



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:36 PM GMT

PDB ID : 1BL9  
Title : CONFORMATIONAL CHANGES OCCURRING UPON REDUCTION IN  
NITRITE REDUCTASE FROM PSEUDOMONAS AERUGINOSA  
Authors : Nurizzo, D.; Cambillau, C.; Tegoni, M.  
Deposited on : 1998-07-20  
Resolution : 2.90 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.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

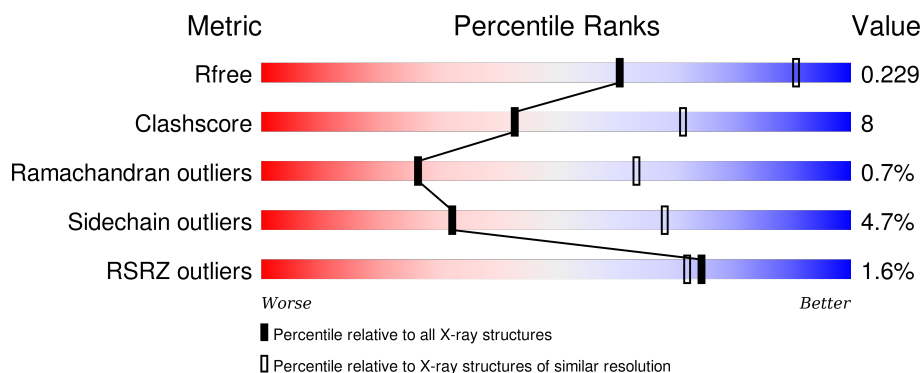
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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.

Mol	Chain	Length	Quality of chain
1	A	543	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 19%, green 77%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>77%</span> <span>19%</span> <span>...</span> </div> </div>
1	B	543	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 19%, green 78%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>78%</span> <span>19%</span> <span>..</span> </div> </div>

## 2 Entry composition [i](#)

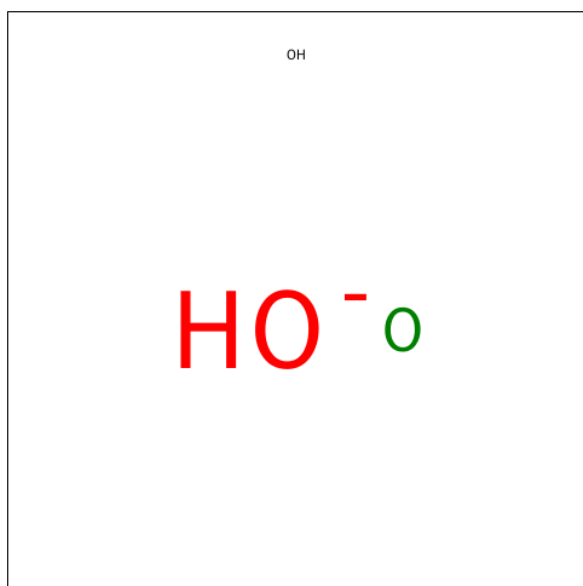
There are 5 unique types of molecules in this entry. The entry contains 8659 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NITRITE REDUCTASE.

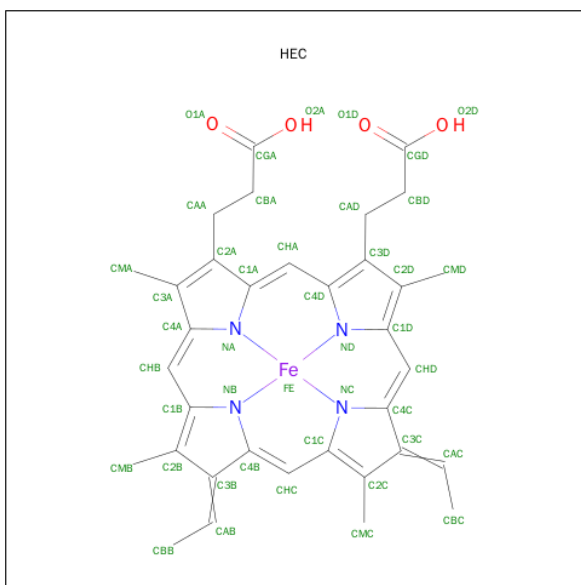
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4198	2662	732	792	12			
1	B	537	Total	C	N	O	S	0	0	0
			4198	2662	732	792	12			

