



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:19 PM GMT

PDB ID : 1OFY  
Title : THREE DIMENSIONAL STRUCTURE OF THE REDUCED FORM OF NINE-HEME CYTOCHROME C AT PH 7.5  
Authors : Bento, I.; Teixeira, V.H.; Baptista, A.M.; Soares, C.M.; Matias, P.M.; Car-rondo, M.A.  
Deposited on : 2003-04-22  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

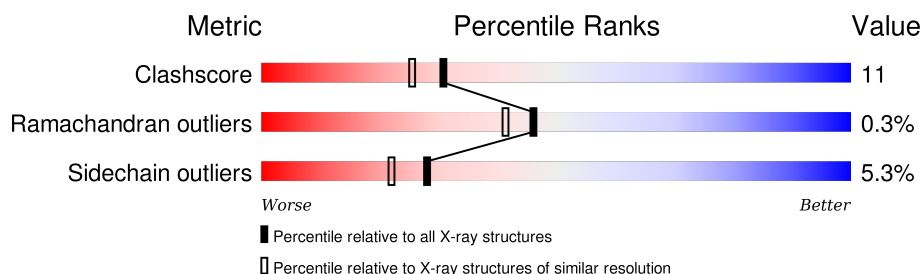
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	296	 82% 15% ..
1	B	296	 76% 21% ..

## 2 Entry composition i

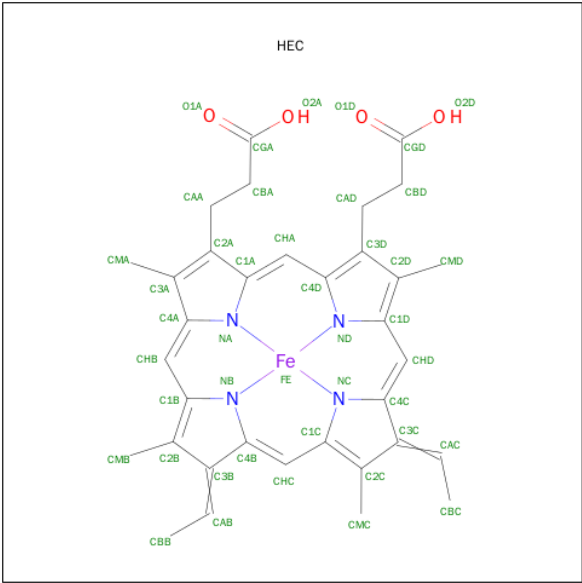
There are 5 unique types of molecules in this entry. The entry contains 5755 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NINE HEME CYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	22	4	1
			2223	1363	412	420	28			
1	B	293	Total	C	N	O	S	21	5	1
			2237	1371	413	425	28			

- 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	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

Continued on next page...

*Continued from previous page...*

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	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

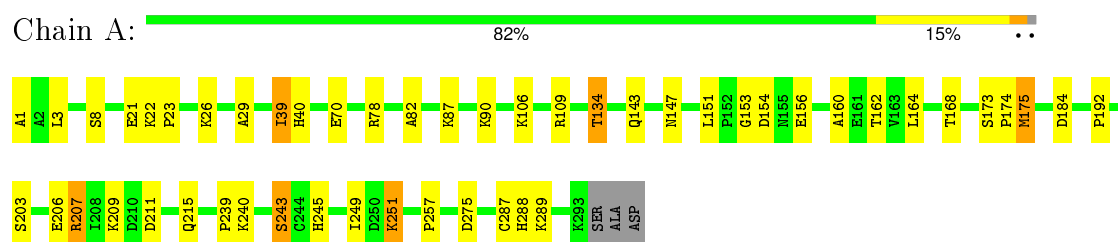
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	263	Total 263	O 263	0	0
5	B	242	Total 242	O 242	0	0

