



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 03:56 PM GMT

PDB ID : 3PMQ  
Title : Crystal structure of the outer membrane decaheme cytochrome MtrF  
Authors : Clarke, T.A.; Edwards, M.J.; Richardson, D.J.  
Deposited on : 2010-11-17  
Resolution : 3.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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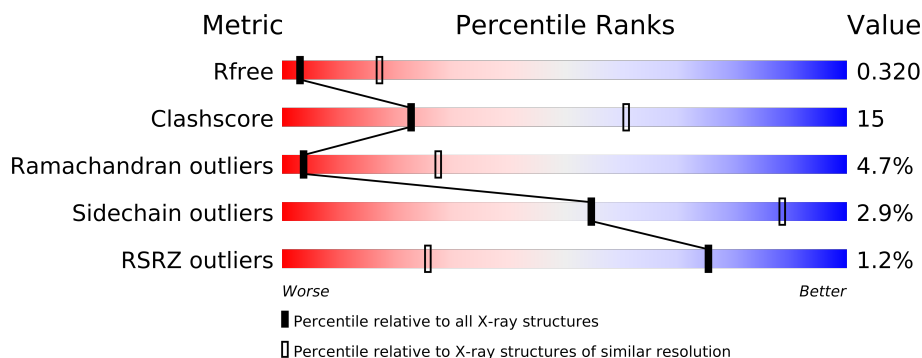
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 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))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	669	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	HEC	A	678	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4826 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Decaheme cytochrome c MtrF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	0	0
			4395	2688	791	883	33			

There are 30 discrepancies between the modelled and reference sequences:

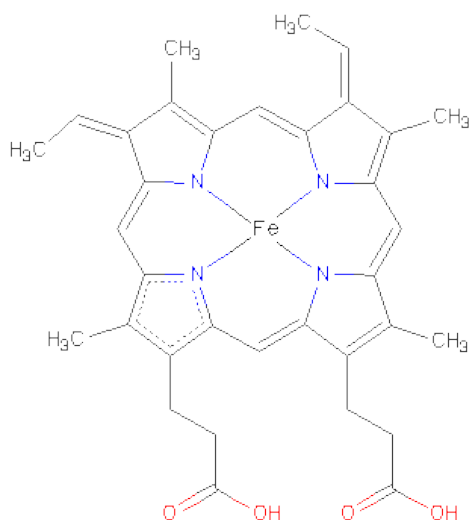
Chain	Residue	Modelled	Actual	Comment	Reference
A	640	LYS	-	EXPRESSION TAG	UNP Q8EG32
A	641	GLY	-	EXPRESSION TAG	UNP Q8EG32
A	642	GLU	-	EXPRESSION TAG	UNP Q8EG32
A	643	LEU	-	EXPRESSION TAG	UNP Q8EG32
A	644	LYS	-	EXPRESSION TAG	UNP Q8EG32
A	645	LEU	-	EXPRESSION TAG	UNP Q8EG32
A	646	GLU	-	EXPRESSION TAG	UNP Q8EG32
A	647	GLY	-	EXPRESSION TAG	UNP Q8EG32
A	648	LYS	-	EXPRESSION TAG	UNP Q8EG32
A	649	PRO	-	EXPRESSION TAG	UNP Q8EG32
A	650	ILE	-	EXPRESSION TAG	UNP Q8EG32
A	651	PRO	-	EXPRESSION TAG	UNP Q8EG32
A	652	ASN	-	EXPRESSION TAG	UNP Q8EG32
A	653	PRO	-	EXPRESSION TAG	UNP Q8EG32
A	654	LEU	-	EXPRESSION TAG	UNP Q8EG32
A	655	LEU	-	EXPRESSION TAG	UNP Q8EG32
A	656	GLY	-	EXPRESSION TAG	UNP Q8EG32
A	657	LEU	-	EXPRESSION TAG	UNP Q8EG32
A	658	ASP	-	EXPRESSION TAG	UNP Q8EG32
A	659	SER	-	EXPRESSION TAG	UNP Q8EG32
A	660	THR	-	EXPRESSION TAG	UNP Q8EG32
A	661	ARG	-	EXPRESSION TAG	UNP Q8EG32
A	662	THR	-	EXPRESSION TAG	UNP Q8EG32
A	663	GLY	-	EXPRESSION TAG	UNP Q8EG32
A	664	HIS	-	EXPRESSION TAG	UNP Q8EG32
A	665	HIS	-	EXPRESSION TAG	UNP Q8EG32
A	666	HIS	-	EXPRESSION TAG	UNP Q8EG32

