



# Full wwPDB X-ray Structure Validation Report

Jun 5, 2014 – 08:21 PM EDT

PDB ID : 4L3Y  
Title : Nitrite complex of TvNiR, high dose data set (NO complex)  
Authors : Trofimov, A.A.; Polyakov, K.M.; Lazarenko, V.A.; Popov, A.N.; Tikhonova, T.V.; Tikhonov, A.V.; Popov, V.O.  
Deposited on : 2013-06-07  
Resolution : 1.95 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>

---

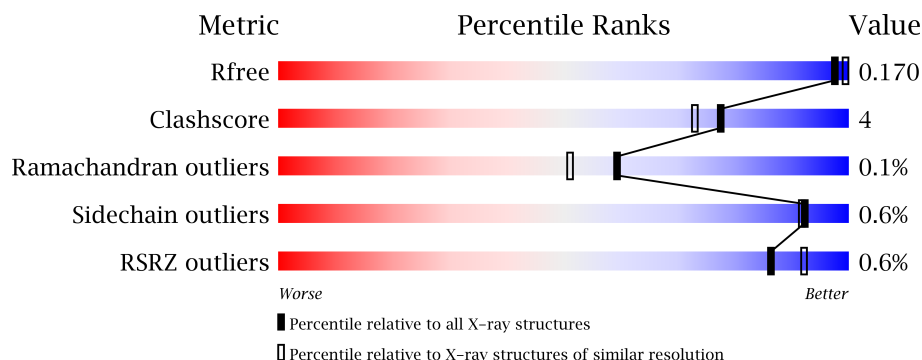
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23161  
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) : stable23161

# 1 Overall quality at a glance

The reported resolution of this entry is 1.95 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	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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	520	
1	B	520	

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	605	-	X
2	HEC	B	604[A]	-	X
2	HEC	B	604[B]	-	X
2	HEC	B	605	-	X
3	NO2	A	609	-	X
5	MPD	A	612	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
5	MPD	B	612	-	X
6	GOL	A	613[A]	-	X
6	GOL	A	613[B]	-	X
6	GOL	A	614	-	X
6	GOL	A	615[A]	-	X
6	GOL	A	615[B]	-	X
6	GOL	B	613[A]	-	X
6	GOL	B	613[B]	-	X
6	GOL	B	614	-	X
7	SO4	A	616	-	X
7	SO4	B	615	-	X

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 10324 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.

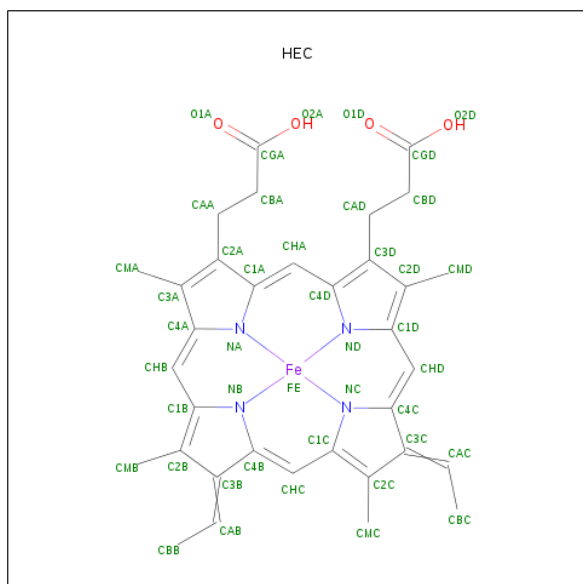
- Molecule 1 is a protein called Eight-heme nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	17	0
			4172	2587	755	796	34			
1	B	520	Total	C	N	O	S	0	16	0
			4179	2591	759	795	34			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	524	VAL	-	EXPRESSION TAG	UNP L0DSL2
B	524	VAL	-	EXPRESSION TAG	UNP L0DSL2

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



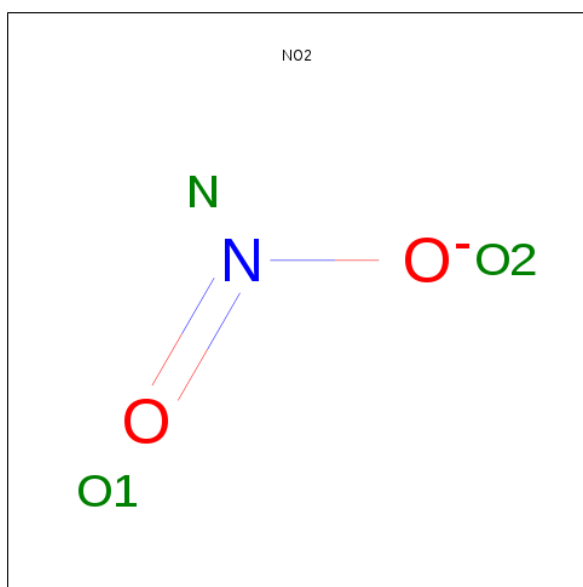
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

*Continued on next page...*

*Continued from previous page...*

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
			38	31	1	4	2		
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	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	1
			47	36	1	4	6		
2	B	1	Total	C	Fe	N	O	0	0
			39	32	1	4	2		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is NITRITE ION (three-letter code: NO2) (formula: NO<sub>2</sub>).