- Molecule 2 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



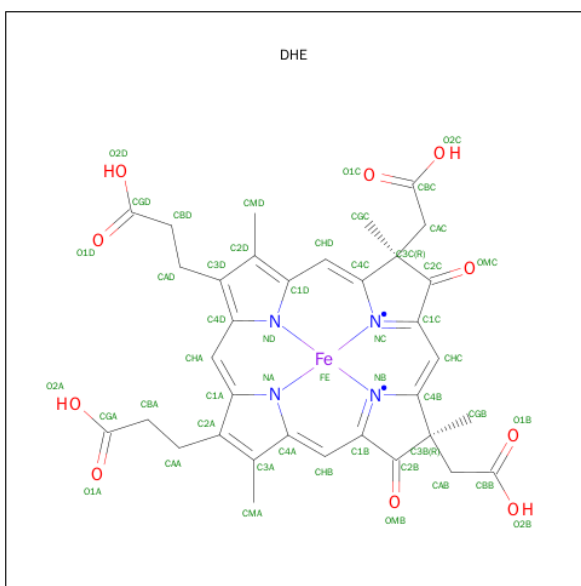
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	O	0	0
			1	1		

- Molecule 3 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 4 is HEME D (three-letter code: DHE) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_{10}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 49	C 34	Fe 1	N 4	O 10	0	0
4	B	1	Total 49	C 34	Fe 1	N 4	O 10	0	0

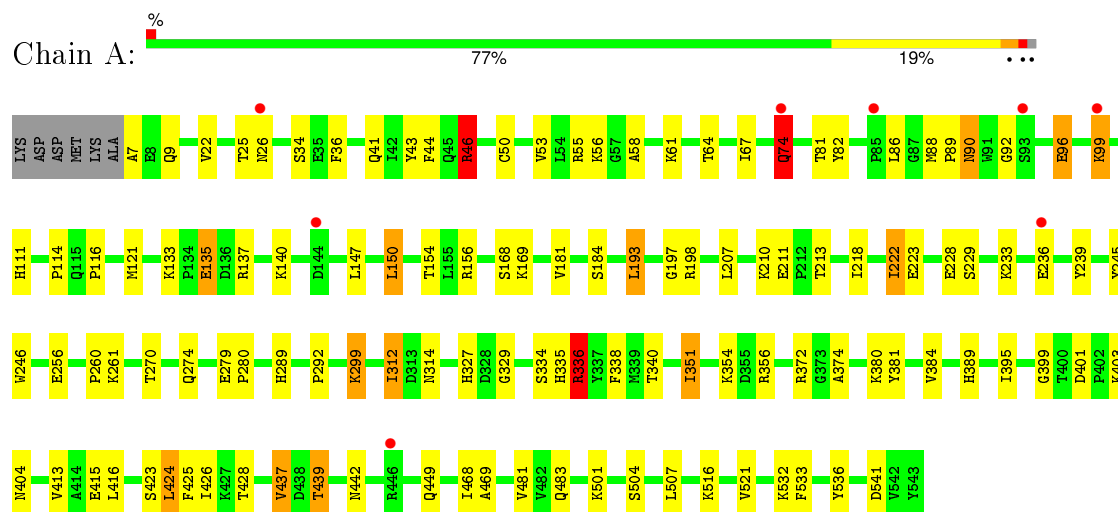
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total 36	O 36	0	0
5	B	42	Total 42	O 42	0	0