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Chain	Residue	Modelled	Actual	Comment	Reference
A	667	HIS	-	EXPRESSION TAG	UNP Q8EG32
A	668	HIS	-	EXPRESSION TAG	UNP Q8EG32
A	669	HIS	-	EXPRESSION TAG	UNP Q8EG32

- Molecule 2 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

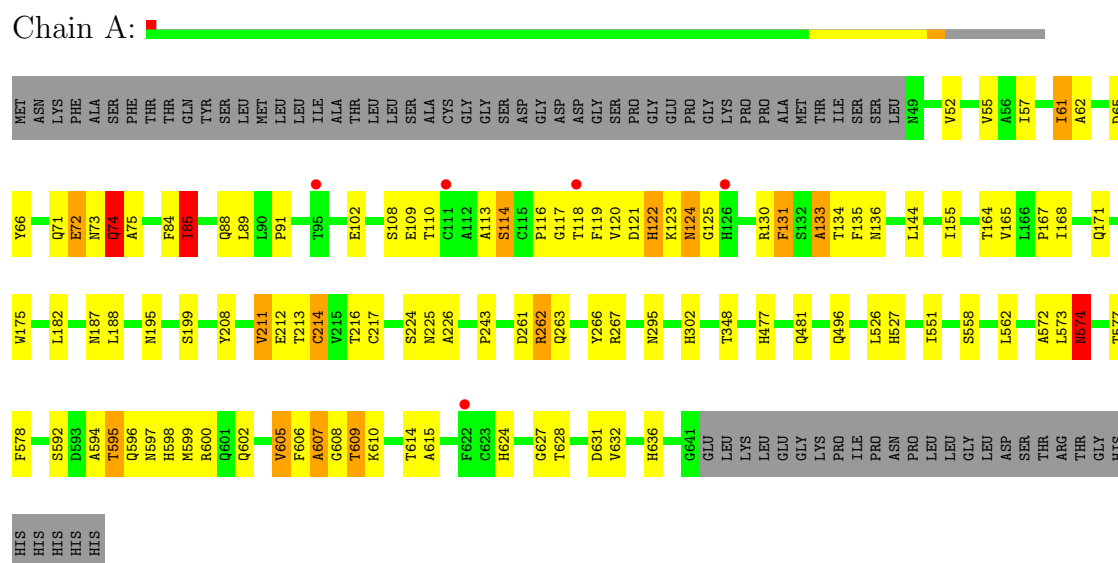
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Decaheme cytochrome c MtrF



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	256.64Å 256.64Å 256.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 57.39 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (40.00-3.20) 97.7 (57.39-3.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.305 , 0.321 0.303 , 0.320	Depositor DCC
$R_{free}$ test set	2291 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	89.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 73.6	EDS
Estimated twinning fraction	0.024 for -l,-k,-h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 45357 reflections	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	4826	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.26	0/4485	0.53	1/6111 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	224	SER	N-CA-C	5.07	124.69	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4395	0	0	70	0
2	A	430	0	0	7	0
3	A	1	0	0	0	0
All	All	4826	0	0	71	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (71) close contacts within the same asymmetric unit are listed below.



Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:614:THR:N	1:A:615:ALA:CA	2.53	0.72
1:A:636:HIS:CE1	2:A:678:HEC:NB	2.63	0.67
1:A:195:ASN:O	1:A:199:SER:N	2.28	0.66
1:A:596:GLN:N	1:A:597:ASN:CA	2.62	0.61
1:A:55:VAL:CG2	1:A:61:ILE:N	2.65	0.60
1:A:262:ARG:CA	1:A:263:GLN:C	2.71	0.59
1:A:88:GLN:NE2	1:A:135:PHE:CD2	2.72	0.58
1:A:597:ASN:C	1:A:599:MET:N	2.56	0.57
1:A:225:ASN:CB	1:A:226:ALA:CA	2.84	0.56
1:A:85:ILE:CG2	1:A:155:ILE:N	2.69	0.55
1:A:592:SER:C	1:A:594:ALA:N	2.59	0.55
1:A:65:ASP:O	1:A:66:TYR:CG	2.58	0.55
1:A:261:ASP:O	1:A:262:ARG:CB	2.53	0.55
1:A:527:HIS:ND1	2:A:677:HEC:CB	2.70	0.54
1:A:597:ASN:O	1:A:599:MET:N	2.41	0.53
1:A:188:LEU:O	1:A:262:ARG:NE	2.41	0.52
1:A:213:THR:OG1	1:A:214:CYS:N	2.42	0.52
1:A:85:ILE:O	1:A:85:ILE:CG2	2.57	0.52
1:A:594:ALA:CA	1:A:595:THR:O	2.58	0.51
1:A:131:PHE:CD2	1:A:131:PHE:N	2.79	0.51
1:A:74:GLN:CG	1:A:75:ALA:N	2.72	0.51
1:A:302:HIS:CD2	2:A:674:HEC:NB	2.78	0.51
1:A:263:GLN:NE2	1:A:267:ARG:CZ	2.74	0.50
1:A:121:ASP:O	1:A:122:HIS:CG	2.65	0.50
1:A:89:LEU:CD1	1:A:216:THR:CA	2.89	0.50
1:A:71:GLN:O	1:A:72:GLU:CB	2.59	0.50
1:A:85:ILE:CD1	1:A:119:PHE:CE2	2.94	0.49
1:A:573:LEU:O	1:A:574:ASN:CB	2.59	0.49
1:A:597:ASN:O	1:A:598:HIS:C	2.50	0.49
1:A:263:GLN:NE2	1:A:266:TYR:OH	2.45	0.49
1:A:572:ALA:O	1:A:573:LEU:C	2.49	0.49
1:A:109:GLU:CG	1:A:110:THR:N	2.75	0.49
1:A:121:ASP:CG	1:A:121:ASP:O	2.48	0.49
1:A:84:PHE:CD1	1:A:119:PHE:CZ	3.00	0.49
1:A:125:GLY:CA	1:A:134:THR:CG2	2.91	0.48
1:A:73:ASN:O	1:A:74:GLN:CB	2.62	0.48
1:A:216:THR:OG1	1:A:217:CYS:N	2.46	0.48
1:A:121:ASP:C	1:A:122:HIS:CG	2.87	0.48
1:A:598:HIS:O	1:A:598:HIS:CG	2.67	0.47
1:A:574:ASN:OD1	1:A:574:ASN:C	2.52	0.47
1:A:577:THR:O	1:A:578:PHE:CD2	2.67	0.47
1:A:155:ILE:CD1	1:A:171:GLN:NE2	2.78	0.47
1:A:636:HIS:CE1	2:A:678:HEC:C1B	2.99	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:627:GLY:O	1:A:628:THR:C	2.54	0.46
1:A:608:GLY:C	1:A:610:LYS:N	2.69	0.45
1:A:624:HIS:CD2	2:A:679:HEC:NC	2.74	0.45
1:A:118:THR:CG2	1:A:119:PHE:N	2.79	0.45
1:A:496:GLN:N	1:A:496:GLN:OE1	2.50	0.45
1:A:605:VAL:CG1	1:A:606:PHE:N	2.79	0.44
2:A:671:HEC:CHA	2:A:671:HEC:CBA	2.96	0.44
1:A:84:PHE:O	1:A:121:ASP:CB	2.66	0.44
1:A:526:LEU:CD1	1:A:527:HIS:CD2	3.01	0.44
1:A:551:ILE:O	1:A:558:SER:N	2.50	0.44
1:A:263:GLN:NE2	1:A:267:ARG:NH2	2.66	0.43
1:A:84:PHE:CB	1:A:85:ILE:CB	2.96	0.43
1:A:211:VAL:CG1	1:A:212:GLU:N	2.81	0.43
1:A:214:CYS:C	1:A:216:THR:N	2.71	0.43
1:A:113:ALA:O	1:A:114:SER:O	2.36	0.42
1:A:595:THR:C	1:A:597:ASN:CA	2.87	0.42
1:A:606:PHE:CG	1:A:607:ALA:N	2.88	0.42
1:A:117:GLY:CA	1:A:136:ASN:OD1	2.68	0.42
1:A:119:PHE:CZ	1:A:208:TYR:OH	2.73	0.42
1:A:133:ALA:CB	1:A:134:THR:CB	2.97	0.42
1:A:600:ARG:NE	1:A:600:ARG:CA	2.83	0.42
1:A:61:ILE:O	1:A:62:ALA:C	2.57	0.41
1:A:74:GLN:C	1:A:74:GLN:NE2	2.74	0.41
1:A:122:HIS:O	1:A:124:ASN:N	2.53	0.41
1:A:477:HIS:CD2	2:A:675:HEC:NB	2.88	0.41
1:A:91:PRO:CA	1:A:102:GLU:O	2.68	0.41
1:A:175:TRP:CZ3	1:A:187:ASN:ND2	2.89	0.41
1:A:117:GLY:CA	1:A:135:PHE:CD1	3.04	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	591/669 (88%)	454 (77%)	109 (18%)	28 (5%)	4 27

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	72	GLU
1	A	114	SER
1	A	120	VAL
1	A	262	ARG
1	A	74	GLN
1	A	85	ILE
1	A	124	ASN
1	A	182	LEU
1	A	211	VAL
1	A	574	ASN
1	A	595	THR
1	A	607	ALA
1	A	631	ASP
1	A	632	VAL
1	A	116	PRO
1	A	123	LYS
1	A	609	THR
1	A	133	ALA
1	A	122	HIS
1	A	168	ILE
1	A	605	VAL
1	A	164	THR
1	A	165	VAL
1	A	243	PRO
1	A	52	VAL
1	A	61	ILE
1	A	167	PRO

