), which is also bonded to a methyl group (CMB) and a vinyl group (C2B).
 - Bottom Right:** A vinyl group (C3C) and a methyl group (CAC) attached to a carbon (C4C), which is also bonded to a methyl group (CMC) and a vinyl group (C2C).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	25	Total O 25 25	0	0
6	C	13	Total O 13 13	0	0
6	E	17	Total O 17 17	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 c6



- Molecule 2: Cytochrome c6



- Molecule 3: Cytochrome c6



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	94.80Å 94.80Å 160.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.53 – 1.70 36.53 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (36.53-1.70) 99.8 (36.53-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.186 , 0.208 0.199 , 0.217	Depositor DCC
R_{free} test set	2903 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.050 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.522 for H, K, L 0.478 for K, H, -L	Depositor
Outliers	0 of 58918 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2116	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MEN, HEC

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	1.99	17/650 (2.6%)	1.64	5/875 (0.6%)
2	C	2.09	20/643 (3.1%)	1.78	12/863 (1.4%)
3	E	1.98	16/657 (2.4%)	1.66	6/884 (0.7%)
All	All	2.02	53/1950 (2.7%)	1.69	23/2622 (0.9%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	74	ALA	N-CA	11.28	1.59	1.46
1	A	36	LEU	C-O	8.36	1.33	1.24
2	C	49	TYR	N-CA	-7.82	1.36	1.46
3	E	6	GLY	N-CA	7.76	1.55	1.45
1	A	33	LYS	C-O	7.62	1.32	1.24
2	C	37	GLU	N-CA	7.44	1.55	1.46
2	C	54	GLY	C-O	7.34	1.35	1.23
3	E	26	MET	CA-C	-7.08	1.45	1.53
3	E	61	PHE	C-O	6.93	1.33	1.24
2	C	33	LYS	N-CA	-6.92	1.38	1.46
2	C	67	ASP	C-O	6.90	1.32	1.24
2	C	47	ILE	N-CA	6.82	1.54	1.46
3	E	60	ALA	N-CA	-6.57	1.37	1.46
1	A	80	GLN	N-CA	6.44	1.54	1.46
3	E	39	PHE	C-O	6.40	1.32	1.24
3	E	65	LEU	N-CA	-6.40	1.38	1.45
2	C	75	ALA	C-O	-6.29	1.16	1.24
1	A	8	LYS	N-CA	-6.28	1.38	1.46
2	C	46	ALA	CA-C	6.25	1.60	1.52
1	A	71	GLN	C-O	6.05	1.31	1.24
3	E	22	GLY	C-O	6.01	1.29	1.23
2	C	6	GLY	N-CA	6.00	1.54	1.45
1	A	34	GLU	C-O	6.00	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	23	ASN	C-O	5.93	1.31	1.24
2	C	46	ALA	C-O	5.93	1.31	1.24
2	C	42	TYR	N-CA	5.92	1.53	1.46
2	C	21	GLY	C-O	5.86	1.31	1.24
2	C	25	VAL	N-CA	-5.76	1.38	1.46
1	A	17	CYS	CA-C	-5.76	1.45	1.52
3	E	59	PRO	C-O	-5.74	1.16	1.23
2	C	71	GLN	N-CA	5.69	1.57	1.46
1	A	81	ALA	CA-C	-5.66	1.45	1.52
2	C	23	ASN	C-O	5.66	1.30	1.23
3	E	24	VAL	CA-CB	5.62	1.61	1.54
2	C	5	ASN	C-O	5.61	1.30	1.24
2	C	23	ASN	CA-CB	5.59	1.60	1.52
2	C	45	GLU	C-N	5.57	1.41	1.33
1	A	75	ALA	C-O	5.52	1.30	1.24
3	E	31	LEU	C-O	-5.51	1.16	1.24
2	C	15	ALA	C-O	5.48	1.31	1.24
2	C	66	THR	N-CA	5.47	1.53	1.45
3	E	46	ALA	N-CA	5.39	1.52	1.46
1	A	70	ILE	CA-C	5.37	1.59	1.52
3	E	61	PHE	CA-C	5.35	1.59	1.52
3	E	24	VAL	C-O	5.31	1.31	1.24
1	A	22	GLY	C-O	5.31	1.29	1.24
3	E	50	GLN	CD-OE1	5.24	1.33	1.23
1	A	67	ASP	C-O	-5.23	1.18	1.24
1	A	18	HIS	CA-CB	-5.17	1.45	1.53
1	A	44	GLU	C-O	5.13	1.29	1.24
1	A	47	ILE	C-O	-5.04	1.18	1.24
1	A	50	GLN	CA-CB	-5.02	1.45	1.53
1	A	45	GLU	N-CA	-5.02	1.40	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	26	MET	CG-SD-CE	-9.21	80.65	100.90
1	A	58	MET	CA-C-N	7.51	127.52	119.78
1	A	58	MET	C-N-CA	7.51	127.52	119.78
3	E	24	VAL	CG1-CB-CG2	7.39	127.06	110.80
2	C	77	VAL	N-CA-C	-7.31	103.33	110.72
2	C	48	ILE	N-CA-C	6.60	117.29	110.36
2	C	6	GLY	N-CA-C	-6.35	106.48	114.16
2	C	44	GLU	N-CA-C	-6.35	104.28	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	41	MET	N-CA-C	6.10	120.85	113.17
2	C	53	HIS	N-CA-C	6.09	120.87	113.38
3	E	65	LEU	N-CA-C	-5.96	100.19	109.72
3	E	53	HIS	CB-CA-C	-5.91	99.37	109.65
3	E	45	ASP	N-CA-C	-5.83	105.00	111.36
1	A	80	GLN	N-CA-CB	5.83	118.78	110.16
1	A	57	ALA	N-CA-C	5.67	119.45	112.54
2	C	4	ALA	CA-C-O	-5.65	113.97	120.24
2	C	8	LYS	N-CA-C	-5.58	105.28	111.36
2	C	4	ALA	N-CA-C	-5.58	104.83	111.69
2	C	18	HIS	N-CA-C	5.54	119.34	112.59
3	E	39	PHE	CA-C-O	5.39	125.87	119.56
2	C	7	ALA	N-CA-C	5.21	117.04	111.36
1	A	39	PHE	N-CA-C	5.17	118.62	112.72
2	C	9	VAL	N-CA-C	-5.14	105.53	110.72