### 3 Residue-property plots

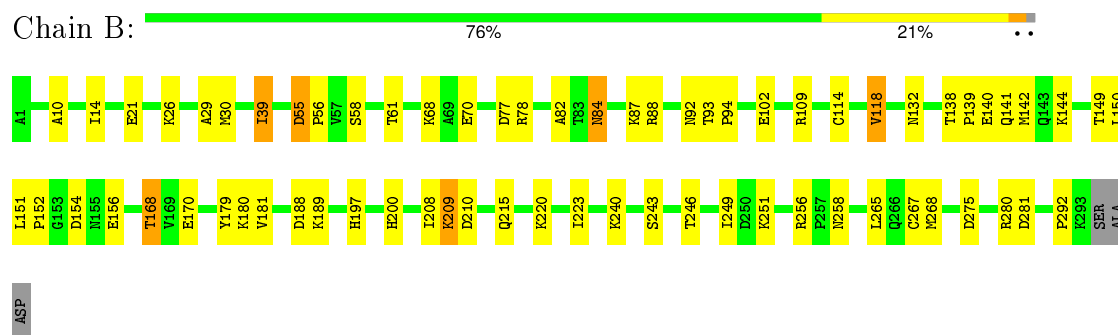
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: NINE HEME CYTOCHROME C



#### • Molecule 1: NINE HEME CYTOCHROME C



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.40 Å   105.66 Å   80.94 Å 90.00°   103.35°   90.00°	Depositor
Resolution (Å)	25.00 – 2.00	Depositor
% Data completeness (in resolution range)	92.7 (25.00-2.00)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.242 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5755	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP



## 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: GOL, HEC, ACT

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	0.36	0/2297	0.91	2/3117 (0.1%)
1	B	0.31	0/2304	0.86	0/3127
All	All	0.34	0/4601	0.89	2/6244 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	A	1	ALA	O-C-N	5.72	131.85	122.70

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	2223	0	2163	33	0
1	B	2237	0	2170	46	0
2	A	387	0	270	23	0
2	B	387	0	270	27	0
3	A	4	0	3	1	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	263	0	0	8	0
5	B	242	0	0	8	0
All	All	5755	0	4892	110	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 11.