### 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	479/542 (88%)	465 (97%)	14 (3%)	55	88

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	85	ILE
1	A	108	SER
1	A	130	ARG
1	A	131	PHE
1	A	144	LEU
1	A	214	CYS
1	A	295	ASN
1	A	348	THR
1	A	481	GLN
1	A	562	LEU
1	A	574	ASN
1	A	602	GLN
1	A	609	THR

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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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
2	HEC	A	670	1	50,50,50	2.81	14 (28%)	56,82,82	1.82	11 (19%)
2	HEC	A	671	1	50,50,50	2.79	14 (28%)	56,82,82	1.89	13 (23%)
2	HEC	A	672	1	50,50,50	2.77	14 (28%)	56,82,82	1.91	13 (23%)
2	HEC	A	673	1	50,50,50	2.76	14 (28%)	56,82,82	1.84	10 (17%)
2	HEC	A	674	1	50,50,50	2.78	14 (28%)	56,82,82	1.89	11 (19%)
2	HEC	A	675	1	50,50,50	2.77	14 (28%)	56,82,82	1.83	10 (17%)
2	HEC	A	676	1	50,50,50	2.79	14 (28%)	56,82,82	1.81	10 (17%)
2	HEC	A	677	1	50,50,50	2.74	14 (28%)	56,82,82	1.99	9 (16%)
2	HEC	A	678	1	50,50,50	2.81	14 (28%)	56,82,82	1.87	11 (19%)
2	HEC	A	679	1	50,50,50	2.74	14 (28%)	56,82,82	1.98	13 (23%)

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	HEC	A	670	1	-	0/10/54/54	0/0/8/8
2	HEC	A	671	1	-	0/10/54/54	0/0/8/8
2	HEC	A	672	1	-	0/10/54/54	0/0/8/8
2	HEC	A	673	1	-	0/10/54/54	0/0/8/8
2	HEC	A	674	1	-	0/10/54/54	0/0/8/8
2	HEC	A	675	1	-	0/10/54/54	0/0/8/8
2	HEC	A	676	1	-	0/10/54/54	0/0/8/8
2	HEC	A	677	1	-	0/10/54/54	0/0/8/8
2	HEC	A	678	1	-	0/10/54/54	0/0/8/8
2	HEC	A	679	1	-	0/10/54/54	0/0/8/8