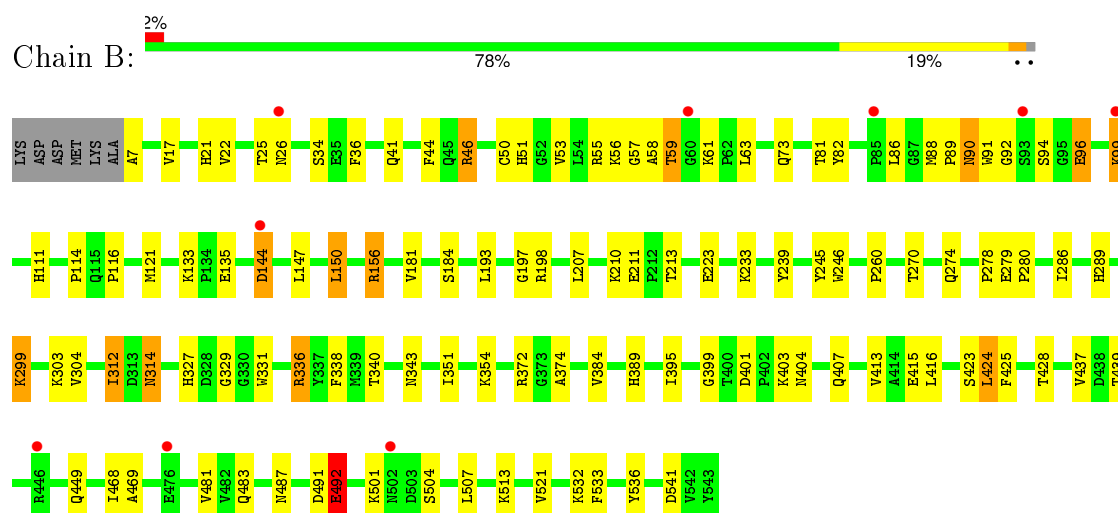
### 3 Residue-property plots

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.

#### • Molecule 1: NITRITE REDUCTASE



#### • Molecule 1: NITRITE REDUCTASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.61Å 89.00Å 112.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.90 11.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.5 (12.00-2.90) 98.6 (11.95-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.92Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.211 , 0.233 0.207 , 0.229	Depositor DCC
$R_{free}$ test set	856 reflections (2.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.4	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 36815 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8659	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.56 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.4536e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: DHE, HEC, OH

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	0.72	18/4303 (0.4%)	0.87	14/5847 (0.2%)
1	B	0.69	18/4303 (0.4%)	0.89	18/5847 (0.3%)
All	All	0.70	36/8606 (0.4%)	0.88	32/11694 (0.3%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	GLN	CD-NE2	-12.52	1.01	1.32
1	A	9	GLN	CD-NE2	-10.65	1.06	1.32
1	B	90	ASN	CG-ND2	-9.88	1.08	1.32
1	A	90	ASN	CG-ND2	-9.55	1.08	1.32
1	A	314	ASN	CG-OD1	-8.75	1.04	1.24
1	B	437	VAL	CB-CG1	-8.72	1.34	1.52
1	B	314	ASN	CG-OD1	-8.66	1.04	1.24
1	B	90	ASN	CG-OD1	-8.64	1.04	1.24
1	B	437	VAL	CB-CG2	-8.36	1.35	1.52
1	A	90	ASN	CG-OD1	-8.16	1.05	1.24
1	A	41	GLN	CD-NE2	-8.11	1.12	1.32
1	A	314	ASN	CG-ND2	-7.53	1.14	1.32
1	B	415	GLU	CD-OE1	-7.45	1.17	1.25
1	A	415	GLU	CD-OE1	-7.29	1.17	1.25
1	B	314	ASN	CG-ND2	-6.92	1.15	1.32
1	A	536	TYR	CE1-CZ	-6.84	1.29	1.38
1	B	536	TYR	CE1-CZ	-6.79	1.29	1.38
1	A	9	GLN	CD-OE1	-6.70	1.09	1.24
1	B	536	TYR	CE2-CZ	-6.62	1.29	1.38
1	A	90	ASN	CB-CG	6.41	1.65	1.51
1	A	536	TYR	CE2-CZ	-6.32	1.30	1.38
1	B	536	TYR	CG-CD1	-5.67	1.31	1.39
1	B	314	ASN	CB-CG	5.59	1.64	1.51
1	B	233	LYS	CB-CG	-5.49	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	GLN	CD-NE2	-5.44	1.19	1.32
1	A	44	PHE	CG-CD2	-5.40	1.30	1.38