All (110) 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:109:ARG:HH21	1:A:275:ASP:HB2	1.45	0.80
1:B:138:THR:OG1	1:B:141:GLN:HG3	1.84	0.78
1:B:68:LYS:HG3	1:B:70:GLU:OE1	1.85	0.76
1:A:39:ILE:HD12	2:A:1295:HEC:HBD1	1.70	0.74
1:B:152:PRO:O	1:B:156:GLU:HG3	1.90	0.71
1:A:109:ARG:NH2	1:A:275:ASP:HB2	2.08	0.68
1:B:21:GLU:HG2	5:B:2028:HOH:O	1.96	0.66
1:B:240:LYS:HG2	5:B:2231:HOH:O	1.97	0.64
1:B:144:LYS:HG2	1:B:149:THR:OG1	1.97	0.64
1:A:160:ALA:O	1:A:164:LEU:HG	1.98	0.63
1:A:211:ASP:O	1:A:215:GLN:HG3	1.98	0.62
1:B:151:LEU:HB2	1:B:154:ASP:OD2	1.99	0.61
1:B:92:ASN:O	1:B:94:PRO:HD3	2.01	0.60
2:A:1301:HEC:HMC1	2:A:1301:HEC:HBC3	1.83	0.60
2:A:1296:HEC:HBC3	2:A:1296:HEC:HMC1	1.84	0.59
1:A:39:ILE:CD1	2:A:1295:HEC:HBD1	2.33	0.58
2:A:1300:HEC:HMB1	2:A:1300:HEC:HBB3	1.84	0.58
2:B:1298:HEC:HMC1	2:B:1298:HEC:HBC3	1.86	0.57
2:B:1301:HEC:HBC3	2:B:1301:HEC:HMC1	1.85	0.57
2:A:1294:HEC:HBC3	2:A:1294:HEC:HMC1	1.87	0.57
1:B:88:ARG:HG2	1:B:93:THR:HA	1.87	0.57
2:A:1300:HEC:HBA2	5:A:2259:HOH:O	2.04	0.56
2:B:1300:HEC:HBB3	2:B:1300:HEC:HMB1	1.87	0.56
1:B:77:ASP:OD1	4:B:1302:GOL:H11	2.06	0.56
1:A:206:GLU:HG2	1:A:209:LYS:HE2	1.86	0.56
1:B:109:ARG:HD3	5:B:2109:HOH:O	2.05	0.56
2:B:1300:HEC:HMC1	2:B:1300:HEC:HBC3	1.88	0.55
1:A:70:GLU:HG2	5:A:2051:HOH:O	2.06	0.55
1:A:153:GLY:HA2	1:A:156:GLU:OE2	2.06	0.55
1:A:287:CYS:HB2	5:A:2240:HOH:O	2.05	0.55
2:B:1295:HEC:HMC1	2:B:1295:HEC:HBC3	1.88	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1295:HEC:HBC3	2:A:1295:HEC:HMC1	1.88	0.54
2:B:1294:HEC:HMC1	2:B:1294:HEC:HBC3	1.90	0.54
2:B:1299:HEC:HMC1	2:B:1299:HEC:HBC3	1.90	0.53
2:A:1300:HEC:HMC1	2:A:1300:HEC:HBC3	1.90	0.52
1:B:246:THR:O	1:B:258:ASN:HB2	2.09	0.52
2:B:1298:HEC:HBB3	2:B:1298:HEC:HMB1	1.91	0.52
1:B:208:ILE:HD13	2:B:1296:HEC:HMC2	1.91	0.52
2:A:1297:HEC:HMC1	2:A:1297:HEC:HBC3	1.90	0.52
2:B:1297:HEC:HBB3	2:B:1297:HEC:HMB1	1.92	0.51
1:B:58:SER:OG	1:B:61:THR:HG23	2.11	0.51
1:B:78:ARG:O	1:B:82:ALA:HB2	2.10	0.51
2:A:1298:HEC:O2A	1:B:26:LYS:HD2	2.10	0.51
1:A:143:GLN:O	1:A:147:ASN:OD1	2.30	0.50
1:A:245:HIS:CE1	1:A:257:PRO:HD2	2.46	0.50
1:B:209[B]:LYS:O	1:B:210[B]:ASP:HB2	2.12	0.50
2:B:1296:HEC:HBC3	2:B:1296:HEC:HMC1	1.93	0.49
2:B:1293:HEC:HMC1	2:B:1293:HEC:HBC3	1.94	0.49
1:A:288:HIS:CD2	2:A:1301:HEC:ND	2.80	0.49
1:B:168:THR:CG2	1:B:215:GLN:HB3	2.42	0.49
2:A:1297:HEC:HBB3	2:A:1297:HEC:HMB1	1.94	0.49
1:A:184:ASP:HB3	1:A:192:PRO:HB3	1.94	0.48
2:B:1301:HEC:HBB3	2:B:1301:HEC:HMB1	1.95	0.48
2:B:1297:HEC:HBC3	2:B:1297:HEC:HMC1	1.95	0.48
1:B:179:TYR:CE2	1:B:180:LYS:HD3	2.49	0.48
1:B:102:GLU:OE1	2:B:1296:HEC:O2A	2.32	0.48
2:A:1298:HEC:HMC1	2:A:1298:HEC:HBC3	1.95	0.48