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	670	HEC	C3C-CAC	9.81	1.55	1.35
2	A	676	HEC	C3C-CAC	9.76	1.55	1.35
2	A	674	HEC	C3C-CAC	9.69	1.55	1.35
2	A	671	HEC	C3C-CAC	9.62	1.55	1.35
2	A	678	HEC	C3B-CAB	9.59	1.55	1.35
2	A	675	HEC	C3C-CAC	9.58	1.55	1.35
2	A	672	HEC	C3B-CAB	9.58	1.55	1.35
2	A	677	HEC	C3B-CAB	9.54	1.55	1.35
2	A	674	HEC	C3B-CAB	9.51	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	673	HEC	C3B-CAB	9.49	1.55	1.35
2	A	679	HEC	C3B-CAB	9.49	1.55	1.35
2	A	676	HEC	C3B-CAB	9.49	1.55	1.35
2	A	670	HEC	C3B-CAB	9.48	1.54	1.35
2	A	679	HEC	C3C-CAC	9.46	1.54	1.35
2	A	678	HEC	C3C-CAC	9.45	1.54	1.35
2	A	673	HEC	C3C-CAC	9.45	1.54	1.35
2	A	675	HEC	C3B-CAB	9.42	1.54	1.35
2	A	671	HEC	C3B-CAB	9.36	1.54	1.35
2	A	672	HEC	C3C-CAC	9.34	1.54	1.35
2	A	677	HEC	C3C-CAC	9.21	1.54	1.35
2	A	671	HEC	C3D-C2D	5.63	1.54	1.37
2	A	674	HEC	C3D-C2D	5.58	1.54	1.37
2	A	672	HEC	C3D-C2D	5.55	1.54	1.37
2	A	670	HEC	C3D-C2D	5.52	1.54	1.37
2	A	676	HEC	C3D-C2D	5.50	1.54	1.37
2	A	679	HEC	C3D-C2D	5.43	1.53	1.37
2	A	678	HEC	C3D-C2D	5.40	1.53	1.37
2	A	673	HEC	C3D-C2D	5.38	1.53	1.37
2	A	677	HEC	C3D-C2D	5.35	1.53	1.37
2	A	675	HEC	C3D-C2D	5.33	1.53	1.37
2	A	678	HEC	FE-ND	4.71	2.12	1.92
2	A	677	HEC	C1B-C2B	4.59	1.45	1.40
2	A	675	HEC	C1B-C2B	4.51	1.45	1.40
2	A	671	HEC	C1B-C2B	4.44	1.45	1.40
2	A	679	HEC	C1C-C2C	4.39	1.45	1.40
2	A	675	HEC	C1C-C2C	4.33	1.45	1.40
2	A	673	HEC	C1B-C2B	4.33	1.45	1.40
2	A	670	HEC	C1C-C2C	4.32	1.45	1.40
2	A	679	HEC	C1B-C2B	4.32	1.45	1.40
2	A	678	HEC	C1C-C2C	4.31	1.45	1.40
2	A	676	HEC	C1C-C2C	4.27	1.45	1.40
2	A	674	HEC	C1C-C2C	4.26	1.45	1.40
2	A	672	HEC	C1B-C2B	4.25	1.45	1.40
2	A	678	HEC	C1B-C2B	4.24	1.45	1.40
2	A	670	HEC	C1D-C2D	4.24	1.45	1.40
2	A	670	HEC	C1B-C2B	4.22	1.45	1.40
2	A	674	HEC	C1D-C2D	4.21	1.45	1.40
2	A	672	HEC	C1D-C2D	4.15	1.45	1.40
2	A	671	HEC	C1C-C2C	4.15	1.45	1.40
2	A	674	HEC	C1B-C2B	4.12	1.45	1.40
2	A	677	HEC	FE-ND	4.12	2.10	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	671	HEC	FE-NA	4.10	2.10	1.92
2	A	676	HEC	C1B-C2B	4.06	1.45	1.40
2	A	672	HEC	C1C-C2C	3.99	1.45	1.40
2	A	674	HEC	FE-ND	3.98	2.09	1.92
2	A	673	HEC	C1D-C2D	3.97	1.45	1.40
2	A	673	HEC	FE-NB	3.96	2.09	1.92
2	A	675	HEC	FE-ND	3.91	2.09	1.92
2	A	676	HEC	FE-NC	3.90	2.09	1.92
2	A	676	HEC	C1D-C2D	3.87	1.45	1.40
2	A	672	HEC	FE-ND	3.85	2.09	1.92
2	A	677	HEC	C1C-C2C	3.81	1.44	1.40
2	A	674	HEC	FE-NC	3.81	2.08	1.92
2	A	679	HEC	C1D-C2D	3.80	1.44	1.40
2	A	675	HEC	FE-NB	3.76	2.08	1.92
2	A	670	HEC	FE-NC	3.75	2.08	1.92
2	A	673	HEC	C1C-C2C	3.75	1.44	1.40
2	A	670	HEC	FE-ND	3.73	2.08	1.92
2	A	678	HEC	C1D-C2D	3.71	1.44	1.40