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	640	0	623	6	0
2	C	643	0	624	14	0
3	E	644	0	630	9	0
4	A	43	0	30	2	0
4	C	43	0	31	8	0
4	E	43	0	31	5	0
5	A	1	0	0	0	0
5	C	4	0	0	0	0
6	A	25	0	0	0	0
6	C	13	0	0	0	0
6	E	17	0	0	0	0
All	All	2116	0	1969	29	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 (29) 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)
2:C:17:CYS:SG	4:C:101:HEC:CAC	2.13	1.36
2:C:17:CYS:SG	4:C:101:HEC:HAC	1.92	1.10
2:C:17:CYS:SG	4:C:101:HEC:C3C	2.78	0.71
3:E:19[B]:MET:H	3:E:19[B]:MET:HE3	1.55	0.70
2:C:17:CYS:SG	4:C:101:HEC:CBC	2.77	0.69
2:C:58:MET:HB2	4:C:101:HEC:C1D	2.29	0.62
3:E:25:VAL:HG21	4:E:101:HEC:CBC	2.28	0.62
2:C:19:MET:HG3	2:C:20:GLY:N	2.16	0.60
4:E:101:HEC:HHD	4:E:101:HEC:HBC3	1.84	0.59
2:C:48:ILE:O	2:C:52:GLN:HG3	2.03	0.59
4:E:101:HEC:CBC	4:E:101:HEC:HHD	2.36	0.55
3:E:25:VAL:HG21	4:E:101:HEC:HBC1	1.88	0.55
2:C:17:CYS:HG	4:C:101:HEC:HAC	1.72	0.50
4:C:101:HEC:HMC3	4:C:101:HEC:HBC3	1.94	0.48
3:E:34:GLU:O	3:E:38:GLN:HG3	2.14	0.46
3:E:15:ALA:O	3:E:19[B]:MET:HE3	2.16	0.45
3:E:66:THR:OG1	3:E:69:GLN:HG3	2.17	0.45
2:C:2:ASP:OD1	2:C:2:ASP:C	2.59	0.45
1:A:86:VAL:CG1	2:C:28:ASN:HD22	2.29	0.45
1:A:58:MET:HB2	4:A:101:HEC:C1D	2.48	0.44
3:E:1:ALA:HB1	3:E:72:ASP:OD1	2.19	0.43
3:E:78:LEU:HA	3:E:78:LEU:HD23	1.70	0.43
2:C:49:TYR:CE2	2:C:53:HIS:CE1	3.07	0.43
1:A:19:MET:HE3	1:A:19:MET:HB2	1.74	0.42
1:A:86:VAL:HG13	2:C:28:ASN:HD22	1.84	0.41
1:A:58:MET:HG3	4:A:101:HEC:NC	2.35	0.41
3:E:58:MET:HG3	4:E:101:HEC:NC	2.36	0.41
1:A:86:VAL:CG1	2:C:28:ASN:HB2	2.50	0.41
2:C:29:LYS:HE2	4:C:101:HEC:O1D	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	84/86 (98%)	78 (93%)	6 (7%)	0	100	100
2	C	84/87 (97%)	80 (95%)	4 (5%)	0	100	100
3	E	85/86 (99%)	82 (96%)	3 (4%)	0	100	100
All	All	253/259 (98%)	240 (95%)	13 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	62/62 (100%)	60 (97%)	2 (3%)	34	17
2	C	60/60 (100%)	56 (93%)	4 (7%)	15	4
3	E	63/62 (102%)	62 (98%)	1 (2%)	55	41
All	All	185/184 (100%)	178 (96%)	7 (4%)	29	13

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	MET
1	A	80	GLN
2	C	19	MET
2	C	29	LYS
2	C	45	GLU
2	C	55	LYS
3	E	26	MET

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

Mol	Chain	Res	Type
2	C	53	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	MEN	C	72	2	7,8,9	1.56	1 (14%)	4,9,11	3.80	2 (50%)

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
2	MEN	C	72	2	-	2/7/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	72	MEN	CA-N	-2.72	1.40	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	72	MEN	OD1-CG-CB	-5.61	113.34	121.54
2	C	72	MEN	CB-CG-ND2	5.02	122.09	115.53