1	B	403	LYS	CG-CD	-5.39	1.34	1.52
1	B	193	LEU	CG-CD2	-5.38	1.31	1.51
1	A	256	GLU	CD-OE2	-5.33	1.19	1.25
1	A	536	TYR	CG-CD2	-5.30	1.32	1.39
1	A	536	TYR	CG-CD1	-5.25	1.32	1.39
1	A	44	PHE	CG-CD1	-5.22	1.30	1.38
1	B	44	PHE	CG-CD1	-5.22	1.30	1.38
1	B	536	TYR	CG-CD2	-5.17	1.32	1.39
1	A	193	LEU	CG-CD2	-5.17	1.32	1.51
1	B	90	ASN	CB-CG	5.13	1.62	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	ARG	NE-CZ-NH2	12.60	126.60	120.30
1	A	336	ARG	NE-CZ-NH2	11.86	126.23	120.30
1	B	403	LYS	CD-CE-NZ	-11.54	85.15	111.70
1	B	46	ARG	NE-CZ-NH2	9.81	125.21	120.30
1	B	437	VAL	CG1-CB-CG2	-9.17	96.22	110.90
1	A	46	ARG	NE-CZ-NH2	8.39	124.50	120.30
1	A	336	ARG	NH1-CZ-NH2	-7.41	111.25	119.40
1	A	415	GLU	OE1-CD-OE2	-7.41	114.41	123.30
1	B	415	GLU	OE1-CD-OE2	-7.21	114.65	123.30
1	B	541	ASP	CB-CG-OD1	7.08	124.67	118.30
1	A	541	ASP	CB-CG-OD1	7.05	124.64	118.30
1	A	372	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	B	336	ARG	NH1-CZ-NH2	-6.76	111.96	119.40
1	B	372	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	B	289	HIS	CG-ND1-CE1	5.96	116.55	108.20
1	B	536	TYR	CD1-CE1-CZ	5.87	125.08	119.80
1	A	44	PHE	CE1-CZ-CE2	-5.85	109.47	120.00
1	A	289	HIS	CG-ND1-CE1	5.83	116.37	108.20
1	A	193	LEU	CD1-CG-CD2	-5.81	93.06	110.50
1	B	111	HIS	CG-ND1-CE1	5.72	116.20	108.20
1	A	111	HIS	CG-ND1-CE1	5.66	116.13	108.20
1	A	536	TYR	CZ-CE2-CD2	5.56	124.80	119.80
1	A	536	TYR	CD1-CE1-CZ	5.55	124.79	119.80
1	B	492	GLU	OE1-CD-OE2	-5.55	116.64	123.30
1	B	536	TYR	CZ-CE2-CD2	5.50	124.75	119.80
1	B	193	LEU	CD1-CG-CD2	-5.50	94.00	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	PHE	CE1-CZ-CE2	-5.45	110.18	120.00
1	A	67	ILE	CG1-CB-CG2	-5.42	99.47	111.40
1	B	46	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
1	B	403	LYS	CG-CD-CE	5.16	127.39	111.90
1	B	343	ASN	O-C-N	-5.05	114.62	122.70
1	A	46	ARG	NH1-CZ-NH2	-5.03	113.87	119.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	4198	0	4153	68	0
1	B	4198	0	4153	73	0
2	B	1	0	0	0	0
3	A	43	0	30	5	0
3	B	43	0	30	5	0
4	A	49	0	24	1	0
4	B	49	0	24	2	0
5	A	36	0	0	2	0
5	B	42	0	0	3	0
All	All	8659	0	8414	140	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.