2	A	679	HEC	FE-ND	3.70	2.08	1.92
2	A	678	HEC	FE-NB	3.69	2.08	1.92
2	A	676	HEC	FE-ND	3.66	2.08	1.92
2	A	671	HEC	C3C-C2C	-3.65	1.33	1.41
2	A	677	HEC	C1D-C2D	3.64	1.44	1.40
2	A	671	HEC	C1D-C2D	3.61	1.44	1.40
2	A	671	HEC	C3B-C2B	-3.58	1.33	1.41
2	A	677	HEC	C3C-C2C	-3.58	1.33	1.41
2	A	675	HEC	C1D-C2D	3.57	1.44	1.40
2	A	670	HEC	FE-NB	3.57	2.07	1.92
2	A	671	HEC	FE-NB	3.57	2.07	1.92
2	A	677	HEC	FE-NC	3.56	2.07	1.92
2	A	673	HEC	C3B-C2B	-3.55	1.33	1.41
2	A	677	HEC	C3B-C2B	-3.54	1.34	1.41
2	A	672	HEC	C3C-C2C	-3.52	1.34	1.41
2	A	675	HEC	C3B-C2B	-3.52	1.34	1.41
2	A	673	HEC	C3C-C2C	-3.51	1.34	1.41
2	A	679	HEC	FE-NA	3.51	2.07	1.92
2	A	678	HEC	C3C-C2C	-3.51	1.34	1.41
2	A	678	HEC	FE-NC	3.48	2.07	1.92
2	A	672	HEC	FE-NB	3.48	2.07	1.92
2	A	670	HEC	C3B-C2B	-3.43	1.34	1.41
2	A	679	HEC	C3C-C2C	-3.42	1.34	1.41
2	A	672	HEC	C3B-C2B	-3.42	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	677	HEC	FE-NB	3.41	2.07	1.92
2	A	671	HEC	FE-ND	3.41	2.07	1.92
2	A	675	HEC	C3C-C2C	-3.40	1.34	1.41
2	A	672	HEC	FE-NC	3.39	2.07	1.92
2	A	676	HEC	C3B-C2B	-3.39	1.34	1.41
2	A	678	HEC	C3B-C2B	-3.38	1.34	1.41
2	A	671	HEC	C3B-C4B	3.34	1.45	1.41
2	A	673	HEC	C3C-C4C	3.34	1.45	1.41
2	A	672	HEC	C3C-C4C	3.31	1.45	1.41
2	A	676	HEC	C3C-C4C	3.31	1.45	1.41
2	A	679	HEC	C3B-C2B	-3.30	1.34	1.41
2	A	676	HEC	C3C-C2C	-3.28	1.34	1.41
2	A	670	HEC	C3C-C2C	-3.26	1.34	1.41
2	A	674	HEC	C3B-C2B	-3.26	1.34	1.41
2	A	676	HEC	FE-NB	3.24	2.06	1.92
2	A	673	HEC	FE-NC	3.23	2.06	1.92
2	A	673	HEC	FE-ND	3.22	2.06	1.92
2	A	674	HEC	C3C-C4C	3.22	1.45	1.41
2	A	670	HEC	C3C-C4C	3.20	1.45	1.41
2	A	674	HEC	C3C-C2C	-3.18	1.34	1.41
2	A	676	HEC	C3B-C4B	3.14	1.45	1.41
2	A	679	HEC	FE-NB	3.12	2.05	1.92
2	A	678	HEC	FE-NA	3.11	2.05	1.92
2	A	670	HEC	C3B-C4B	3.10	1.45	1.41
2	A	674	HEC	FE-NB	3.07	2.05	1.92
2	A	674	HEC	C3B-C4B	3.02	1.45	1.41
2	A	675	HEC	FE-NC	3.01	2.05	1.92
2	A	679	HEC	C3B-C4B	2.97	1.45	1.41
2	A	678	HEC	C3B-C4B	2.96	1.45	1.41
2	A	675	HEC	C3C-C4C	2.95	1.45	1.41
2	A	677	HEC	C3C-C4C	2.93	1.45	1.41
2	A	675	HEC	FE-NA	2.92	2.05	1.92
2	A	673	HEC	C3B-C4B	2.90	1.45	1.41
2	A	671	HEC	C3C-C4C	2.89	1.45	1.41
2	A	678	HEC	C3C-C4C	2.89	1.45	1.41
2	A	676	HEC	FE-NA	2.88	2.04	1.92
2	A	670	HEC	FE-NA	2.87	2.04	1.92
2	A	672	HEC	C3B-C4B	2.83	1.45	1.41
2	A	673	HEC	FE-NA	2.79	2.04	1.92
2	A	679	HEC	C3C-C4C	2.78	1.45	1.41
2	A	672	HEC	FE-NA	2.74	2.04	1.92
2	A	675	HEC	C3B-C4B	2.71	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	677	HEC	C3B-C4B	2.46	1.44	1.41
2	A	674	HEC	FE-NA	2.30	2.02	1.92
2	A	671	HEC	FE-NC	2.29	2.02	1.92
2	A	677	HEC	FE-NA	2.22	2.01	1.92
2	A	679	HEC	FE-NC	2.17	2.01	1.92