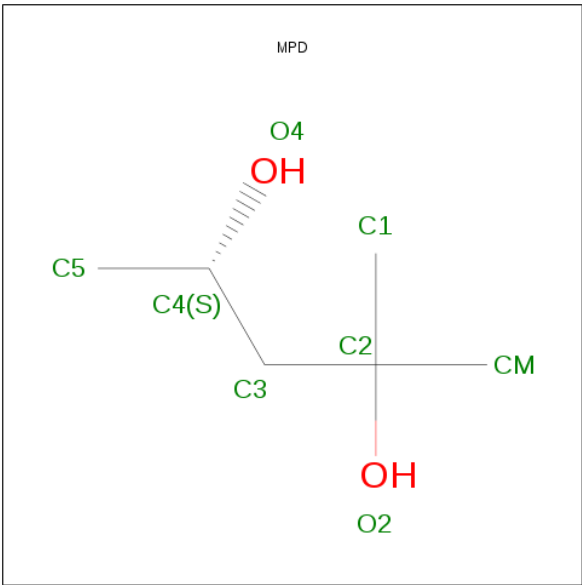


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			2	1	1		
3	A	1	Total	N	O	0	0
			3	1	2		
3	A	1	Total	N	O	0	0
			3	1	2		
3	B	1	Total	N	O	0	0
			2	1	1		
3	B	1	Total	N	O	0	0
			3	1	2		
3	B	1	Total	N	O	0	0
			3	1	2		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

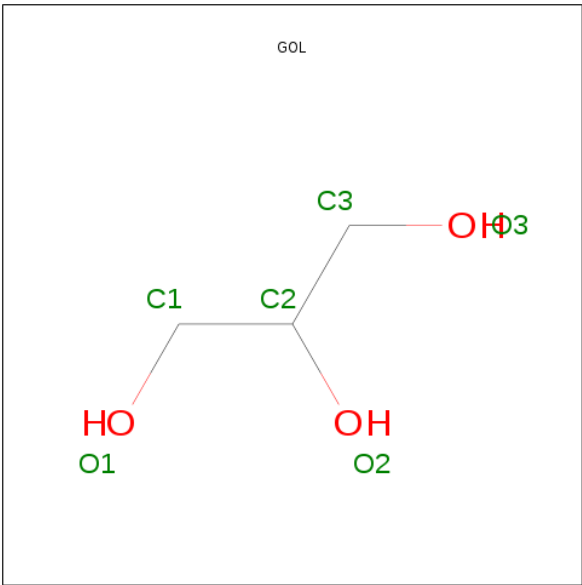
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ca	0	0
			2	2		
4	A	2	Total	Ca	0	0
			2	2		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



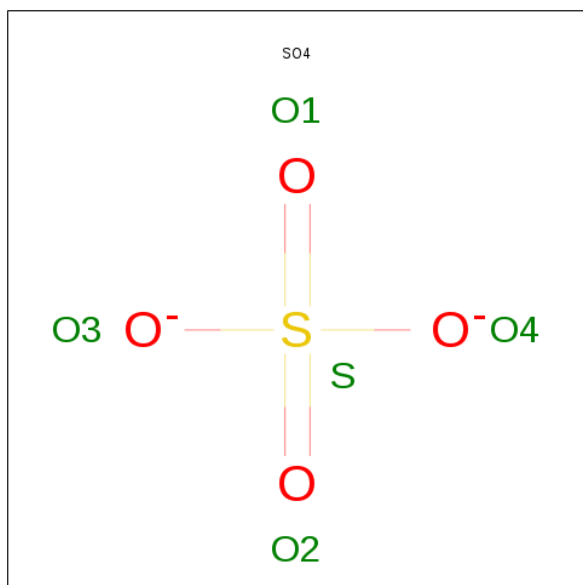
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			7	3	4		
6	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			7	3	4		
6	B	1	Total	C	O	0	1
			7	3	4		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	594	Total	O	0	0
			594	594		
8	B	617	Total	O	0	0
			617	617		



### 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: Eight-heme nitrite reductase

Chain A: 



- Molecule 1: Eight-heme nitrite reductase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.98Å 194.98Å 194.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.08 – 1.95 29.07 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.08-1.95) 99.5 (29.07-1.95)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.151 , 0.170 0.151 , 0.170	Depositor DCC
$R_{free}$ test set	8889 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 39.6	EDS
Estimated twinning fraction	0.050 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 177422 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10324	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: GOL, MPD, CA, SO4, HEC, NO2

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	0/4370	0.76	2/5930 (0.0%)
1	B	0.72	1/4369 (0.0%)	0.76	2/5928 (0.0%)
All	All	0.72	1/8739 (0.0%)	0.76	4/11858 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	GLU	CD-OE1	6.16	1.32	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	LYS	CD-CE-NZ	5.35	124.00	111.70
1	B	411	CYS	CB-CA-C	-5.33	99.74	110.40
1	A	153	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	201	ASP	CB-CG-OD1	5.05	122.85	118.30

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	4172	0	3878	28	0
1	B	4179	0	3892	27	0
2	A	339	0	236	9	0
2	B	344	0	214	7	0
3	A	8	0	0	0	0
3	B	8	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	8	0	14	1	0
5	B	8	0	14	3	0
6	A	20	0	18	0	0
6	B	13	0	12	0	0
7	A	5	0	0	0	0
7	B	5	0	0	1	0
8	A	594	0	0	10	1
8	B	617	0	0	13	1
All	All	10324	0	8278	63	1

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 4.