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	72	MEN	CA-CB-CG-OD1
2	C	72	MEN	CA-CB-CG-ND2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	HEC	C	101	2	46,50,50	2.04	15 (32%)	58,82,82	2.18	18 (31%)
4	HEC	A	101	1	46,50,50	2.14	16 (34%)	58,82,82	2.03	17 (29%)
4	HEC	E	101	3	46,50,50	2.25	20 (43%)	58,82,82	2.11	20 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEC	C	101	2	-	7/14/54/54	-
4	HEC	A	101	1	-	6/14/54/54	-
4	HEC	E	101	3	-	5/14/54/54	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	101	HEC	C4B-NB	-5.70	1.28	1.39
4	A	101	HEC	CAC-C3C	4.72	1.50	1.35
4	E	101	HEC	CBC-CAC	-4.57	1.32	1.49
4	C	101	HEC	O1A-CGA	4.31	1.36	1.22
4	E	101	HEC	C1D-ND	-4.30	1.31	1.39
4	C	101	HEC	CBC-CAC	-4.30	1.33	1.49
4	C	101	HEC	CAB-C3B	4.29	1.48	1.35
4	E	101	HEC	CAB-C3B	4.25	1.48	1.35
4	A	101	HEC	C1C-NC	-4.16	1.31	1.39
4	A	101	HEC	CHC-C4B	4.11	1.46	1.38
4	A	101	HEC	O2A-CGA	-3.96	1.17	1.30
4	C	101	HEC	C4A-NA	-3.79	1.32	1.39
4	A	101	HEC	C4B-NB	-3.72	1.32	1.39
4	C	101	HEC	CMD-C2D	-3.61	1.43	1.50
4	A	101	HEC	CBD-CAD	3.56	1.64	1.51
4	C	101	HEC	CBA-CAA	3.54	1.64	1.51
4	A	101	HEC	CBB-CAB	-3.41	1.36	1.49
4	A	101	HEC	CAB-C3B	3.35	1.45	1.35
4	E	101	HEC	CHC-C4B	3.26	1.44	1.38
4	A	101	HEC	C1A-NA	-3.26	1.33	1.39
4	E	101	HEC	C1D-C2D	3.13	1.50	1.43
4	E	101	HEC	CAC-C3C	3.12	1.45	1.35
4	E	101	HEC	CHD-C4C	2.94	1.44	1.38
4	A	101	HEC	CHB-C1B	2.91	1.45	1.39
4	E	101	HEC	C3C-C2C	-2.76	1.31	1.41
4	E	101	HEC	CBA-CAA	2.75	1.61	1.51
4	C	101	HEC	C1A-NA	2.69	1.44	1.39
4	E	101	HEC	C1C-NC	-2.67	1.34	1.39
4	A	101	HEC	O1A-CGA	2.66	1.30	1.22
4	C	101	HEC	C1D-ND	-2.62	1.34	1.39
4	C	101	HEC	CAC-C3C	2.58	1.43	1.35
4	E	101	HEC	C4D-ND	-2.57	1.34	1.39
4	C	101	HEC	C3C-C4C	2.56	1.50	1.46
4	A	101	HEC	CMA-C3A	-2.53	1.45	1.50
4	E	101	HEC	O2D-CGD	-2.53	1.22	1.30
4	C	101	HEC	CHB-C1B	2.48	1.45	1.39
4	C	101	HEC	C3D-C2D	-2.37	1.32	1.38
4	A	101	HEC	C4C-NC	-2.36	1.35	1.39
4	A	101	HEC	CMC-C2C	2.36	1.55	1.50
4	A	101	HEC	CHC-C1C	-2.30	1.34	1.39
4	E	101	HEC	CMD-C2D	-2.28	1.46	1.50
4	E	101	HEC	CMB-C2B	-2.25	1.46	1.50
4	C	101	HEC	CBA-CGA	2.19	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	101	HEC	C4A-NA	-2.18	1.35	1.39
4	C	101	HEC	C4C-NC	-2.18	1.35	1.39
4	E	101	HEC	CBD-CAD	2.16	1.59	1.51
4	E	101	HEC	C1B-C2B	2.14	1.48	1.43
4	C	101	HEC	C2A-C3A	2.11	1.41	1.36
4	E	101	HEC	C3B-C4B	2.10	1.49	1.46
4	E	101	HEC	C1B-NB	-2.04	1.35	1.39
4	E	101	HEC	CAD-C3D	2.01	1.56	1.51