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	677	HEC	CBC-CAC-C3C	-8.15	105.49	128.44
2	A	672	HEC	CBC-CAC-C3C	-7.04	108.62	128.44
2	A	679	HEC	CBC-CAC-C3C	-6.93	108.93	128.44
2	A	679	HEC	CBB-CAB-C3B	-6.90	109.02	128.44
2	A	674	HEC	CBB-CAB-C3B	-6.65	109.71	128.44
2	A	678	HEC	CBB-CAB-C3B	-6.60	109.85	128.44
2	A	675	HEC	CBB-CAB-C3B	-6.60	109.85	128.44
2	A	670	HEC	CBB-CAB-C3B	-6.60	109.87	128.44
2	A	672	HEC	CBB-CAB-C3B	-6.57	109.93	128.44
2	A	678	HEC	CBC-CAC-C3C	-6.54	110.04	128.44
2	A	673	HEC	CBB-CAB-C3B	-6.50	110.15	128.44
2	A	671	HEC	CBC-CAC-C3C	-6.45	110.28	128.44
2	A	671	HEC	CBB-CAB-C3B	-6.44	110.30	128.44
2	A	676	HEC	CBB-CAB-C3B	-6.40	110.41	128.44
2	A	677	HEC	CBB-CAB-C3B	-6.38	110.47	128.44
2	A	673	HEC	CBC-CAC-C3C	-6.32	110.65	128.44
2	A	675	HEC	CBC-CAC-C3C	-6.23	110.90	128.44
2	A	674	HEC	CBC-CAC-C3C	-6.15	111.13	128.44
2	A	676	HEC	CBC-CAC-C3C	-5.56	112.78	128.44
2	A	670	HEC	CBC-CAC-C3C	-5.15	113.93	128.44
2	A	670	HEC	CMC-C2C-C1C	-4.11	122.31	128.62
2	A	679	HEC	C4D-ND-C1D	3.96	111.98	106.76
2	A	674	HEC	C4D-ND-C1D	3.95	111.97	106.76
2	A	677	HEC	C4D-ND-C1D	3.77	111.73	106.76
2	A	672	HEC	C4D-ND-C1D	3.74	111.69	106.76
2	A	673	HEC	C4D-ND-C1D	3.74	111.69	106.76
2	A	675	HEC	C4D-ND-C1D	3.72	111.66	106.76
2	A	671	HEC	C4D-ND-C1D	3.55	111.44	106.76
2	A	670	HEC	C4D-ND-C1D	3.53	111.42	106.76
2	A	676	HEC	C4D-ND-C1D	3.51	111.39	106.76
2	A	678	HEC	C4D-ND-C1D	3.48	111.35	106.76
2	A	677	HEC	CMC-C2C-C1C	-2.93	124.12	128.62
2	A	672	HEC	CBA-CAA-C2A	-2.81	107.10	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	675	HEC	CMC-C2C-C1C	-2.79	124.33	128.62
2	A	677	HEC	C2A-C1A-NA	-2.70	107.61	109.64
2	A	676	HEC	CMC-C2C-C1C	-2.68	124.50	128.62
2	A	670	HEC	C3B-C4B-NB	-2.64	107.70	111.52
2	A	679	HEC	C3C-C4C-NC	-2.63	107.71	111.52
2	A	679	HEC	C3B-C4B-NB	-2.62	107.73	111.52
2	A	679	HEC	CMC-C2C-C1C	-2.62	124.59	128.62
2	A	677	HEC	C4C-C3C-C2C	2.60	108.34	106.68
2	A	679	HEC	C4B-C3B-C2B	2.58	108.32	106.68
2	A	676	HEC	CMB-C2B-C1B	-2.58	124.66	128.62
2	A	672	HEC	CMC-C2C-C1C	-2.57	124.66	128.62
2	A	672	HEC	C3C-C4C-NC	-2.57	107.81	111.52
2	A	670	HEC	C4B-C3B-C2B	2.56	108.31	106.68
2	A	671	HEC	C1D-C2D-C3D	-2.56	105.22	107.00
2	A	677	HEC	C3C-C4C-NC	-2.54	107.85	111.52
2	A	672	HEC	C2A-C1A-NA	-2.54	107.73	109.64
2	A	673	HEC	CMC-C2C-C1C	-2.51	124.76	128.62
2	A	671	HEC	C4A-C3A-C2A	2.51	108.49	106.89
2	A	674	HEC	C3B-C4B-NB	-2.50	107.91	111.52
2	A	678	HEC	CMC-C2C-C1C	-2.48	124.80	128.62
2	A	674	HEC	C4A-CHB-C1B	-2.48	124.21	127.47
2	A	674	HEC	C3C-C4C-NC	-2.48	107.94	111.52
2	A	679	HEC	C2A-C1A-NA	-2.46	107.79	109.64
2	A	676	HEC	C2A-C1A-NA	-2.43	107.81	109.64
2	A	670	HEC	C3C-C4C-NC	-2.43	108.02	111.52
2	A	671	HEC	C3C-C4C-NC	-2.42	108.02	111.52
2	A	674	HEC	CMC-C2C-C1C	-2.41	124.91	128.62
2	A	673	HEC	C3C-C4C-NC	-2.41	108.05	111.52
2	A	671	HEC	CMC-C2C-C1C	-2.38	124.96	128.62
2	A	678	HEC	C3B-C4B-NB	-2.37	108.09	111.52
2	A	675	HEC	C4B-C3B-C2B	2.36	108.18	106.68
2	A	676	HEC	C3B-C4B-NB	-2.35	108.12	111.52