1:B:268:MET:HB3	1:B:281:ASP:OD1	2.14	0.48
5:A:2147:HOH:O	1:B:26:LYS:HE3	2.14	0.47
1:B:138:THR:HB	1:B:140:GLU:OE1	2.13	0.47
2:A:1293:HEC:HMC1	2:A:1293:HEC:HBC3	1.97	0.46
1:B:200:HIS:HD2	2:B:1300:HEC:NC	2.07	0.46
1:A:22:LYS:HA	1:A:23:PRO:HD3	1.85	0.46
1:A:239:PRO:HA	1:B:29:ALA:HA	1.98	0.46
2:B:1296:HEC:HBB3	2:B:1296:HEC:HMB1	1.99	0.45
1:A:173:SER:OG	1:A:175:MET:HB2	2.16	0.45
2:A:1296:HEC:HMB1	2:A:1296:HEC:HBB3	1.98	0.45
2:B:1295:HEC:HBB3	2:B:1295:HEC:HMB1	1.99	0.45
1:B:144:LYS:HB3	1:B:150:LEU:HB2	1.99	0.45
1:B:114:CYS:O	1:B:118:VAL:HG13	2.17	0.45
3:A:1302:ACT:H1	5:A:2263:HOH:O	2.16	0.45
1:B:156:GLU:HG2	5:B:2023:HOH:O	2.16	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLU:N	1:A:70:GLU:OE1	2.49	0.44
1:B:249:ILE:HD11	5:B:2098:HOH:O	2.16	0.44
1:B:84:ASN:OD1	1:B:84:ASN:N	2.50	0.44
1:A:203:SER:OG	1:A:207:ARG:NH2	2.50	0.44
1:A:40:HIS:CE1	2:A:1295:HEC:NA	2.86	0.44
1:A:106:LYS:NZ	5:A:2091:HOH:O	2.50	0.44
1:A:3:LEU:HD13	5:A:2029:HOH:O	2.18	0.44
1:B:30:MET:HG3	2:B:1297:HEC:C4A	2.48	0.43
1:B:197:HIS:CE1	2:B:1298:HEC:NB	2.86	0.43
1:A:8:SER:HB2	2:A:1293:HEC:HMB2	2.00	0.43
1:B:220:LYS:NZ	1:B:223:ILE:HD12	2.33	0.43
1:B:55:ASP:HA	1:B:56:PRO:HD3	1.92	0.43
1:A:240:LYS:O	1:A:243:SER:HB2	2.19	0.43
1:B:88:ARG:HH21	2:B:1294:HEC:CGD	2.31	0.43
1:A:78:ARG:O	1:A:82:ALA:HB2	2.19	0.43
1:A:29:ALA:HB1	2:A:1297:HEC:O2A	2.18	0.42
1:A:245:HIS:HE1	1:A:257:PRO:HD2	1.83	0.42
1:B:181:VAL:HG11	2:B:1298:HEC:HAD1	2.02	0.42
2:A:1299:HEC:HBC3	2:A:1299:HEC:HMC1	2.01	0.42
1:B:39:ILE:HD12	2:B:1295:HEC:HBD1	2.01	0.41
1:A:251:LYS:HB2	5:A:2211:HOH:O	2.18	0.41
2:A:1293:HEC:HBB3	2:A:1293:HEC:HMB1	2.01	0.41
1:B:265:LEU:HB2	2:B:1299:HEC:HMA3	2.03	0.41
1:B:132:ASN:HB2	5:B:2126:HOH:O	2.20	0.41
1:B:267:CYS:HA	2:B:1300:HEC:HHC	2.03	0.41
1:A:151:LEU:O	1:A:154:ASP:N	2.51	0.41
1:B:68:LYS:HE3	5:B:2078:HOH:O	2.20	0.41
1:A:134:THR:HG22	1:A:162:THR:OG1	2.20	0.41
1:B:58:SER:O	1:B:61:THR:HG23	2.20	0.41
1:B:10:ALA:HB2	2:B:1293:HEC:C4A	2.51	0.41
2:A:1294:HEC:HMB1	2:A:1294:HEC:HBB3	2.03	0.40
1:A:245:HIS:CE1	2:A:1299:HEC:NA	2.89	0.40
2:B:1298:HEC:HBD2	5:B:2231:HOH:O	2.21	0.40
1:A:168:THR:CG2	1:A:215:GLN:HB3	2.51	0.40
1:A:173:SER:HA	1:A:174:PRO:HD3	1.98	0.40
1:B:139:PRO:O	1:B:142:MET:HB3	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	295/296 (100%)	288 (98%)	7 (2%)	0	100	100
1	B	296/296 (100%)	281 (95%)	13 (4%)	2 (1%)	26	19
All	All	591/592 (100%)	569 (96%)	20 (3%)	2 (0%)	46	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	ASP
1	B	292	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	250/249 (100%)	239 (96%)	11 (4%)	35	30
1	B	251/249 (101%)	235 (94%)	16 (6%)	22	15
All	All	501/498 (101%)	474 (95%)	27 (5%)	28	21