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	101	HEC	CBB-CAB-C3B	-6.89	113.66	127.43
4	C	101	HEC	CBB-CAB-C3B	-6.52	114.41	127.43
4	C	101	HEC	CHB-C4A-NA	5.75	130.72	124.45
4	A	101	HEC	CBC-CAC-C3C	-5.45	116.55	127.43
4	C	101	HEC	C2A-C1A-NA	-5.30	105.21	110.32
4	E	101	HEC	C3D-C4D-ND	5.03	115.73	110.15
4	A	101	HEC	CHC-C4B-NB	-4.34	119.72	124.45
4	A	101	HEC	CAD-C3D-C4D	3.97	132.68	124.94
4	C	101	HEC	CHD-C4C-NC	3.93	128.73	124.45
4	A	101	HEC	C2A-C1A-NA	-3.90	106.56	110.32
4	E	101	HEC	CMD-C2D-C3D	3.76	133.59	125.62
4	A	101	HEC	C2D-C1D-ND	3.68	116.04	110.14
4	E	101	HEC	CHA-C1A-NA	-3.68	120.45	124.45
4	A	101	HEC	CBD-CAD-C3D	-3.52	102.79	112.53
4	C	101	HEC	C4C-NC-C1C	3.45	111.44	105.82
4	E	101	HEC	C1D-C2D-C3D	-3.32	103.02	106.82
4	C	101	HEC	C4A-NA-C1A	3.29	111.19	105.82
4	C	101	HEC	CMC-C2C-C1C	3.19	130.28	125.42
4	C	101	HEC	CBC-CAC-C3C	-3.16	121.11	127.43
4	E	101	HEC	C2C-C1C-NC	3.16	115.20	110.14
4	E	101	HEC	CBA-CAA-C2A	-3.13	103.88	112.53
4	E	101	HEC	O2A-CGA-CBA	3.12	123.84	114.00
4	C	101	HEC	CAD-C3D-C2D	-3.11	120.10	127.07
4	C	101	HEC	CMD-C2D-C1D	3.09	130.12	125.42
4	A	101	HEC	C3D-C4D-ND	3.05	113.54	110.15
4	E	101	HEC	C4C-NC-C1C	-3.03	100.88	105.82
4	C	101	HEC	O1D-CGD-CBD	-3.00	113.58	123.09
4	A	101	HEC	CAA-CBA-CGA	2.96	121.53	113.67
4	A	101	HEC	C1C-CHC-C4B	2.92	133.67	124.66
4	A	101	HEC	C4C-NC-C1C	2.91	110.57	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	101	HEC	C4D-ND-C1D	-2.90	101.10	105.82
4	E	101	HEC	CHA-C1A-C2A	2.90	129.44	124.86
4	A	101	HEC	CMD-C2D-C1D	2.85	129.76	125.42
4	A	101	HEC	O2D-CGD-CBD	2.85	123.00	114.00
4	C	101	HEC	CAD-C3D-C4D	2.84	130.49	124.94
4	E	101	HEC	CHB-C4A-NA	2.75	127.45	124.45
4	E	101	HEC	CHD-C1D-C2D	-2.74	119.48	127.43
4	C	101	HEC	O2D-CGD-CBD	2.73	122.64	114.00
4	E	101	HEC	CBD-CAD-C3D	-2.73	104.99	112.53
4	A	101	HEC	CBB-CAB-C3B	-2.71	122.02	127.43
4	E	101	HEC	C4D-ND-C1D	-2.63	101.53	105.82
4	E	101	HEC	O1A-CGA-CBA	-2.58	114.91	123.09
4	E	101	HEC	CHD-C4C-NC	-2.47	121.76	124.45
4	A	101	HEC	C1D-C2D-C3D	-2.38	104.09	106.82
4	E	101	HEC	C2D-C1D-ND	2.30	113.83	110.14
4	E	101	HEC	C4B-NB-C1B	2.30	109.56	105.82
4	A	101	HEC	CHA-C1A-NA	2.28	126.94	124.45
4	C	101	HEC	C1D-C2D-C3D	-2.23	104.26	106.82
4	C	101	HEC	CMA-C3A-C4A	2.23	128.65	124.73
4	C	101	HEC	CHA-C1A-C2A	2.22	128.36	124.86
4	C	101	HEC	CBD-CAD-C3D	-2.19	106.48	112.53
4	A	101	HEC	CAD-C3D-C2D	-2.18	122.19	127.07
4	C	101	HEC	CHB-C4A-C3A	-2.17	120.97	125.49
4	E	101	HEC	CHC-C1C-NC	-2.15	119.97	123.86
4	E	101	HEC	CHA-C4D-C3D	-2.02	120.87	125.30

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	101	HEC	C2B-C3B-CAB-CBB
4	A	101	HEC	C4B-C3B-CAB-CBB
4	A	101	HEC	C2C-C3C-CAC-CBC
4	A	101	HEC	C4C-C3C-CAC-CBC
4	C	101	HEC	C2B-C3B-CAB-CBB
4	C	101	HEC	C4B-C3B-CAB-CBB
4	C	101	HEC	C2C-C3C-CAC-CBC
4	C	101	HEC	C4C-C3C-CAC-CBC
4	E	101	HEC	C2B-C3B-CAB-CBB
4	E	101	HEC	C4B-C3B-CAB-CBB
4	C	101	HEC	CAD-CBD-CGD-O2D
4	C	101	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
4	A	101	HEC	CAD-CBD-CGD-O1D
4	A	101	HEC	CAD-CBD-CGD-O2D
4	E	101	HEC	CAD-CBD-CGD-O2D
4	E	101	HEC	CAD-CBD-CGD-O1D
4	C	101	HEC	CAA-CBA-CGA-O2A
4	E	101	HEC	CAA-CBA-CGA-O1A

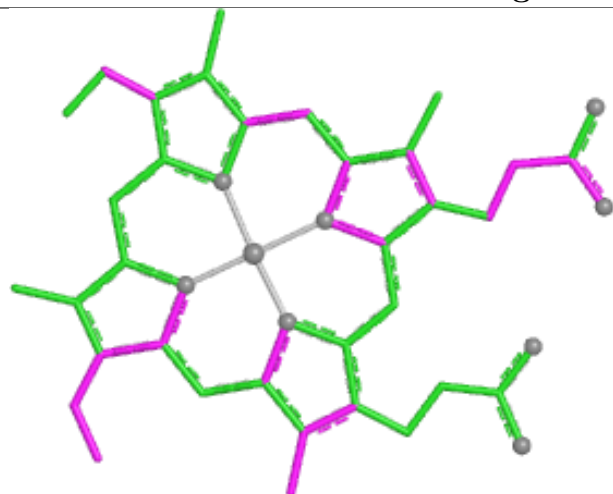
There are no ring outliers.

