

wwPDB X-ray Structure Validation Summary Report (i)

Sep 14, 2020 - 08:43 AM BST

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

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) were used in the production of this report:

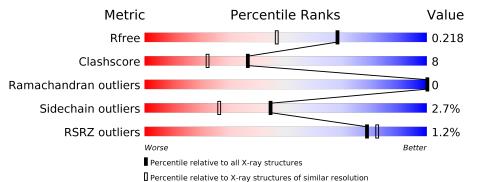
Mogul Xtriage (Phenix) EDS buster-report	::	1.8.5 (274361), CSD as541be (2020) 1.13 2.14.4.dev1
CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	:	7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	$2.14.4\mathrm{dev1}$

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 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R _{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695(1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 on 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	А	86	92%		7%•					
2	С	87	74%	25%	•					
3	Е	86	% 77%	20%	•					



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	А	86	Total 640	C 401	N 111	0 122	S 6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	45	GLU	ASP	$\operatorname{conflict}$	UNP P0A3X9
А	86	VAL	ALA	$\operatorname{conflict}$	UNP P0A3X9

• Molecule 2 is a protein called Cytochrome c6.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	45	GLU	ASP	$\operatorname{conflict}$	UNP P0A3X9
С	72	MEN	ASP	conflict	UNP P0A3X9

• Molecule 3 is a protein called Cytochrome c6.

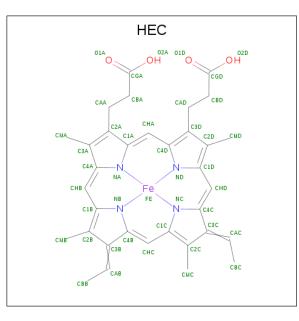
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Е	86	Total 644	C 404	N 111	0 122	S 7	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	86	VAL	ALA	$\operatorname{conflict}$	UNP P0A3X9



• Molecule 4 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	A	Atoms			ZeroOcc	AltConf
4	А	1	Total (43 3	C Fe 4 1		O 4	0	0
4	С	1	Total (43 3		N 4	O 4	0	0
4	Е	1	Total C 43 3	$\begin{array}{cc} \mathrm{Fe} \\ \mathrm{4} & 1 \end{array}$	N 4	0 4	0	0

• Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Na 1 1	0	0
5	С	4	Total Na 4 4	0	0

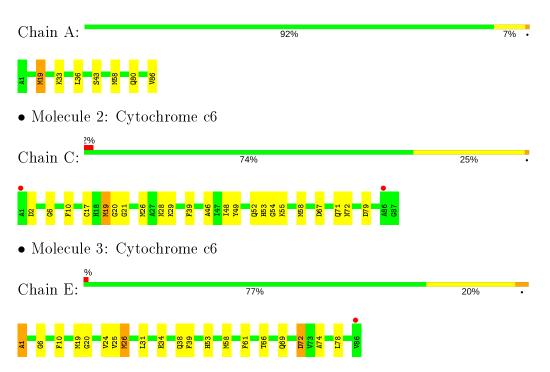
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	25	$\begin{array}{cc} \text{Total} & \text{O} \\ 25 & 25 \end{array}$	0	0
6	С	13	Total O 13 13	0	0
6	Е	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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants	94.80Å 94.80 Å 160.22 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.53 - 1.70	Depositor
Resolution (A)	36.53 - 1.70	EDS
% Data completeness	98.2 (36.53-1.70)	Depositor
(in resolution range)	99.8 (36.53 - 1.70)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	3.84 (at 1.70 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
D D	0.186 , 0.208	Depositor
R, R_{free}	0.200 , 0.218	DCC
R_{free} test set	2903 reflections (4.93%)	wwPDB-VP
Wilson B-factor $(Å^2)$	19.1	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.40 , 45.8	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.050 for h,-h-k,-l	Xtriage
Depented twinning fraction	0.522 for H, K, L	Deperitor
Reported twinning fraction	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.

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.



¹Intensities estimated from amplitudes.

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: 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	Bo	nd lengths	Bond angles		
	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.48	3/650~(0.5%)	1.20	0/875	
2	С	1.62	5/643~(0.8%)	1.41	5/863~(0.6%)	
3	Е	1.53	4/657~(0.6%)	1.41	8/884~(0.9%)	
All	All	1.54	12/1950~(0.6%)	1.35	13/2622~(0.5%)	

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	С	54	GLY	C-O	7.13	1.35	1.23
3	Е	74	ALA	N-CA	6.72	1.59	1.46
3	Е	6	GLY	N-CA	6.25	1.55	1.46
2	С	39	PHE	CG-CD1	5.85	1.47	1.38
1	А	43	SER	CB-OG	-5.49	1.35	1.42