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	26	LYS
1	A	39	ILE
1	A	87	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	90	LYS
1	A	134	THR
1	A	175	MET
1	A	243	SER
1	A	249	ILE
1	A	251	LYS
1	A	289	LYS
1	B	14	ILE
1	B	39	ILE
1	B	55	ASP
1	B	84	ASN
1	B	87	LYS
1	B	118	VAL
1	B	168	THR
1	B	170	GLU
1	B	189	LYS
1	B	209[A]	LYS
1	B	209[B]	LYS
1	B	243	SER
1	B	251	LYS
1	B	256	ARG
1	B	275	ASP
1	B	280	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	B	72	ASN
1	B	194	ASN
1	B	215	GLN
1	B	266	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	HEC	A	1293	1	24,50,50	1.88	2 (8%)	19,82,82	2.38	5 (26%)
2	HEC	A	1294	1	24,50,50	1.90	4 (16%)	19,82,82	2.47	4 (21%)
2	HEC	A	1295	1	24,50,50	1.87	2 (8%)	19,82,82	2.50	7 (36%)
2	HEC	A	1296	1	24,50,50	1.87	2 (8%)	19,82,82	2.47	7 (36%)
2	HEC	A	1297	1	24,50,50	1.84	3 (12%)	19,82,82	2.24	6 (31%)
2	HEC	A	1298	1	24,50,50	1.93	2 (8%)	19,82,82	2.37	5 (26%)
2	HEC	A	1299	1	24,50,50	1.86	2 (8%)	19,82,82	2.67	8 (42%)
2	HEC	A	1300	1	24,50,50	1.96	2 (8%)	19,82,82	2.31	5 (26%)
2	HEC	A	1301	1	24,50,50	1.95	3 (12%)	19,82,82	2.88	8 (42%)
3	ACT	A	1302	-	1,3,3	0.37	0	0,3,3	0.00	-
4	GOL	A	1303	-	5,5,5	0.22	0	5,5,5	0.40	0
2	HEC	B	1293	1	24,50,50	1.78	2 (8%)	19,82,82	2.50	4 (21%)
2	HEC	B	1294	1	24,50,50	1.81	2 (8%)	19,82,82	2.34	4 (21%)
2	HEC	B	1295	1	24,50,50	2.04	4 (16%)	19,82,82	2.39	7 (36%)
2	HEC	B	1296	1	24,50,50	1.83	2 (8%)	19,82,82	2.39	7 (36%)
2	HEC	B	1297	1	24,50,50	1.94	3 (12%)	19,82,82	2.53	5 (26%)
2	HEC	B	1298	1	24,50,50	1.87	2 (8%)	19,82,82	2.62	6 (31%)
2	HEC	B	1299	1	24,50,50	1.87	4 (16%)	19,82,82	2.57	6 (31%)
2	HEC	B	1300	1	24,50,50	1.96	2 (8%)	19,82,82	2.14	5 (26%)
2	HEC	B	1301	1	24,50,50	1.89	2 (8%)	19,82,82	2.57	7 (36%)
4	GOL	B	1302	-	5,5,5	0.23	0	5,5,5	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	1293	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1294	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1295	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1296	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1297	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1298	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1299	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1300	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1301	1	-	0/6/54/54	0/0/8/8
3	ACT	A	1302	-	-	0/0/0/0	0/0/0/0
4	GOL	A	1303	-	-	0/4/4/4	0/0/0/0
2	HEC	B	1293	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1294	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1295	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1296	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1297	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1298	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1299	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1300	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1301	1	-	0/6/54/54	0/0/8/8
4	GOL	B	1302	-	-	0/4/4/4	0/0/0/0