All (63) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:259[B]:HIS:HD2	8:B:956:HOH:O	0.82	1.17
1:A:222[A]:ASN:ND2	8:A:1186:HOH:O	1.85	1.10
1:B:138[B]:GLN:CD	8:B:1128:HOH:O	1.90	1.09
1:B:138[B]:GLN:NE2	8:B:1128:HOH:O	1.85	1.08
1:B:138[B]:GLN:OE1	8:B:1128:HOH:O	1.72	1.07
7:B:615:SO4:O1	8:B:1236:HOH:O	1.72	1.06
1:B:222[B]:ASN:ND2	8:B:1015:HOH:O	1.98	0.94
1:B:222[A]:ASN:OD1	8:B:1150:HOH:O	1.85	0.93
1:B:259[B]:HIS:CD2	8:B:956:HOH:O	1.66	0.92
1:A:204:GLU:OE2	8:A:1064:HOH:O	1.87	0.91
2:B:605:HEC:HMC1	2:B:605:HEC:HBC3	1.56	0.87
1:A:222[B]:ASN:OD1	8:A:1120:HOH:O	1.97	0.81
1:B:138[B]:GLN:NE2	5:B:612:MPD:H32	1.96	0.81
1:A:413:ASN:HB2	8:A:1118:HOH:O	1.84	0.76
1:B:474[A]:ASP:OD2	8:B:1225:HOH:O	2.07	0.73
2:A:605:HEC:HBC3	2:A:605:HEC:HMC1	1.75	0.68
2:A:606:HEC:HBC3	2:A:606:HEC:HMC1	1.77	0.67
1:A:521:GLN:O	1:A:524:VAL:HG22	1.94	0.67
2:B:606:HEC:HMC1	2:B:606:HEC:HBC3	1.83	0.60
1:B:413:ASN:HB2	8:B:1148:HOH:O	2.03	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:138[B]:GLN:HE21	5:B:612:MPD:H32	1.68	0.57
1:A:140:LYS:HG2	1:A:160[B]:THR:HG23	1.84	0.57
1:A:19[B]:THR:HG23	8:A:1226:HOH:O	2.03	0.57
1:A:68[B]:THR:HG23	8:A:1228:HOH:O	2.07	0.54
1:A:303:TYR:CE2	2:A:601:HEC:HMC2	2.43	0.54
1:A:140:LYS:HG2	1:A:160[B]:THR:CG2	2.39	0.53
2:B:603:HEC:HMA3	2:B:604[B]:HEC:HBA2	1.91	0.53
1:A:394[B]:VAL:HG12	8:A:950:HOH:O	2.10	0.52
1:A:384:MET:HB2	1:A:397:SER:O	2.10	0.51
1:B:138[B]:GLN:NE2	5:B:612:MPD:C3	2.70	0.51
1:B:129:VAL:HG11	2:B:601:HEC:HMA1	1.93	0.51
2:B:606:HEC:HBD2	2:B:606:HEC:HHA	1.93	0.51
1:B:524:VAL:HG13	8:B:1132:HOH:O	2.11	0.50
1:B:303:TYR:CE2	2:B:601:HEC:HMC2	2.48	0.48
1:A:367:PHE:CZ	2:A:604:HEC:HMC2	2.49	0.47
1:B:466:ASN:HD22	1:B:469:ARG:HD2	1.77	0.47
1:A:273[B]:THR:HG22	8:A:949:HOH:O	2.14	0.47
1:A:68[A]:THR:HG23	1:A:69:CYS:N	2.29	0.47
1:B:384:MET:HB2	1:B:397:SER:O	2.15	0.47
1:B:466:ASN:ND2	1:B:469:ARG:HH11	2.13	0.47
1:B:413:ASN:ND2	8:B:1142:HOH:O	2.48	0.46
1:A:487:SER:HB3	1:A:491:HIS:CE1	2.52	0.45
1:B:140:LYS:HG2	1:B:160[B]:THR:HG23	1.99	0.45
1:A:520:ALA:O	1:A:524:VAL:HG13	2.17	0.45
1:A:138:GLN:HG2	8:A:1098:HOH:O	2.18	0.44
1:A:225:LEU:HD11	2:A:602:HEC:HMC1	1.99	0.44
2:A:603:HEC:HMA3	2:A:604:HEC:HBA2	1.99	0.44
1:A:486:ASN:HB3	2:A:604:HEC:HAA1	2.00	0.44
1:B:487:SER:HB3	1:B:491:HIS:CE1	2.52	0.44
1:B:361:HIS:NE2	3:B:609:NO2:O2	2.39	0.44
1:A:46:GLU:HG3	8:A:1232:HOH:O	2.18	0.43
1:A:486:ASN:HB3	2:A:604:HEC:CAA	2.49	0.42
1:A:430:ILE:HG21	1:A:490:PHE:HA	2.02	0.42
1:B:119:HIS:CD2	2:B:603:HEC:ND	2.88	0.42
1:A:78[A]:VAL:HG12	1:A:152:VAL:HG21	2.02	0.41
1:A:119:HIS:CD2	2:A:603:HEC:ND	2.89	0.41
1:B:337:GLU:HG2	8:B:1252:HOH:O	2.21	0.41
1:A:482:TRP:HE1	1:A:499:SER:CB	2.34	0.41
1:A:142:TRP:CE3	5:A:612:MPD:H11	2.56	0.40
1:B:167:SER:HB2	1:B:216[B]:GLU:HG2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:A:1242:HOH:O	8:B:870:HOH:O[7.555]	1.49	0.71

## 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	535/520 (103%)	508 (95%)	26 (5%)	1 (0%)	56	46
1	B	534/520 (103%)	510 (96%)	24 (4%)	0	100	100
All	All	1069/1040 (103%)	1018 (95%)	50 (5%)	1 (0%)	59	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	HIS