All (140) 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:336:ARG:HH11	1:A:354:LYS:HB3	1.29	0.97
1:A:114:PRO:HB2	1:B:22:VAL:HG12	1.57	0.86
1:A:22:VAL:HG12	1:B:114:PRO:HB2	1.66	0.77
1:B:336:ARG:NH1	1:B:354:LYS:HD3	1.99	0.77
1:B:53:VAL:HG11	1:B:116:PRO:HG3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ILE:HG13	1:A:437:VAL:HG12	1.68	0.74
1:A:236:GLU:HG3	5:A:611:HOH:O	1.90	0.71
3:B:601:HEC:HBC3	3:B:601:HEC:HMC1	1.75	0.69
1:B:50:CYS:O	1:B:58:ALA:HB3	1.93	0.68
1:A:336:ARG:NH1	1:A:354:LYS:HB3	2.06	0.68
1:A:96:GLU:HA	1:A:96:GLU:OE1	1.94	0.67
1:B:96:GLU:OE1	1:B:96:GLU:HA	1.96	0.65
1:A:56:LYS:HE3	1:A:64:THR:HG21	1.77	0.65
1:A:121:MET:SD	1:A:260:PRO:HB2	2.37	0.65
1:B:223:GLU:HG2	1:B:245:TYR:HB2	1.78	0.65
1:B:56:LYS:HG3	1:B:278:PRO:CG	2.26	0.65
1:B:46:ARG:HH11	1:B:91:TRP:HZ3	1.44	0.64
1:B:61:LYS:HE2	3:B:601:HEC:O2D	1.96	0.64
3:A:601:HEC:HMC1	3:A:601:HEC:HBC3	1.78	0.64
1:A:223:GLU:HG2	1:A:245:TYR:HB2	1.82	0.61
1:A:53:VAL:HG11	1:A:116:PRO:HG3	1.81	0.61
1:A:46:ARG:NH1	1:A:96:GLU:HG3	2.15	0.61
1:B:99:LYS:HA	1:B:99:LYS:HE2	1.82	0.61
1:A:7:ALA:N	5:A:636:HOH:O	2.33	0.61
1:A:181:VAL:HA	1:A:197:GLY:HA2	1.81	0.61
1:B:7:ALA:N	5:B:640:HOH:O	2.33	0.61
1:B:181:VAL:HA	1:B:197:GLY:HA2	1.82	0.60
1:A:99:LYS:HA	1:A:99:LYS:HE2	1.82	0.60
1:B:133:LYS:HB3	1:B:135:GLU:OE1	2.02	0.60
1:A:423:SER:HA	1:A:439:THR:HA	1.84	0.60
1:B:55:ARG:CD	1:B:63:LEU:HB2	2.32	0.59
1:A:43:TYR:OH	1:A:55:ARG:HG2	2.03	0.59
1:B:90:ASN:ND2	1:B:94:SER:HB3	2.18	0.58
1:A:61:LYS:HG3	3:A:601:HEC:HAD2	1.85	0.58
1:B:304:VAL:HG11	1:B:351:ILE:HG13	1.86	0.57
1:A:261:LYS:HB3	1:A:312:ILE:HD11	1.87	0.56
1:A:211:GLU:O	1:A:213:THR:HG23	2.05	0.56
1:A:116:PRO:HG2	1:A:246:TRP:CE2	2.41	0.55
1:B:116:PRO:HG2	1:B:246:TRP:CE2	2.42	0.55
1:B:211:GLU:O	1:B:213:THR:HG23	2.06	0.55
1:A:50:CYS:O	1:A:58:ALA:HB3	2.06	0.55
1:A:218:ILE:HD11	1:A:260:PRO:HG3	1.88	0.55
1:B:239:TYR:CZ	1:B:312:ILE:HG21	2.41	0.55
1:B:55:ARG:HD2	1:B:63:LEU:HB2	1.89	0.54
1:B:121:MET:SD	1:B:260:PRO:HB2	2.48	0.54
1:B:46:ARG:HD2	1:B:91:TRP:CZ3	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:601:HEC:HBB3	3:B:601:HEC:HMB1	1.89	0.53
1:B:279:GLU:N	1:B:280:PRO:HD3	2.22	0.53
1:A:279:GLU:N	1:A:280:PRO:HD3	2.23	0.53
1:A:81:THR:HG23	1:A:92:GLY:HA3	1.92	0.52
1:B:144:ASP:OD1	1:B:144:ASP:N	2.43	0.52
1:B:239:TYR:CE1	1:B:312:ILE:HG21	2.45	0.52
1:A:380:LYS:HE2	1:A:381:TYR:CE1	2.44	0.52
1:A:468:ILE:HB	1:A:481:VAL:HG21	1.92	0.52
1:B:338:PHE:HB3	1:B:351:ILE:HB	1.93	0.51
1:B:468:ILE:HB	1:B:481:VAL:HG21	1.92	0.51
1:B:384:VAL:HG12	1:B:399:GLY:HA2	1.93	0.51
1:A:384:VAL:HG12	1:A:399:GLY:HA2	1.93	0.50
1:B:86:LEU:HB2	3:B:601:HEC:O1D	2.12	0.50
1:A:336:ARG:NH1	1:A:354:LYS:HD3	2.26	0.50
1:A:239:TYR:CZ	1:A:312:ILE:HG21	2.46	0.49
1:B:82:TYR:O	1:B:90:ASN:HB3	2.12	0.49
1:B:423:SER:HA	1:B:439:THR:HA	1.94	0.49
1:B:55:ARG:C	1:B:57:GLY:N	2.66	0.49
1:B:424:LEU:HB3	1:B:425:PHE:CD2	2.48	0.48
1:B:449:GLN:HB3	1:B:469:ALA:HB3	1.95	0.48
1:A:424:LEU:HB3	1:A:425:PHE:CD2	2.47	0.48
1:A:449:GLN:HB3	1:A:469:ALA:HB3	1.96	0.48
1:B:81:THR:HG23	1:B:92:GLY:HA3	1.96	0.47
1:B:395:ILE:HB	1:B:416:LEU:HB2	1.97	0.47
1:B:46:ARG:NH1	1:B:91:TRP:HZ3	2.11	0.47
1:A:198:ARG:HH22	4:A:602:DHE:CBB	2.27	0.47
1:A:184:SER:HB2	1:A:533:PHE:CD2	2.50	0.47