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1300	HEC	C3C-C2C	-6.25	1.34	1.40
2	B	1295	HEC	C3C-C2C	-6.23	1.34	1.40
2	B	1297	HEC	C3B-C2B	-6.19	1.34	1.40
2	A	1298	HEC	C3C-C2C	-6.04	1.34	1.40
2	A	1301	HEC	C3B-C2B	-6.01	1.34	1.40
2	B	1300	HEC	C3C-C2C	-5.95	1.34	1.40
2	B	1295	HEC	C3B-C2B	-5.86	1.34	1.40
2	B	1301	HEC	C3C-C2C	-5.83	1.34	1.40
2	B	1300	HEC	C3B-C2B	-5.82	1.34	1.40
2	A	1295	HEC	C3B-C2B	-5.80	1.34	1.40
2	A	1293	HEC	C3B-C2B	-5.77	1.34	1.40
2	B	1298	HEC	C3C-C2C	-5.76	1.34	1.40
2	B	1296	HEC	C3C-C2C	-5.75	1.34	1.40
2	A	1299	HEC	C3C-C2C	-5.75	1.34	1.40
2	A	1296	HEC	C3C-C2C	-5.68	1.34	1.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1293	HEC	C3B-C2B	-5.67	1.34	1.40
2	A	1300	HEC	C3B-C2B	-5.63	1.34	1.40
2	A	1294	HEC	C3B-C2B	-5.59	1.34	1.40
2	A	1293	HEC	C3C-C2C	-5.57	1.34	1.40
2	A	1295	HEC	C3C-C2C	-5.55	1.35	1.40
2	A	1296	HEC	C3B-C2B	-5.54	1.35	1.40
2	A	1298	HEC	C3B-C2B	-5.49	1.35	1.40
2	B	1301	HEC	C3B-C2B	-5.45	1.35	1.40
2	B	1299	HEC	C3B-C2B	-5.42	1.35	1.40
2	A	1297	HEC	C3B-C2B	-5.41	1.35	1.40
2	B	1299	HEC	C3C-C2C	-5.38	1.35	1.40
2	A	1299	HEC	C3B-C2B	-5.38	1.35	1.40
2	A	1301	HEC	C3C-C2C	-5.36	1.35	1.40
2	B	1294	HEC	C3B-C2B	-5.29	1.35	1.40
2	A	1294	HEC	C3C-C2C	-5.28	1.35	1.40
2	B	1296	HEC	C3B-C2B	-5.20	1.35	1.40
2	B	1298	HEC	C3B-C2B	-5.17	1.35	1.40
2	B	1294	HEC	C3C-C2C	-5.16	1.35	1.40
2	B	1297	HEC	C3C-C2C	-5.12	1.35	1.40
2	A	1297	HEC	C3C-C2C	-5.02	1.35	1.40
2	B	1293	HEC	C3C-C2C	-4.97	1.35	1.40
2	B	1299	HEC	C4A-NA	2.00	1.39	1.36
2	B	1295	HEC	C4A-NA	2.07	1.39	1.36
2	B	1297	HEC	C4C-NC	2.14	1.39	1.36
2	B	1299	HEC	C4C-NC	2.16	1.39	1.36
2	A	1294	HEC	C4C-NC	2.27	1.39	1.36
2	A	1294	HEC	C4A-NA	2.32	1.39	1.36
2	B	1295	HEC	C1A-NA	2.44	1.40	1.36
2	A	1301	HEC	C1A-NA	2.47	1.40	1.36
2	A	1297	HEC	C1A-NA	2.81	1.40	1.36