3 monomers are involved in 15 short contacts:

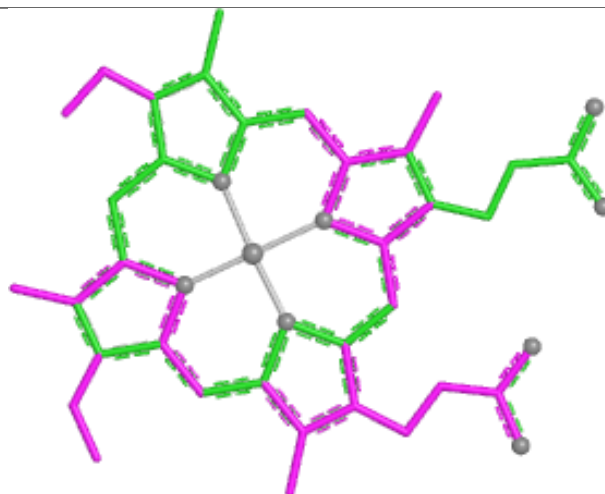
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	101	HEC	8	0
4	A	101	HEC	2	0
4	E	101	HEC	5	0

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

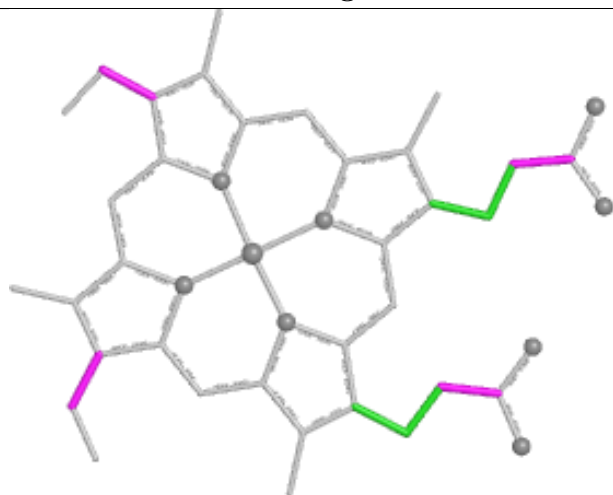
Ligand HEC C 101



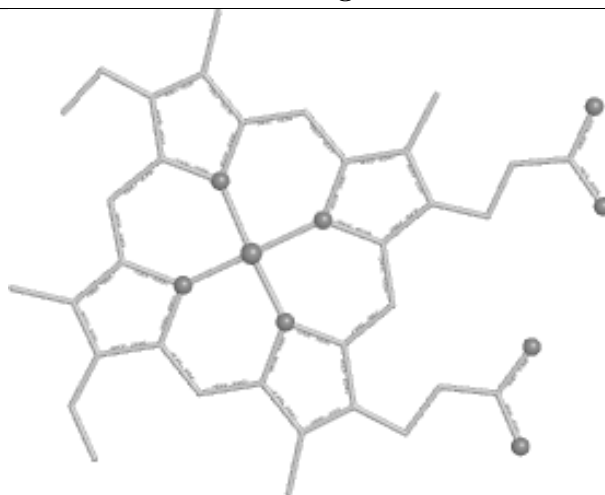
Bond lengths



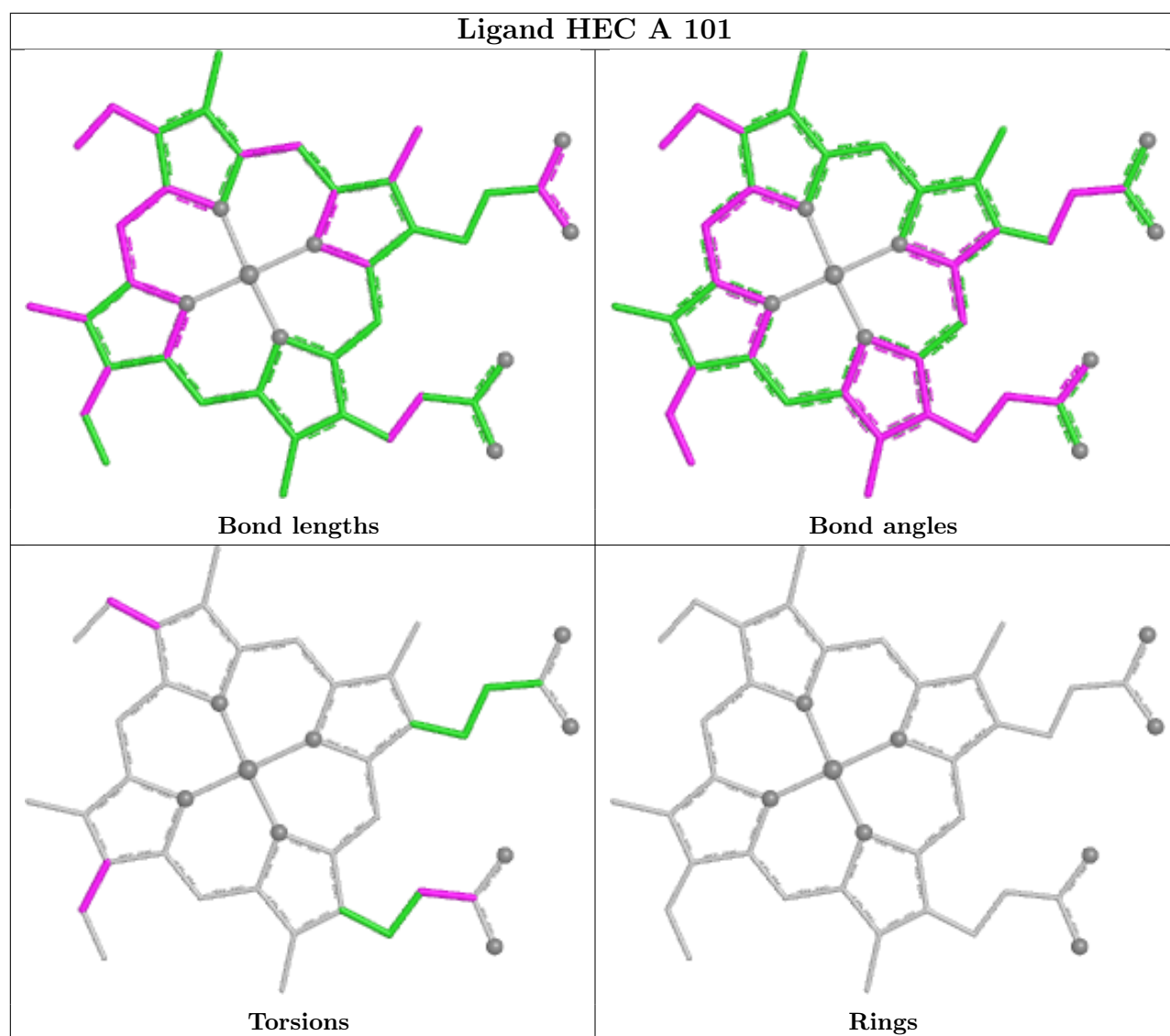
Bond angles

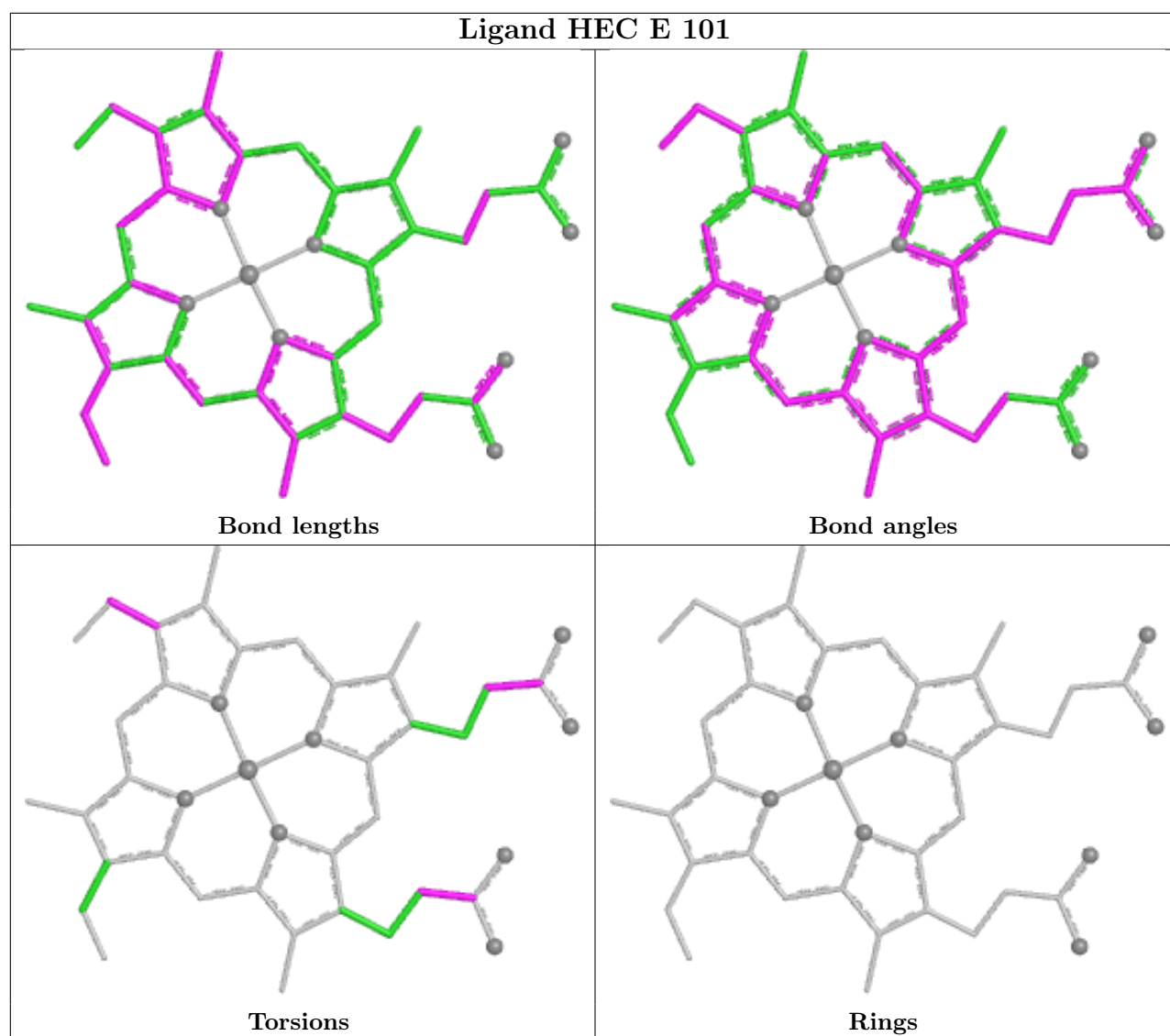


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	86/86 (100%)	0.30	3 (3%) 47 52	14, 20, 30, 36	0