2	A	679	HEC	C2C-C1C-NC	-2.35	107.64	109.41
2	A	678	HEC	C4A-CHB-C1B	-2.34	124.40	127.47
2	A	675	HEC	C3B-C4B-NB	-2.32	108.17	111.52
2	A	678	HEC	C3C-C4C-NC	-2.31	108.18	111.52
2	A	672	HEC	C4C-C3C-C2C	2.30	108.14	106.68
2	A	674	HEC	CMB-C2B-C1B	-2.27	125.13	128.62
2	A	671	HEC	C3B-C4B-NB	-2.25	108.27	111.52
2	A	673	HEC	CBA-CAA-C2A	-2.23	108.17	112.35
2	A	675	HEC	C3C-C4C-NC	-2.22	108.31	111.52
2	A	679	HEC	C4C-C3C-C2C	2.21	108.08	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	676	HEC	C4A-C3A-C2A	2.20	108.29	106.89
2	A	671	HEC	CMD-C2D-C3D	2.19	129.08	124.94
2	A	671	HEC	C2A-C1A-NA	-2.18	108.00	109.64
2	A	672	HEC	C1D-C2D-C3D	-2.16	105.49	107.00
2	A	674	HEC	C3A-C4A-NA	-2.16	107.78	109.41
2	A	675	HEC	C2A-C1A-NA	-2.16	108.02	109.64
2	A	673	HEC	C3B-C4B-NB	-2.15	108.41	111.52
2	A	676	HEC	C3C-C4C-NC	-2.14	108.43	111.52
2	A	679	HEC	C1D-C2D-C3D	-2.13	105.51	107.00
2	A	673	HEC	C4A-C3A-C2A	2.13	108.25	106.89
2	A	673	HEC	C2A-C1A-NA	-2.12	108.04	109.64
2	A	672	HEC	C4A-C3A-C2A	2.11	108.24	106.89
2	A	677	HEC	C3A-C4A-NA	-2.11	107.82	109.41
2	A	679	HEC	C4A-C3A-C2A	2.10	108.23	106.89
2	A	671	HEC	CAA-C2A-C1A	2.09	128.44	124.67
2	A	674	HEC	C2B-C1B-NB	-2.08	107.84	109.41
2	A	672	HEC	C3B-C4B-NB	-2.07	108.53	111.52
2	A	671	HEC	C4C-C3C-C2C	2.07	108.00	106.68
2	A	671	HEC	CMB-C2B-C1B	-2.06	125.46	128.62
2	A	670	HEC	C2B-C1B-NB	-2.06	107.86	109.41
2	A	677	HEC	C1A-C2A-C3A	2.04	108.30	106.69
2	A	678	HEC	C4C-C3C-C2C	2.04	107.98	106.68
2	A	675	HEC	C3A-C4A-NA	-2.04	107.87	109.41
2	A	670	HEC	C4A-C3A-C2A	2.03	108.19	106.89
2	A	672	HEC	C3A-C4A-NA	-2.03	107.88	109.41
2	A	672	HEC	CMB-C2B-C1B	-2.03	125.50	128.62
2	A	678	HEC	C2A-C1A-NA	-2.02	108.12	109.64
2	A	670	HEC	C1D-C2D-C3D	-2.02	105.59	107.00
2	A	670	HEC	C3A-C4A-NA	-2.02	107.89	109.41
2	A	674	HEC	C4B-C3B-C2B	2.01	107.96	106.68
2	A	679	HEC	C2B-C1B-NB	-2.01	107.89	109.41
2	A	673	HEC	C3A-C4A-NA	-2.01	107.89	109.41
2	A	675	HEC	C2B-C1B-NB	-2.01	107.89	109.41
2	A	678	HEC	C3A-C4A-NA	-2.01	107.90	109.41
2	A	678	HEC	C4B-C3B-C2B	2.00	107.95	106.68
2	A	676	HEC	C1D-C2D-C3D	-2.00	105.60	107.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	593/669 (88%)	0.05	5 (0%) 83 35	46, 99, 206, 272	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	CYS	3.5
1	A	126	HIS	3.0
1	A	95	THR	2.1
1	A	118	THR	2.0
1	A	622	PHE	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	HEC	A	678	43/43	0.42	3.46	114,162,187,202	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEC	A	679	43/43	0.43	1.94	106,176,195,203	0
2	HEC	A	670	43/43	0.28	1.42	55,90,118,129	0
2	HEC	A	677	43/43	0.27	1.18	73,103,115,122	0
2	HEC	A	672	43/43	0.28	1.00	40,69,89,104	0
2	HEC	A	673	43/43	0.24	0.73	29,61,98,106	0
2	HEC	A	674	43/43	0.21	0.26	31,52,83,105	0
2	HEC	A	676	43/43	0.26	0.24	39,73,127,151	0
2	HEC	A	675	43/43	0.24	0.02	53,83,105,143	0
2	HEC	A	671	43/43	0.25	-0.03	63,86,140,148	0
3	CA	A	680	1/1	0.14	-1.17	101,101,101,101	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.