1:A:389:HIS:O	1:A:423:SER:HB3	2.15	0.47
1:B:374:ALA:HB1	1:B:428:THR:HG22	1.97	0.47
1:A:395:ILE:HB	1:A:416:LEU:HB2	1.98	0.46
1:A:507:LEU:HB2	1:A:521:VAL:HB	1.97	0.46
1:B:389:HIS:O	1:B:423:SER:HB3	2.16	0.46
3:A:601:HEC:HBB3	3:A:601:HEC:HMB1	1.96	0.46
1:B:184:SER:HB2	1:B:533:PHE:CD2	2.51	0.46
1:B:51:HIS:O	1:B:55:ARG:HA	2.15	0.45
1:A:114:PRO:HB2	1:B:22:VAL:CG1	2.39	0.45
1:B:532:LYS:HE2	1:B:532:LYS:HB2	1.79	0.45
1:A:374:ALA:HB1	1:A:428:THR:HG22	1.99	0.45
1:B:90:ASN:O	1:B:90:ASN:ND2	2.50	0.45
1:A:270:THR:O	1:A:274:GLN:HA	2.17	0.45
1:A:46:ARG:HH11	1:A:96:GLU:HG3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:LEU:HB2	1:B:521:VAL:HB	1.98	0.44
1:A:82:TYR:O	1:A:90:ASN:HB3	2.16	0.44
1:B:56:LYS:HG3	1:B:278:PRO:HG3	1.99	0.44
1:A:222:ILE:CG2	1:B:17:VAL:HG22	2.48	0.44
1:A:99:LYS:CE	1:A:99:LYS:HA	2.46	0.44
1:B:61:LYS:HB3	5:B:638:HOH:O	2.18	0.44
1:A:532:LYS:HB2	1:A:532:LYS:HE2	1.79	0.44
1:B:116:PRO:HG2	1:B:246:TRP:NE1	2.32	0.44
1:B:156:ARG:HD3	5:B:618:HOH:O	2.16	0.44
1:B:99:LYS:HA	1:B:99:LYS:CE	2.48	0.43
1:A:147:LEU:HD22	1:A:207:LEU:HB3	1.99	0.43
1:A:150:LEU:HD12	1:A:150:LEU:HA	1.84	0.43
1:A:133:LYS:HB3	1:A:135:GLU:OE1	2.17	0.43
1:A:36:PHE:HZ	1:A:114:PRO:HG3	1.83	0.43
1:B:329:GLY:HA3	1:B:340:THR:HA	2.00	0.43
1:A:239:TYR:CE1	1:A:312:ILE:HG21	2.53	0.43
1:A:116:PRO:HG2	1:A:246:TRP:NE1	2.32	0.43
1:B:270:THR:O	1:B:274:GLN:HA	2.18	0.43
1:B:88:MET:HB2	3:B:601:HEC:C4D	2.48	0.43
1:B:487:ASN:CG	1:B:492:GLU:HG3	2.39	0.43
1:B:401:ASP:OD2	1:B:404:ASN:HB2	2.18	0.43
1:B:198:ARG:HH22	4:B:602:DHE:CBB	2.31	0.43
1:A:439:THR:OG1	1:A:442:ASN:HB2	2.18	0.43
1:B:56:LYS:HG3	1:B:278:PRO:CD	2.49	0.43
1:B:25:THR:O	1:B:26:ASN:HB2	2.18	0.43
1:B:150:LEU:HD12	1:B:150:LEU:HA	1.84	0.43
1:B:36:PHE:HZ	1:B:114:PRO:HG3	1.84	0.42
1:A:401:ASP:OD2	1:A:404:ASN:HB2	2.19	0.42
1:B:286:ILE:HD11	1:B:331:TRP:CD1	2.55	0.42
1:A:88:MET:HA	1:A:89:PRO:HD2	1.89	0.42
1:B:55:ARG:HD3	1:B:63:LEU:HB2	2.00	0.42
1:B:198:ARG:NH2	4:B:602:DHE:O2B	2.52	0.42
1:A:25:THR:O	1:A:26:ASN:HB2	2.19	0.42
1:A:86:LEU:HB2	3:A:601:HEC:O1D	2.20	0.42
1:A:354:LYS:O	1:A:356:ARG:HG3	2.19	0.42
1:B:491:ASP:OD1	1:B:492:GLU:HG2	2.20	0.42
1:B:88:MET:HA	1:B:89:PRO:HD2	1.88	0.41
1:A:228:GLU:HG3	1:A:229:SER:N	2.35	0.41
1:B:46:ARG:HD3	1:B:46:ARG:HA	1.94	0.41
1:B:55:ARG:NH1	1:B:63:LEU:O	2.52	0.41
1:A:133:LYS:O	1:A:137:ARG:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:HD22	1:B:207:LEU:HB3	2.02	0.41
3:A:601:HEC:HMD1	3:A:601:HEC:HAD1	1.96	0.41
1:A:299:LYS:NZ	1:A:327:HIS:HD2	2.19	0.41
1:A:222:ILE:HG21	1:B:17:VAL:HG22	2.02	0.41
1:B:299:LYS:NZ	1:B:327:HIS:HD2	2.20	0.40
1:A:338:PHE:HB3	1:A:351:ILE:HB	2.02	0.40
1:A:334:SER:O	1:A:335:HIS:HB2	2.22	0.40
1:A:74:GLN:HG2	1:A:74:GLN:H	1.46	0.40
1:A:22:VAL:HG22	1:B:116:PRO:HB3	2.03	0.40
1:A:154:THR:HG21	1:A:181:VAL:O	2.21	0.40
1:A:329:GLY:HA3	1:A:340:THR:HA	2.03	0.40
1:A:168:SER:O	1:A:169:LYS:HB2	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	535/543 (98%)	496 (93%)	36 (7%)	3 (1%)	30	67
1	B	535/543 (98%)	494 (92%)	37 (7%)	4 (1%)	26	63
All	All	1070/1086 (98%)	990 (92%)	73 (7%)	7 (1%)	26	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	LYS
1	B	299	LYS
1	B	156	ARG
1	A	156	ARG
1	B	59	THR
1	A	483	GLN