2	C	86/87 (98%)	0.33	3 (3%) 47 52	14, 19, 32, 50	0
3	E	86/86 (100%)	0.15	2 (2%) 61 65	13, 20, 31, 38	1 (1%)
All	All	258/259 (99%)	0.26	8 (3%) 51 55	13, 20, 31, 50	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	VAL	4.4
2	C	87	GLY	3.5
2	C	1	ALA	3.4
2	C	86	ALA	3.4
3	E	1	ALA	3.0
1	A	1	ALA	2.3
3	E	86	VAL	2.2
1	A	19	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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
2	MEN	C	72	9/10	0.94	0.10	15,17,25,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

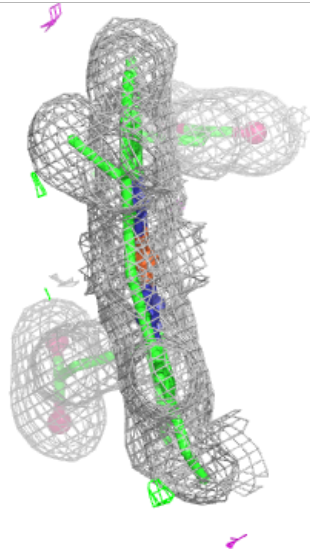
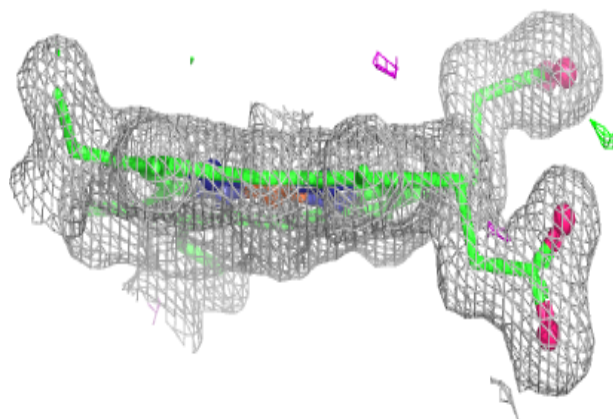
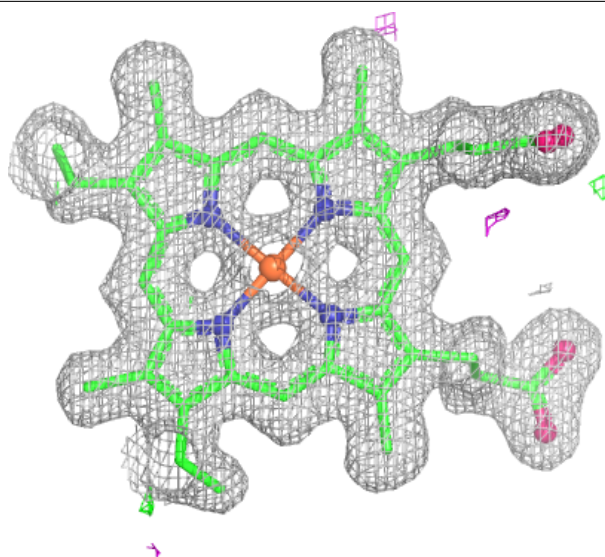
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	C	104	1/1	0.95	0.11	36,36,36,36	0
5	NA	C	105	1/1	0.95	0.19	40,40,40,40	0
5	NA	C	103	1/1	0.97	0.08	36,36,36,36	0
5	NA	A	102	1/1	0.97	0.10	37,37,37,37	0
5	NA	C	102	1/1	0.97	0.07	33,33,33,33	0
4	HEC	E	101	43/43	0.99	0.05	10,12,19,22	0
4	HEC	A	101	43/43	0.99	0.06	12,15,20,23	0
4	HEC	C	101	43/43	0.99	0.06	10,14,18,21	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.