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	HEC	CBB-CAB-C3B	-7.88	109.85	127.35
2	B	1297	HEC	CBB-CAB-C3B	-7.45	110.79	127.35
2	B	1298	HEC	CBB-CAB-C3B	-7.43	110.84	127.35
2	A	1294	HEC	CBC-CAC-C3C	-6.72	112.43	127.35
2	A	1299	HEC	CBB-CAB-C3B	-6.66	112.54	127.35
2	B	1301	HEC	CBC-CAC-C3C	-6.58	112.74	127.35
2	A	1298	HEC	CBB-CAB-C3B	-6.42	113.09	127.35
2	B	1299	HEC	CBB-CAB-C3B	-6.36	113.21	127.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1295	HEC	CBB-CAB-C3B	-6.36	113.22	127.35
2	A	1297	HEC	CBB-CAB-C3B	-6.34	113.27	127.35
2	A	1293	HEC	CBB-CAB-C3B	-6.31	113.34	127.35
2	A	1299	HEC	CBC-CAC-C3C	-6.17	113.64	127.35
2	B	1294	HEC	CBB-CAB-C3B	-6.15	113.69	127.35
2	B	1294	HEC	CBC-CAC-C3C	-6.14	113.70	127.35
2	A	1294	HEC	CBB-CAB-C3B	-6.12	113.75	127.35
2	A	1298	HEC	CBC-CAC-C3C	-6.10	113.79	127.35
2	B	1297	HEC	CBC-CAC-C3C	-6.03	113.95	127.35
2	B	1299	HEC	CBC-CAC-C3C	-6.00	114.02	127.35
2	A	1296	HEC	CBB-CAB-C3B	-5.96	114.10	127.35
2	B	1293	HEC	CBB-CAB-C3B	-5.89	114.27	127.35
2	B	1301	HEC	CBB-CAB-C3B	-5.87	114.32	127.35
2	B	1298	HEC	CBC-CAC-C3C	-5.84	114.37	127.35
2	A	1296	HEC	CBC-CAC-C3C	-5.82	114.41	127.35
2	B	1300	HEC	CBB-CAB-C3B	-5.69	114.71	127.35
2	B	1296	HEC	CBB-CAB-C3B	-5.53	115.06	127.35
2	B	1293	HEC	CBC-CAC-C3C	-5.47	115.21	127.35
2	A	1293	HEC	CBC-CAC-C3C	-5.46	115.21	127.35
2	B	1296	HEC	CBC-CAC-C3C	-5.41	115.33	127.35
2	A	1300	HEC	CBC-CAC-C3C	-5.34	115.48	127.35
2	A	1300	HEC	CBB-CAB-C3B	-5.24	115.71	127.35
2	A	1301	HEC	CBC-CAC-C3C	-5.12	115.98	127.35
2	A	1297	HEC	CBC-CAC-C3C	-5.08	116.07	127.35
2	A	1295	HEC	CBB-CAB-C3B	-5.07	116.10	127.35
2	A	1295	HEC	CBC-CAC-C3C	-4.70	116.91	127.35
2	B	1293	HEC	CMB-C2B-C1B	-4.39	121.09	128.36
2	B	1300	HEC	CBC-CAC-C3C	-4.22	117.98	127.35
2	A	1301	HEC	CMD-C2D-C1D	-4.18	121.45	128.36
2	B	1296	HEC	CAA-C2A-C1A	-4.11	122.54	127.01
2	A	1295	HEC	CAA-C2A-C1A	-4.08	122.58	127.01
2	A	1295	HEC	CMC-C2C-C1C	-3.96	121.81	128.36
2	A	1299	HEC	CAA-C2A-C1A	-3.93	122.74	127.01
2	A	1300	HEC	CMC-C2C-C1C	-3.86	121.98	128.36
2	B	1295	HEC	CBC-CAC-C3C	-3.70	119.12	127.35
2	B	1295	HEC	CMB-C2B-C1B	-3.61	122.39	128.36
2	B	1301	HEC	CMC-C2C-C1C	-3.61	122.39	128.36
2	A	1301	HEC	CMB-C2B-C1B	-3.53	122.53	128.36
2	A	1294	HEC	CMC-C2C-C1C	-3.51	122.56	128.36
2	A	1299	HEC	CMC-C2C-C1C	-3.50	122.57	128.36
2	B	1300	HEC	CMC-C2C-C1C	-3.48	122.61	128.36
2	B	1299	HEC	CMC-C2C-C1C	-3.48	122.61	128.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1296	HEC	CAA-C2A-C1A	-3.45	123.26	127.01
2	A	1301	HEC	CAD-C3D-C4D	-3.37	123.34	127.01
2	A	1295	HEC	CMB-C2B-C1B	-3.33	122.86	128.36
2	B	1298	HEC	CMD-C2D-C1D	-3.30	122.91	128.36
2	A	1300	HEC	CAA-C2A-C1A	-3.28	123.45	127.01
2	B	1299	HEC	CMB-C2B-C1B	-3.19	123.09	128.36
2	B	1295	HEC	CMC-C2C-C1C	-3.13	123.19	128.36
2	B	1295	HEC	CMD-C2D-C1D	-3.11	123.22	128.36
2	A	1295	HEC	CAD-C3D-C4D	-3.10	123.64	127.01
2	B	1298	HEC	CMB-C2B-C1B	-2.95	123.49	128.36
2	A	1298	HEC	CMC-C2C-C1C	-2.90	123.57	128.36
2	B	1296	HEC	CAD-C3D-C4D	-2.89	123.87	127.01
2	A	1293	HEC	CAD-C3D-C4D	-2.87	123.89	127.01
2	B	1299	HEC	CMD-C2D-C1D	-2.86	123.63	128.36
2	B	1295	HEC	CAD-C3D-C4D	-2.84	123.92	127.01
2	B	1293	HEC	CAA-CBA-CGA	-2.82	107.58	112.75
2	A	1298	HEC	CMB-C2B-C1B	-2.73	123.84	128.36
2	A	1300	HEC	CMB-C2B-C1B	-2.72	123.86	128.36
2	B	1301	HEC	CAA-C2A-C1A	-2.71	124.07	127.01
2	A	1296	HEC	CAD-C3D-C4D	-2.62	124.16	127.01
2	B	1301	HEC	CAD-C3D-C4D	-2.61	124.17	127.01
2	B	1297	HEC	CMC-C2C-C1C	-2.59	124.07	128.36
2	A	1301	HEC	CMC-C2C-C1C	-2.57	124.11	128.36
2	A	1297	HEC	CAD-C3D-C4D	-2.56	124.23	127.01
2	B	1300	HEC	CAD-C3D-C4D	-2.52	124.27	127.01
2	A	1293	HEC	CMD-C2D-C1D	-2.47	124.27	128.36
2	B	1297	HEC	CMB-C2B-C1B	-2.43	124.34	128.36
2	A	1295	HEC	CMD-C2D-C1D	-2.40	124.39	128.36
2	A	1293	HEC	CAA-C2A-C1A	-2.39	124.41	127.01
2	B	1300	HEC	CMB-C2B-C1B	-2.36	124.46	128.36
2	B	1296	HEC	CMB-C2B-C1B	-2.32	124.53	128.36
2	B	1296	HEC	CMD-C2D-C1D	-2.28	124.59	128.36
2	B	1296	HEC	CMC-C2C-C1C	-2.25	124.64	128.36
2	A	1296	HEC	CMB-C2B-C1B	-2.23	124.68	128.36
2	A	1296	HEC	CMC-C2C-C1C	-2.23	124.68	128.36
2	B	1299	HEC	CAD-C3D-C4D	-2.21	124.61	127.01
2	B	1297	HEC	CBD-CAD-C3D	-2.20	108.58	112.53
2	A	1296	HEC	CMD-C2D-C1D	-2.20	124.73	128.36
2	A	1299	HEC	CMD-C2D-C1D	-2.19	124.74	128.36
2	A	1299	HEC	CMB-C2B-C1B	-2.18	124.76	128.36
2	A	1297	HEC	CMC-C2C-C1C	-2.14	124.83	128.36
2	A	1299	HEC	CAD-C3D-C4D	-2.10	124.72	127.01