### 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	455/439 (104%)	453 (100%)	2 (0%)	95	94
1	B	454/439 (103%)	450 (99%)	4 (1%)	87	86
All	All	909/878 (104%)	903 (99%)	6 (1%)	92	90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	ARG
1	A	406	MET
1	B	68[A]	THR
1	B	68[B]	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	316	ARG
1	B	406	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	B	388	GLN
1	B	413	ASN
1	B	466	ASN

### 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 39 ligands modelled in this entry, 4 are monoatomic and 6 are modelled with single atom - leaving 29 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	601	1,8,3	50,50,50	3.20	21 (42%)	56,82,82	3.44	25 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEC	A	602	1	50,50,50	3.18	21 (42%)	56,82,82	3.65	30 (53%)
2	HEC	A	603	1,4	50,50,50	3.26	26 (52%)	56,82,82	3.89	30 (53%)
2	HEC	A	604	1	50,50,50	3.07	20 (40%)	56,82,82	3.60	25 (44%)
2	HEC	A	605	1	44,45,50	14.28	23 (52%)	44,75,82	3.66	17 (38%)
2	HEC	A	606	1	50,50,50	3.40	24 (48%)	56,82,82	3.70	27 (48%)
2	HEC	A	607	1	50,50,50	3.07	21 (42%)	56,82,82	3.38	27 (48%)
2	HEC	A	608	1	50,50,50	3.44	25 (50%)	56,82,82	3.56	31 (55%)
3	NO2	A	609	2	0,1,2	0.00	-	0,0,1	0.00	-
5	MPD	A	612	-	7,7,7	0.67	0	10,10,10	0.56	0
6	GOL	A	614	-	5,5,5	0.56	0	5,5,5	0.40	0
7	SO4	A	616	-	4,4,4	0.50	0	6,6,6	0.68	0
3	NO2	A	617	-	2,2,2	0.91	0	1,1,1	0.13	0
3	NO2	A	618	-	2,2,2	0.76	0	1,1,1	0.01	0
2	HEC	B	601	1,8,3	50,50,50	3.12	19 (38%)	56,82,82	3.70	27 (48%)
2	HEC	B	602	1	50,50,50	3.13	23 (46%)	56,82,82	3.64	30 (53%)
2	HEC	B	603	1,4	50,50,50	3.14	19 (38%)	56,82,82	3.92	27 (48%)
2	HEC	B	604[A]	-	2,3,50	1.99	1 (50%)	1,3,82	1.37	0
2	HEC	B	604[B]	4	2,3,50	1.46	0	1,3,82	1.36	0
2	HEC	B	605	1	46,46,50	3.85	25 (54%)	49,77,82	3.82	22 (44%)
2	HEC	B	606	1	50,50,50	3.43	24 (48%)	56,82,82	3.56	28 (50%)
2	HEC	B	607	1	50,50,50	3.05	19 (38%)	56,82,82	3.44	27 (48%)
2	HEC	B	608	1	50,50,50	3.47	26 (52%)	56,82,82	3.89	26 (46%)
3	NO2	B	609	2	0,1,2	0.00	-	0,0,1	0.00	-
5	MPD	B	612	-	7,7,7	0.62	0	10,10,10	0.85	0
6	GOL	B	614	-	5,5,5	0.42	0	5,5,5	0.35	0
7	SO4	B	615	-	4,4,4	0.66	0	6,6,6	0.43	0
3	NO2	B	616	-	2,2,2	0.86	0	1,1,1	0.16	0
3	NO2	B	617	-	2,2,2	0.85	0	1,1,1	0.12	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	601	1,8,3	-	0/10/54/54	0/0/8/8
2	HEC	A	602	1	-	0/10/54/54	0/0/8/8
2	HEC	A	603	1,4	-	0/10/54/54	0/0/8/8
2	HEC	A	604	1	-	0/10/54/54	0/0/8/8

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	605	1	-	0/5/49/54	0/0/8/8
2	HEC	A	606	1	-	0/10/54/54	0/0/8/8
2	HEC	A	607	1	-	0/10/54/54	0/0/8/8
2	HEC	A	608	1	-	0/10/54/54	0/0/8/8
3	NO2	A	609	2	-	0/0/0/0	0/0/0/0
5	MPD	A	612	-	-	0/5/5/5	0/0/0/0
6	GOL	A	614	-	-	0/4/4/4	0/0/0/0
7	SO4	A	616	-	-	0/0/0/0	0/0/0/0
3	NO2	A	617	-	-	0/0/0/0	0/0/0/0
3	NO2	A	618	-	-	0/0/0/0	0/0/0/0
2	HEC	B	601	1,8,3	-	0/10/54/54	0/0/8/8
2	HEC	B	602	1	-	0/10/54/54	0/0/8/8
2	HEC	B	603	1,4	-	0/10/54/54	0/0/8/8
2	HEC	B	604[A]	-	-	0/0/0/54	0/0/0/8
2	HEC	B	604[B]	4	-	0/0/0/54	0/0/0/8
2	HEC	B	605	1	-	0/5/49/54	0/0/8/8
2	HEC	B	606	1	-	0/10/54/54	0/0/8/8
2	HEC	B	607	1	-	0/10/54/54	0/0/8/8
2	HEC	B	608	1	-	0/10/54/54	0/0/8/8
3	NO2	B	609	2	-	0/0/0/0	0/0/0/0
5	MPD	B	612	-	-	0/5/5/5	0/0/0/0
6	GOL	B	614	-	-	0/4/4/4	0/0/0/0
7	SO4	B	615	-	-	0/0/0/0	0/0/0/0
3	NO2	B	616	-	-	0/0/0/0	0/0/0/0
3	NO2	B	617	-	-	0/0/0/0	0/0/0/0