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	С	26	MET	CG-SD-CE	-12.22	80.65	100.20
3	Е	24	VAL	CG1-CB-CG2	10.10	127.06	110.90
2	С	67	ASP	CB-CG-OD1	7.08	124.67	118.30
3	Е	39	PHE	CB-CG-CD1	5.67	124.77	120.80
3	Е	53	HIS	CB-CA-C	-5.52	99.37	110.40

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	А	640	0	623	6	0
2	С	643	0	624	14	0
3	Е	644	0	630	9	0
4	А	43	0	30	3	0
4	С	43	0	31	9	0
4	Е	43	0	31	6	0
5	А	1	0	0	0	0
5	С	4	0	0	0	0
6	А	25	0	0	0	0
6	С	13	0	0	0	0
6	Е	17	0	0	0	0
All	All	2116	0	1969	32	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 8.

The worst 5 of 32 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
2:C:17:CYS:SG	4:C:101:HEC:CBC	2.77	0.69
3:E:19[B]:MET:HE3	3:E:19[B]:MET:H	1.57	0.69

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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	Percentiles	
1	А	84/86~(98%)	78~(93%)	6 (7%)	0	100	100	
2	С	84/87~(97%)	80~(95%)	4 (5%)	0	100	100	
3	Е	85/86~(99%)	82 (96%)	3 (4%)	0	100	100	
All	All	253/259~(98%)	240 (95%)	13~(5%)	0	100	100	

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	62/62~(100%)	60~(97%)	2(3%)	39 20		
2	С	60/60~(100%)	58 (97%)	2(3%)	38 19		
3	Ε	63/62~(102%)	62~(98%)	1 (2%)	62 48		
All	All	185/184~(100%)	$180 \ (97\%)$	5(3%)	44 26		

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

Mol	Chain	Res	Type
1	А	19	MET
1	А	80	GLN
2	С	19	MET
2	С	55	LYS
3	Е	26	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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).

ſ	Mol	Tuno	Type Chain Res	Chain Res		Link	B	ond leng	gths	В	ond ang	gles
	WIOI	туре	Unam	Chain Res		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
	2	MEN	С	72	2	7,8,9	1.48	1 (14%)	$6,\!9,\!11$	<mark>3.09</mark>	2 (33%)	

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
2	MEN	С	72	2	-	2/7/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	С	72	MEN	CA-N	-2.55	1.40	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	С	72	MEN	OD1-CG-CB	-5.57	113.34	121.50
2	С	72	MEN	CB-CG-ND2	4.91	122.09	115.48

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	С	72	MEN	CA-CB-CG-OD1
2	С	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 monosaccharides 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	Bo	Bond lengths			Bond angles		
Moi Type		nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2		
4	HEC	А	101	1	26,50,50	1.76	7 (26%)	18,82,82	2.58	<mark>6 (33%)</mark>	
4	HEC	С	101	2	26,50,50	2.08	6 (23%)	18,82,82	1.81	<mark>5 (27%)</mark>	
4	HEC	Е	101	3	26,50,50	2.42	8 (30%)	18,82,82	<mark>2.78</mark>	7 (38%)	

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	А	101	1	-	0/6/54/54	-
4	HEC	С	101	2	-	0/6/54/54	-
4	HEC	Е	101	3	-	0/6/54/54	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
4	Ε	101	HEC	C3C-C2C	-8.51	1.31	1.40
4	Ε	101	HEC	CBC-CAC	-4.51	1.32	1.49
4	С	101	HEC	CBC-CAC	-4.24	1.33	1.49
4	С	101	HEC	C3B-C2B	-4.16	1.36	1.40
4	С	101	HEC	C3C-C4C	4.10	1.50	1.43



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	Е	101	HEC	C1D-C2D-C3D	-5.72	103.02	107.00
4	А	101	HEC	CAA-CBA-CGA	5.28	121.53	112.67
4	А	101	HEC	CBD-CAD-C3D	-5.26	102.79	112.49
4	Е	101	HEC	CBA-CAA-C2A	-4.67	103.88	112.48
4	Е	101	HEC	CMD-C2D-C3D	4.59	133.59	124.94

The worst 5 of 18 bond angle outliers are listed below:

There are no chirality outliers.

There are no torsion outliers.