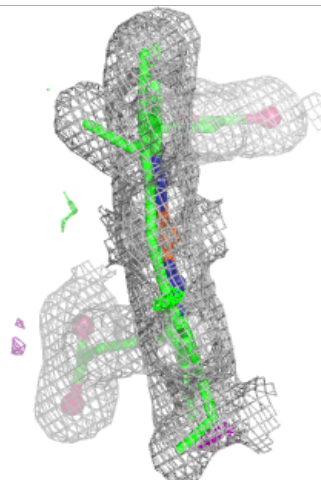
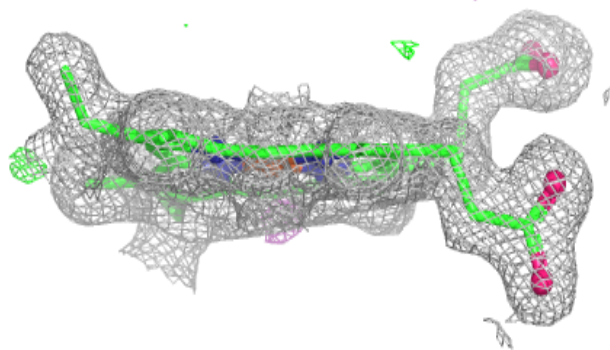
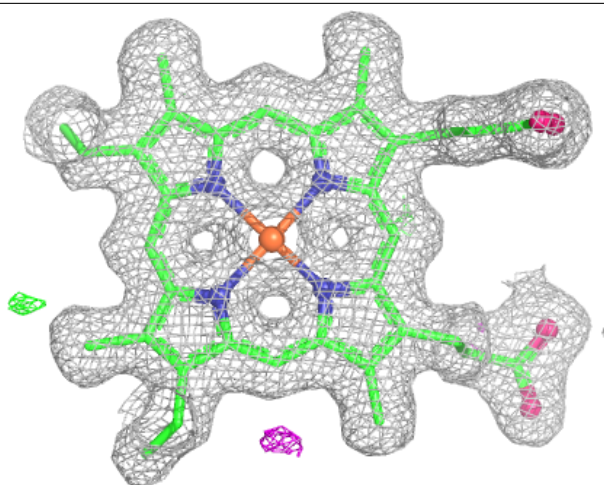
Electron density around HEC E 101:

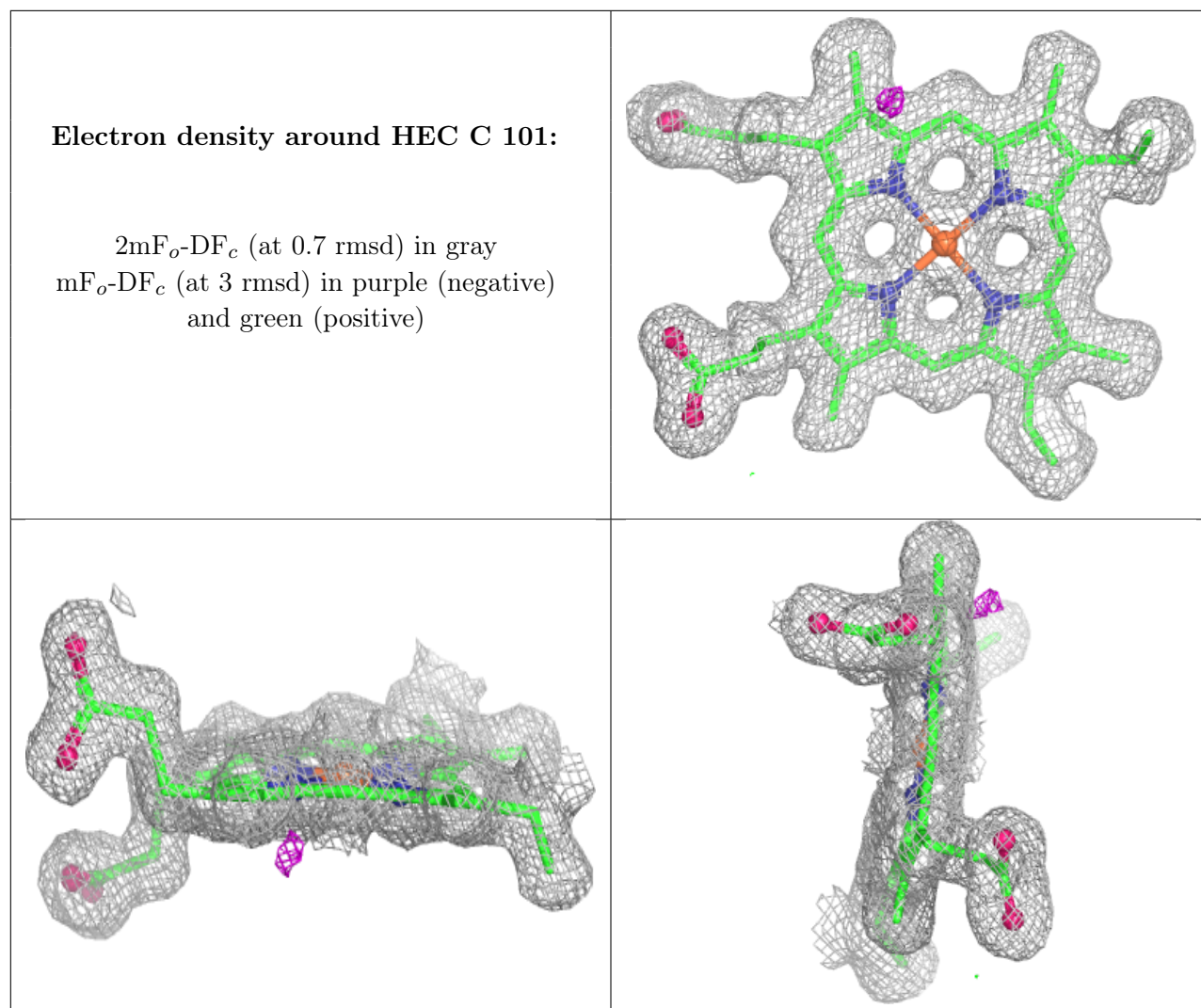
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 101:

$2mF_o-DF_c$ (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.