All (337) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEC	C3D-C4D	91.95	1.51	1.38
2	B	606	HEC	C3B-CAB	13.52	1.53	1.34
2	B	602	HEC	C3C-CAC	13.01	1.52	1.34
2	A	602	HEC	C3C-CAC	12.76	1.52	1.34
2	A	601	HEC	C3B-CAB	12.64	1.51	1.34
2	A	608	HEC	C3B-CAB	12.56	1.51	1.34
2	A	605	HEC	C3C-CAC	12.45	1.51	1.34
2	A	603	HEC	C3B-CAB	12.43	1.51	1.34
2	A	607	HEC	C3C-CAC	12.31	1.51	1.34
2	A	608	HEC	C3C-CAC	12.31	1.51	1.34
2	A	606	HEC	C3B-CAB	12.26	1.51	1.34
2	B	608	HEC	C3C-CAC	12.22	1.51	1.34
2	B	605	HEC	C3C-CAC	12.21	1.51	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	603	HEC	C3C-CAC	12.14	1.51	1.34
2	A	606	HEC	C3C-CAC	11.94	1.50	1.34
2	B	605	HEC	C3D-C4D	11.60	1.50	1.44
2	B	608	HEC	C3B-CAB	11.53	1.50	1.34
2	A	604	HEC	C3C-CAC	11.48	1.50	1.34
2	A	603	HEC	C3C-CAC	11.44	1.50	1.34
2	B	607	HEC	C3B-CAB	11.41	1.50	1.34
2	B	603	HEC	C3B-CAB	11.34	1.50	1.34
2	B	601	HEC	C3C-CAC	11.28	1.49	1.34
2	A	601	HEC	C3C-CAC	11.17	1.49	1.34
2	B	606	HEC	C3C-CAC	11.06	1.49	1.34
2	B	602	HEC	C3B-CAB	10.78	1.49	1.34
2	B	607	HEC	C3C-CAC	10.70	1.49	1.34
2	A	604	HEC	C3B-CAB	10.65	1.49	1.34
2	A	607	HEC	C3B-CAB	10.45	1.48	1.34
2	B	601	HEC	C3B-CAB	10.43	1.48	1.34
2	A	602	HEC	C3B-CAB	9.90	1.48	1.34
2	B	605	HEC	C3B-CAB	9.69	1.47	1.34
2	A	605	HEC	C3B-CAB	9.48	1.47	1.34
2	B	608	HEC	C3C-C2C	7.26	1.48	1.40
2	B	606	HEC	C3C-C2C	7.24	1.48	1.40
2	B	601	HEC	C3B-C2B	6.96	1.47	1.40
2	B	606	HEC	C3B-C2B	6.79	1.47	1.40
2	A	602	HEC	C3C-C2C	6.68	1.47	1.40
2	B	608	HEC	C3B-C2B	6.57	1.47	1.40
2	A	606	HEC	C3B-C2B	6.49	1.47	1.40
2	A	606	HEC	C3C-C2C	6.33	1.47	1.40
2	B	603	HEC	C3C-C2C	6.30	1.47	1.40
2	A	608	HEC	C3C-C2C	6.29	1.47	1.40
2	B	605	HEC	C3C-C2C	6.26	1.47	1.40
2	A	604	HEC	C3C-C2C	6.00	1.46	1.40
2	A	601	HEC	C3C-C2C	5.91	1.46	1.40
2	B	603	HEC	C3B-C2B	5.90	1.46	1.40
2	B	602	HEC	C3C-C2C	5.88	1.46	1.40
2	A	605	HEC	C3B-C2B	5.85	1.46	1.40
2	B	601	HEC	C3C-C2C	5.76	1.46	1.40
2	B	607	HEC	C3B-C2B	5.73	1.46	1.40
2	A	602	HEC	C3B-C2B	5.44	1.46	1.40
2	A	605	HEC	C3C-C2C	5.42	1.46	1.40
2	A	603	HEC	C3C-C2C	5.28	1.46	1.40
2	A	608	HEC	C3B-C2B	5.25	1.46	1.40
2	A	603	HEC	C3B-C2B	5.23	1.46	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	607	HEC	C3C-C2C	5.21	1.46	1.40
2	B	605	HEC	C1D-C2D	5.20	1.51	1.43
2	A	607	HEC	C3B-C2B	5.11	1.46	1.40
2	B	605	HEC	C3D-C2D	4.97	1.50	1.41
2	B	607	HEC	C3C-C2C	4.87	1.45	1.40
2	B	605	HEC	C3B-C2B	4.73	1.45	1.40
2	B	602	HEC	C3B-C2B	4.70	1.45	1.40
2	A	604	HEC	C3B-C2B	4.61	1.45	1.40
2	A	601	HEC	C3B-C2B	4.60	1.45	1.40
2	A	605	HEC	FE-NA	4.38	2.11	1.92
2	A	605	HEC	FE-ND	4.29	2.10	1.92
2	B	605	HEC	FE-ND	4.26	2.10	1.92
2	A	608	HEC	FE-NC	4.17	2.10	1.92
2	A	608	HEC	FE-NB	4.10	2.10	1.92
2	B	605	HEC	FE-NA	4.08	2.10	1.92
2	A	608	HEC	C1B-C2B	4.05	1.50	1.43