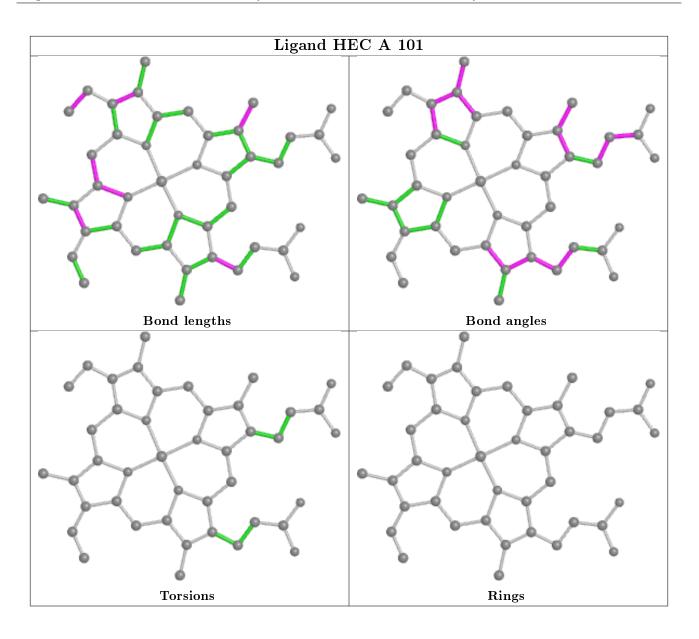
There are no ring outliers.

3 monomers are involved in 18 short contacts:

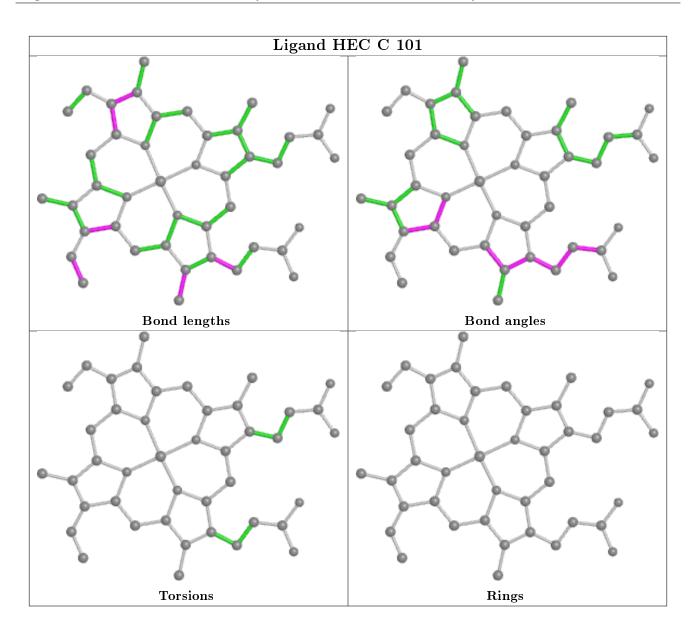
Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
4	А	101	HEC	3	0
4	С	101	HEC	9	0
4	Е	101	HEC	6	0

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.

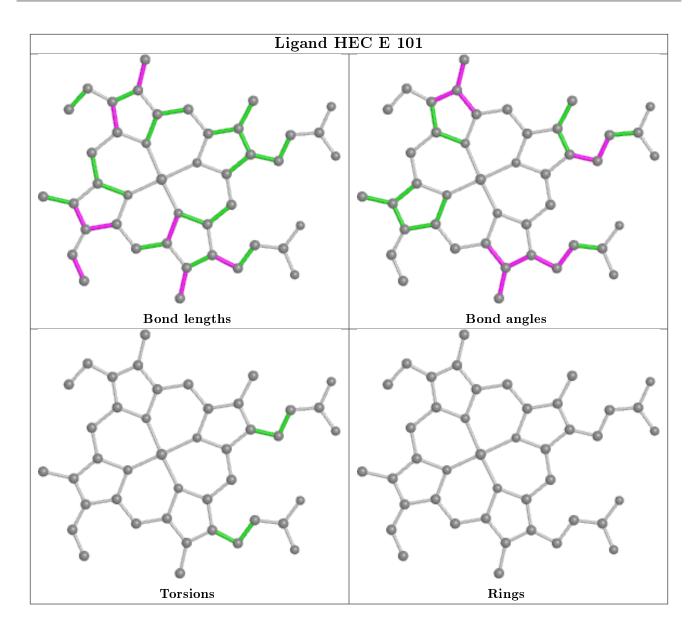












5.7 Other polymers (i)

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, 95^{th} 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 $>$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	86/86~(100%)	-0.33	0 100 100	14, 20, 30, 36	0
2	С	86/87~(98%)	-0.26	2 (2%) 60 65	14, 19, 32, 50	0
3	Е	86/86 (100%)	-0.23	1 (1%) 79 82	13, 20, 31, 38	0
All	All	258/259~(99%)	-0.27	3 (1%) 79 82	13, 20, 31, 50	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Е	86	VAL	3.2
2	С	1	ALA	2.9
2	С	86	ALA	2.4

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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	\mathbf{RSR}	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	$Q{<}0.9$
2	MEN	С	72	9/10	0.96	0.07	$15,\!17,\!25,\!33$	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