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Mol	Chain	Res	Type
1	B	483	GLN

### 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	453/458 (99%)	429 (95%)	24 (5%)	28	63
1	B	453/458 (99%)	434 (96%)	19 (4%)	36	73
All	All	906/916 (99%)	863 (95%)	43 (5%)	32	68

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	46	ARG
1	A	74	GLN
1	A	96	GLU
1	A	99	LYS
1	A	135	GLU
1	A	140	LYS
1	A	150	LEU
1	A	193	LEU
1	A	210	LYS
1	A	222	ILE
1	A	233	LYS
1	A	292	PRO
1	A	312	ILE
1	A	336	ARG
1	A	351	ILE
1	A	403	LYS
1	A	413	VAL
1	A	424	LEU
1	A	437	VAL
1	A	439	THR
1	A	501	LYS

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Mol	Chain	Res	Type
1	A	504	SER
1	A	516	LYS
1	B	21	HIS
1	B	34	SER
1	B	59	THR
1	B	73	GLN
1	B	96	GLU
1	B	99	LYS
1	B	144	ASP
1	B	150	LEU
1	B	210	LYS
1	B	303	LYS
1	B	312	ILE
1	B	314	ASN
1	B	407	GLN
1	B	413	VAL
1	B	424	LEU
1	B	492	GLU
1	B	501	LYS
1	B	504	SER
1	B	513	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	111	HIS
1	A	115	GLN
1	A	160	GLN
1	A	327	HIS
1	B	73	GLN
1	B	110	GLN
1	B	115	GLN
1	B	160	GLN
1	B	314	ASN
1	B	327	HIS

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is modelled with single atom - leaving 4 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$
3	HEC	A	601	1	24,50,50	1.63	2 (8%)	19,82,82	1.45	3 (15%)
4	DHE	A	602	1	29,56,56	2.04	8 (27%)	27,94,94	3.19	8 (29%)
3	HEC	B	601	1	24,50,50	1.72	2 (8%)	19,82,82	1.71	4 (21%)
4	DHE	B	602	1,2	29,56,56	2.04	7 (24%)	27,94,94	3.12	10 (37%)

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
3	HEC	A	601	1	-	0/6/54/54	0/0/8/8
4	DHE	A	602	1	-	0/12/108/108	0/0/8/8
3	HEC	B	601	1	-	0/6/54/54	0/0/8/8
4	DHE	B	602	1,2	-	0/12/108/108	0/0/8/8