2	B	608	HEC	FE-NC	4.03	2.09	1.92
2	A	605	HEC	C1D-C2D	4.01	1.50	1.44
2	B	606	HEC	FE-ND	4.01	2.09	1.92
2	B	606	HEC	FE-NB	3.91	2.09	1.92
2	B	608	HEC	FE-NB	3.89	2.09	1.92
2	B	607	HEC	C1C-C2C	3.88	1.49	1.43
2	B	608	HEC	C1C-C2C	3.86	1.49	1.43
2	A	606	HEC	FE-ND	3.86	2.09	1.92
2	B	608	HEC	FE-NA	3.82	2.08	1.92
2	A	606	HEC	FE-NA	3.80	2.08	1.92
2	B	605	HEC	C2A-C3A	3.80	1.48	1.37
2	A	605	HEC	C2A-C3A	3.79	1.48	1.37
2	A	608	HEC	FE-NA	3.77	2.08	1.92
2	A	608	HEC	FE-ND	3.75	2.08	1.92
2	A	605	HEC	FE-NC	3.75	2.08	1.92
2	A	601	HEC	C1B-C2B	3.75	1.49	1.43
2	A	602	HEC	FE-NA	3.73	2.08	1.92
2	B	601	HEC	C1B-C2B	3.68	1.49	1.43
2	A	606	HEC	FE-NB	3.67	2.08	1.92
2	A	605	HEC	FE-NB	3.66	2.08	1.92
2	A	607	HEC	C1C-C2C	3.64	1.49	1.43
2	B	605	HEC	FE-NB	3.62	2.08	1.92
2	A	601	HEC	FE-NC	3.61	2.08	1.92
2	A	601	HEC	FE-NB	3.60	2.07	1.92
2	A	605	HEC	C4D-CHA	3.60	1.49	1.39
2	A	603	HEC	FE-NC	3.59	2.07	1.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	606	HEC	FE-NC	3.56	2.07	1.92
2	A	604	HEC	FE-NB	3.56	2.07	1.92
2	B	605	HEC	FE-NC	3.55	2.07	1.92
2	A	604	HEC	FE-ND	3.55	2.07	1.92
2	A	606	HEC	C4D-C3D	3.55	1.49	1.43
2	B	608	HEC	FE-ND	3.54	2.07	1.92
2	B	601	HEC	FE-NC	3.53	2.07	1.92
2	B	608	HEC	C4D-C3D	3.50	1.49	1.43
2	A	602	HEC	C3D-C2D	3.50	1.48	1.37
2	A	604	HEC	C1B-C2B	3.50	1.49	1.43
2	B	608	HEC	C3C-C4C	3.49	1.50	1.42
2	A	605	HEC	C3C-C4C	3.46	1.50	1.42
2	A	605	HEC	C1D-CHD	3.46	1.49	1.39
2	A	607	HEC	FE-NC	3.45	2.07	1.92
2	B	601	HEC	C1D-C2D	3.43	1.49	1.43
2	A	608	HEC	C1C-C2C	3.42	1.49	1.43
2	B	607	HEC	FE-NB	3.42	2.07	1.92
2	A	603	HEC	FE-NA	3.40	2.07	1.92
2	B	602	HEC	FE-NA	3.40	2.07	1.92
2	A	607	HEC	FE-NB	3.39	2.07	1.92
2	B	605	HEC	C4D-CHA	3.38	1.49	1.39
2	A	608	HEC	C2A-C3A	3.38	1.47	1.37
2	A	603	HEC	C4D-C3D	3.37	1.49	1.43
2	B	606	HEC	FE-NA	3.36	2.06	1.92
2	B	603	HEC	FE-NA	3.35	2.06	1.92
2	A	608	HEC	C3D-C2D	3.35	1.47	1.37
2	B	606	HEC	C3D-C2D	3.34	1.47	1.37
2	A	603	HEC	C3D-C2D	3.34	1.47	1.37
2	A	606	HEC	C3D-C2D	3.33	1.47	1.37
2	B	601	HEC	FE-NB	3.32	2.06	1.92
2	B	605	HEC	C1D-CHD	3.32	1.49	1.39
2	B	605	HEC	C3C-C4C	3.32	1.50	1.42
2	B	607	HEC	FE-NC	3.32	2.06	1.92
2	A	601	HEC	FE-NA	3.31	2.06	1.92
2	A	603	HEC	FE-NB	3.31	2.06	1.92
2	B	603	HEC	FE-NC	3.30	2.06	1.92
2	A	606	HEC	C2A-C3A	3.29	1.47	1.37
2	A	602	HEC	FE-NC	3.26	2.06	1.92
2	B	608	HEC	C3D-C2D	3.26	1.47	1.37
2	A	605	HEC	C1A-C2A	3.25	1.50	1.42
2	B	601	HEC	FE-NA	3.24	2.06	1.92
2	B	601	HEC	C2A-C3A	3.23	1.47	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	HEC	FE-NC	3.21	2.06	1.92
2	A	604	HEC	C2A-C3A	3.20	1.47	1.37
2	B	601	HEC	C3D-C2D	3.18	1.47	1.37
2	B	606	HEC	FE-NC	3.17	2.06	1.92
2	A	602	HEC	FE-NB	3.17	2.06	1.92
2	B	603	HEC	C3D-C2D	3.17	1.47	1.37
2	B	608	HEC	C1D-C2D	3.15	1.48	1.43