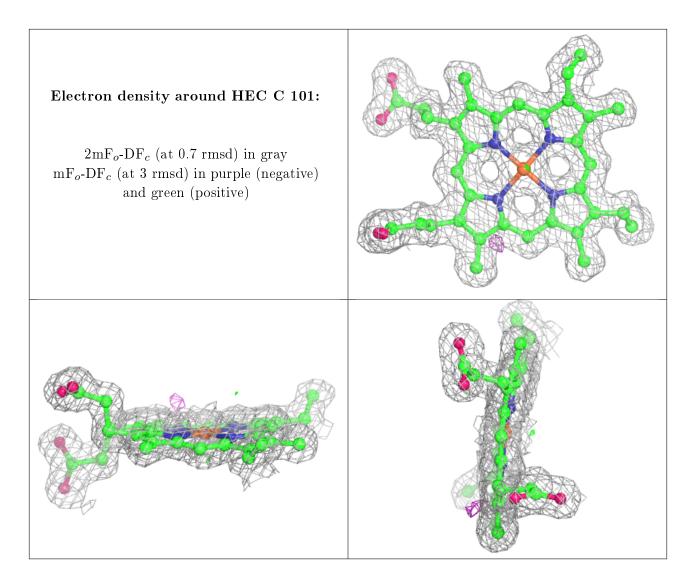
6.4 Ligands (i)

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, 95^{th} 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.

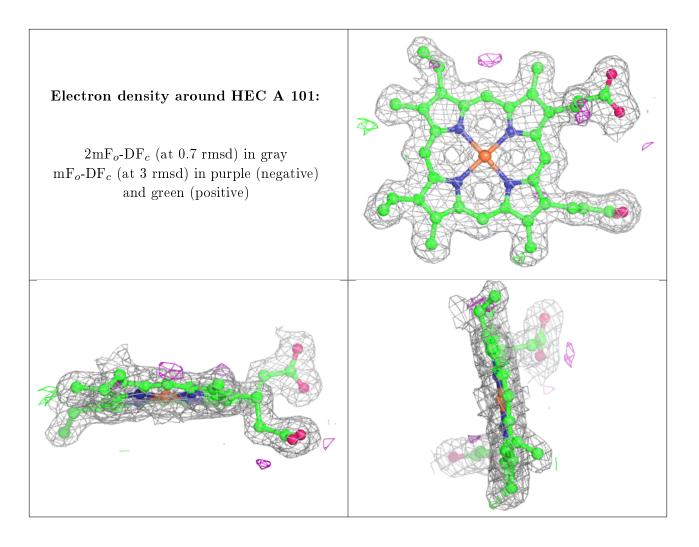
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	$Q{<}0.9$
5	NA	С	105	1/1	0.94	0.12	$40,\!40,\!40,\!40$	0
5	NA	С	104	1/1	0.97	0.09	$36,\!36,\!36,\!36$	0
5	NA	С	103	1/1	0.97	0.08	$36,\!36,\!36,\!36$	0
4	HEC	С	101	43/43	0.98	0.08	$10,\!14,\!18,\!21$	0
5	NA	А	102	1/1	0.98	0.07	37,37,37,37	0
5	NA	С	102	1/1	0.98	0.11	$33,\!33,\!33,\!33$	0
4	HEC	А	101	43/43	0.98	0.08	12,15,20,23	0
4	HEC	Е	101	43/43	0.99	0.08	$10,\!12,\!19,\!22$	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.

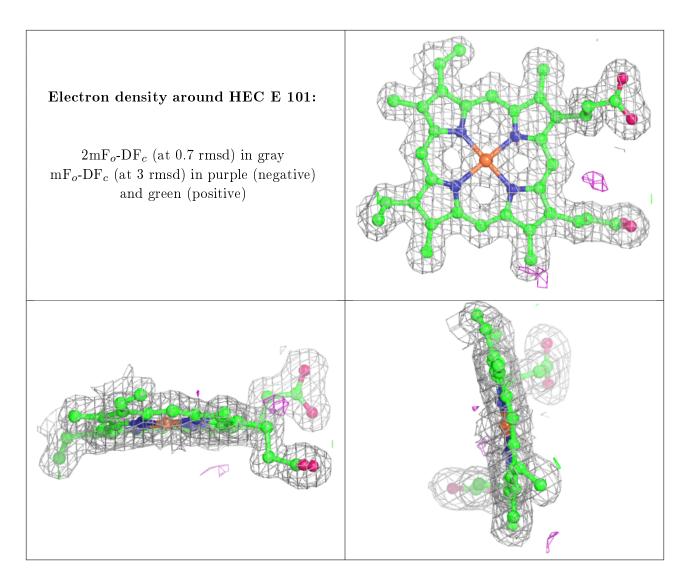












6.5 Other polymers (i)

There are no such residues in this entry.