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1298	HEC	CAD-C3D-C4D	-2.07	124.76	127.01
2	A	1299	HEC	CBA-CAA-C2A	-2.06	108.84	112.53
2	A	1297	HEC	CMB-C2B-C1B	-2.06	124.96	128.36
2	B	1294	HEC	CBD-CAD-C3D	-2.05	108.85	112.53
2	A	1297	HEC	CMD-C2D-C1D	-2.04	124.99	128.36
2	A	1298	HEC	CAA-C2A-C1A	-2.03	124.81	127.01
2	A	1294	HEC	CMB-C2B-C1B	-2.02	125.02	128.36
2	B	1294	HEC	CMD-C2D-C1D	-2.01	125.04	128.36
2	B	1301	HEC	CMA-C3A-C2A	2.10	129.63	125.24
2	B	1301	HEC	C4C-C3C-C2C	2.14	108.66	106.35
2	B	1295	HEC	CMD-C2D-C3D	2.14	129.71	125.24
2	B	1298	HEC	CMD-C2D-C3D	2.48	130.41	125.24
2	A	1301	HEC	CMA-C3A-C2A	2.61	130.70	125.24
2	A	1301	HEC	CMD-C2D-C3D	3.09	131.71	125.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1293	HEC	3	0
2	A	1294	HEC	2	0
2	A	1295	HEC	4	0
2	A	1296	HEC	2	0
2	A	1297	HEC	3	0
2	A	1298	HEC	2	0
2	A	1299	HEC	2	0
2	A	1300	HEC	3	0
2	A	1301	HEC	2	0
3	A	1302	ACT	1	0
2	B	1293	HEC	2	0
2	B	1294	HEC	2	0
2	B	1295	HEC	3	0
2	B	1296	HEC	4	0
2	B	1297	HEC	3	0
2	B	1298	HEC	5	0
2	B	1299	HEC	2	0
2	B	1300	HEC	4	0
2	B	1301	HEC	2	0
4	B	1302	GOL	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.