2	A	606	HEC	C1B-C2B	3.13	1.48	1.43
2	A	604	HEC	C4B-NB	-3.11	1.32	1.36
2	A	607	HEC	FE-NA	3.09	2.05	1.92
2	B	607	HEC	FE-NA	3.07	2.05	1.92
2	A	602	HEC	C2A-C3A	3.07	1.46	1.37
2	B	607	HEC	C1D-C2D	3.07	1.48	1.43
2	B	605	HEC	C4A-C3A	3.06	1.50	1.42
2	A	603	HEC	C1B-C2B	3.05	1.48	1.43
2	A	601	HEC	FE-ND	3.03	2.05	1.92
2	A	606	HEC	C3B-C4B	3.02	1.49	1.42
2	A	601	HEC	C2A-C3A	3.02	1.46	1.37
2	A	604	HEC	C1D-C2D	3.01	1.48	1.43
2	B	603	HEC	C2A-C3A	3.01	1.46	1.37
2	A	603	HEC	C4D-CHA	2.99	1.48	1.39
2	B	608	HEC	C2A-C3A	3.00	1.46	1.37
2	A	608	HEC	C3B-C4B	2.95	1.49	1.42
2	A	607	HEC	C1D-C2D	2.95	1.48	1.43
2	A	607	HEC	FE-ND	2.94	2.05	1.92
2	B	606	HEC	C4A-C3A	2.93	1.50	1.42
2	A	602	HEC	C1D-CHD	2.93	1.47	1.39
2	B	608	HEC	C1B-C2B	2.93	1.48	1.43
2	B	605	HEC	C1A-C2A	2.92	1.49	1.42
2	A	603	HEC	FE-ND	2.92	2.04	1.92
2	B	607	HEC	C1B-C2B	2.91	1.48	1.43
2	B	601	HEC	FE-ND	2.90	2.04	1.92
2	B	603	HEC	C4D-CHA	2.90	1.47	1.39
2	A	606	HEC	C1C-C2C	2.90	1.48	1.43
2	A	608	HEC	C3C-C4C	2.88	1.49	1.42
2	A	602	HEC	FE-ND	2.88	2.04	1.92
2	B	607	HEC	C3B-C4B	2.86	1.49	1.42
2	A	601	HEC	C3D-C2D	2.85	1.46	1.37
2	A	607	HEC	C2A-C3A	2.83	1.46	1.37
2	A	605	HEC	C1A-CHA	2.83	1.50	1.37
2	B	606	HEC	C1A-C2A	2.83	1.49	1.42
2	B	607	HEC	C1B-CHB	2.83	1.47	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	607	HEC	C1C-CHC	2.83	1.47	1.39
2	A	608	HEC	C1D-C2D	2.82	1.48	1.43
2	A	602	HEC	C1C-C2C	2.80	1.48	1.43
2	A	606	HEC	C3C-C4C	2.80	1.49	1.42
2	A	606	HEC	C4A-C3A	2.79	1.49	1.42
2	B	607	HEC	FE-ND	2.79	2.04	1.92
2	A	604	HEC	FE-NC	2.79	2.04	1.92
2	A	601	HEC	C1B-CHB	2.78	1.47	1.39
2	B	607	HEC	C2A-C3A	2.78	1.45	1.37
2	A	602	HEC	O2D-CGD	-2.75	1.20	1.30
2	B	606	HEC	C1B-CHB	2.74	1.47	1.39
2	A	608	HEC	C4D-CHA	2.73	1.47	1.39
2	A	601	HEC	C1A-C2A	2.73	1.49	1.42
2	B	603	HEC	FE-NB	2.73	2.04	1.92
2	B	602	HEC	C2A-C3A	2.73	1.45	1.37
2	A	605	HEC	C4A-C3A	2.71	1.49	1.42
2	B	608	HEC	C4D-CHA	2.71	1.47	1.39
2	B	606	HEC	C3B-C4B	2.71	1.49	1.42
2	B	607	HEC	C3D-C2D	2.71	1.45	1.37
2	B	606	HEC	C4D-C3D	2.71	1.48	1.43
2	B	608	HEC	C1C-CHC	2.69	1.47	1.39
2	B	605	HEC	C4B-NB	-2.68	1.33	1.36
2	A	605	HEC	C1B-CHB	2.68	1.47	1.39
2	A	602	HEC	C4D-CHA	2.66	1.47	1.39
2	B	606	HEC	C2A-C3A	2.66	1.45	1.37
2	B	602	HEC	C1B-C2B	2.65	1.47	1.43
2	B	602	HEC	FE-NB	2.65	2.03	1.92
2	A	603	HEC	C4C-NC	-2.65	1.33	1.36
2	A	603	HEC	C1B-CHB	2.64	1.47	1.39
2	B	602	HEC	O2D-CGD	-2.64	1.21	1.30
2	B	601	HEC	C4D-C3D	2.63	1.47	1.43
2	B	608	HEC	C3B-C4B	2.63	1.48	1.42
2	A	608	HEC	C1A-C2A	2.62	1.49	1.42
2	B	606	HEC	C1D-C2D	2.62	1.47	1.43
2	B	605	HEC	C1A-CHA	2.61	1.49	1.37
2	A	607	HEC	C1B-CHB	2.61	1.47	1.39
2	A	605	HEC	C1C-C2C	2.61	1.47	1.43
2	A	604	HEC	C3D-C2D	2.61	1.45	1.37
2	A	606	HEC	C4C-NC	-2.60	1.33	1.36
2	A	604	HEC	C1C-C2C	2.60	1.47	1.43