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	HEC	C3B-C2B	-5.84	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	HEC	C3C-C2C	-5.24	1.35	1.40
4	A	602	DHE	CAC-C3C	-5.00	1.48	1.56
4	B	602	DHE	CAC-C3C	-4.75	1.48	1.56
4	B	602	DHE	CAB-C3B	-4.74	1.48	1.56
4	A	602	DHE	CAB-C3B	-4.69	1.48	1.56
3	A	601	HEC	C3B-C2B	-4.54	1.36	1.40
3	B	601	HEC	C3C-C2C	-4.43	1.36	1.40
4	B	602	DHE	CBD-CAD	-3.61	1.28	1.53
4	A	602	DHE	CBD-CAD	-3.56	1.29	1.53
4	A	602	DHE	CAD-C3D	-3.03	1.46	1.52
4	B	602	DHE	CAD-C3D	-2.70	1.47	1.52
4	A	602	DHE	CHB-C1B	2.37	1.39	1.35
4	A	602	DHE	CGB-C3B	2.83	1.60	1.54
4	B	602	DHE	CGB-C3B	2.90	1.60	1.54
4	A	602	DHE	CGC-C3C	3.13	1.61	1.54
4	B	602	DHE	CGC-C3C	3.46	1.62	1.54
4	A	602	DHE	FE-NB	3.52	2.09	1.95
4	B	602	DHE	FE-NB	3.67	2.10	1.95

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	HEC	CBB-CAB-C3B	-3.58	119.40	127.35
3	B	601	HEC	CBC-CAC-C3C	-3.26	120.11	127.35
4	A	602	DHE	CMA-C3A-C4A	-3.09	123.25	128.36
4	B	602	DHE	CMD-C2D-C1D	-2.98	123.43	128.36
3	B	601	HEC	CBB-CAB-C3B	-2.86	121.00	127.35
3	A	601	HEC	CBD-CAD-C3D	-2.78	107.54	112.53
4	B	602	DHE	CMA-C3A-C4A	-2.77	123.78	128.36
3	B	601	HEC	CAA-C2A-C3A	-2.68	121.36	129.00
4	A	602	DHE	CMD-C2D-C1D	-2.65	123.98	128.36
4	B	602	DHE	CAD-C3D-C4D	-2.50	124.29	127.01
3	A	601	HEC	CBC-CAC-C3C	-2.23	122.39	127.35
4	B	602	DHE	CHB-C1B-NB	2.23	126.79	124.42
4	A	602	DHE	CAA-CBA-CGA	2.48	117.29	112.75
4	B	602	DHE	CAA-CBA-CGA	2.53	117.39	112.75
4	A	602	DHE	CHB-C1B-NB	2.66	127.24	124.42
4	B	602	DHE	CHC-C1C-NC	2.70	127.60	124.45
3	B	601	HEC	CAA-C2A-C1A	4.17	131.54	127.01
4	B	602	DHE	C1C-NC-C4C	6.27	110.70	105.00
4	B	602	DHE	C1B-NB-C4B	6.27	110.31	106.90
4	A	602	DHE	C1C-NC-C4C	6.65	111.05	105.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	DHE	CAD-CBD-CGD	7.03	125.64	112.75
4	B	602	DHE	CAD-CBD-CGD	7.18	125.91	112.75
4	A	602	DHE	C1B-NB-C4B	7.45	110.95	106.90
4	A	602	DHE	CBD-CAD-C3D	8.37	127.54	112.53
4	B	602	DHE	CBD-CAD-C3D	8.63	127.99	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	HEC	5	0
4	A	602	DHE	1	0
3	B	601	HEC	5	0
4	B	602	DHE	2	0

## 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, 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	537/543 (98%)	-0.46	8 (1%) 76 74	15, 39, 65, 84	0
1	B	537/543 (98%)	-0.48	9 (1%) 73 70	21, 38, 65, 83	0
All	All	1074/1086 (98%)	-0.47	17 (1%) 74 72	15, 38, 65, 84	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	GLY	4.1
1	B	144	ASP	3.3
1	A	93	SER	2.9
1	A	236	GLU	2.7
1	A	144	ASP	2.5
1	A	26	ASN	2.5
1	B	502	ASN	2.4
1	B	93	SER	2.4
1	B	26	ASN	2.4
1	B	446	ARG	2.3
1	A	85	PRO	2.2
1	A	74	GLN	2.2
1	B	85	PRO	2.2
1	A	446	ARG	2.2
1	B	99	LYS	2.1
1	A	99	LYS	2.1
1	B	476	GLU	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 [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DHE	A	602	49/49	0.97	0.12	-0.22	24,32,43,45	0
3	HEC	B	601	43/43	0.96	0.14	-0.61	26,34,45,47	0
4	DHE	B	602	49/49	0.97	0.11	-0.74	16,29,42,47	0
3	HEC	A	601	43/43	0.97	0.13	-0.87	19,35,56,65	0
2	OH	B	603	1/1	0.98	0.35	-	42,42,42,42	0

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

There are no such residues in this entry.