2	B	602	HEC	C3D-C2D	2.60	1.45	1.37
2	B	605	HEC	C1B-CHB	2.59	1.47	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	604	HEC	C4D-C3D	2.59	1.47	1.43
2	A	602	HEC	C4A-C3A	2.58	1.49	1.42
2	A	602	HEC	C1A-C2A	2.58	1.49	1.42
2	A	603	HEC	C1C-CHC	2.57	1.46	1.39
2	A	603	HEC	C3B-C4B	2.57	1.48	1.42
2	B	606	HEC	C3C-C4C	2.53	1.48	1.42
2	A	608	HEC	C1C-CHC	2.52	1.46	1.39
2	B	608	HEC	C4A-C3A	2.52	1.48	1.42
2	A	601	HEC	C4A-C3A	2.51	1.48	1.42
2	A	606	HEC	C1D-CHD	2.51	1.46	1.39
2	B	605	HEC	CAD-C3D	2.50	1.52	1.40
2	A	604	HEC	C4C-NC	-2.50	1.33	1.36
2	B	603	HEC	FE-ND	2.49	2.03	1.92
2	A	604	HEC	FE-NA	2.49	2.03	1.92
2	A	606	HEC	C1C-CHC	2.49	1.46	1.39
2	B	605	HEC	C4C-CHD	2.48	1.48	1.37
2	A	602	HEC	C1B-C2B	2.48	1.47	1.43
2	A	603	HEC	C1C-C2C	2.47	1.47	1.43
2	B	605	HEC	C1C-C2C	2.46	1.47	1.43
2	B	608	HEC	C1D-CHD	2.46	1.46	1.39
2	A	603	HEC	C2A-C3A	2.45	1.44	1.37
2	A	602	HEC	C4D-C3D	2.45	1.47	1.43
2	B	606	HEC	C1C-CHC	2.45	1.46	1.39
2	A	603	HEC	C1D-CHD	2.45	1.46	1.39
2	B	602	HEC	C1A-C2A	2.45	1.48	1.42
2	B	608	HEC	C1A-NA	-2.44	1.33	1.36
2	A	601	HEC	C1C-CHC	2.44	1.46	1.39
2	A	607	HEC	C1C-CHC	2.42	1.46	1.39
2	B	602	HEC	C1B-CHB	2.41	1.46	1.39
2	B	603	HEC	C1A-C2A	2.41	1.48	1.42
2	B	602	HEC	C1C-C2C	2.40	1.47	1.43
2	A	601	HEC	C4D-C3D	2.40	1.47	1.43
2	A	607	HEC	C4A-C3A	2.39	1.48	1.42
2	A	607	HEC	C3D-C2D	2.38	1.44	1.37
2	B	606	HEC	C1B-C2B	2.38	1.47	1.43
2	A	606	HEC	C1A-CHA	2.38	1.48	1.37
2	A	608	HEC	C4A-CHB	2.37	1.48	1.37
2	A	603	HEC	C3C-C4C	2.35	1.48	1.42
2	B	608	HEC	C1A-C2A	2.35	1.48	1.42
2	A	607	HEC	C1D-CHD	2.35	1.46	1.39
2	A	603	HEC	C4B-CHC	2.34	1.48	1.37
2	A	606	HEC	C4D-CHA	2.33	1.46	1.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	HEC	C1C-CHC	2.33	1.46	1.39
2	A	603	HEC	C1A-C2A	2.33	1.48	1.42
2	A	602	HEC	C1C-CHC	2.33	1.46	1.39
2	A	608	HEC	C1B-CHB	2.32	1.46	1.39
2	B	606	HEC	C4A-CHB	2.32	1.48	1.37
2	A	608	HEC	C4A-C3A	2.31	1.48	1.42
2	B	601	HEC	C1C-C2C	2.29	1.47	1.43
2	A	603	HEC	C1A-NA	-2.29	1.33	1.36
2	A	601	HEC	C3B-C4B	2.29	1.48	1.42
2	B	603	HEC	C1C-CHC	2.29	1.46	1.39
2	B	602	HEC	C1A-CHA	2.28	1.47	1.37
2	A	608	HEC	C4B-CHC	2.28	1.47	1.37
2	B	605	HEC	C3B-C4B	2.27	1.48	1.42
2	B	602	HEC	C4D-CHA	2.27	1.46	1.39
2	B	607	HEC	C4D-CHA	2.27	1.46	1.39
2	A	607	HEC	C1A-CHA	2.27	1.47	1.37
2	A	608	HEC	C1D-CHD	2.27	1.46	1.39
2	B	603	HEC	C1C-C2C	2.26	1.47	1.43
2	B	606	HEC	C1C-C2C	2.26	1.47	1.43
2	B	603	HEC	C1B-CHB	2.26	1.46	1.39
2	B	603	HEC	CBA-CGA	2.25	1.56	1.50
2	A	605	HEC	C4B-CHC	2.24	1.47	1.37
2	B	606	HEC	C1A-CHA	2.23	1.47	1.37
2	B	608	HEC	C1A-CHA	2.22	1.47	1.37
2	A	606	HEC	C4B-CHC	2.21	1.47	1.37
2	A	608	HEC	C1A-CHA	2.21	1.47	1.37
2	B	601	HEC	C1B-CHB	2.21	1.45	1.39
2	B	606	HEC	C4D-CHA	2.21	1.45	1.39
2	A	605	HEC	C4C-CHD	2.20	1.47	1.37
2	B	604[A]	HEC	O1A-CGA	2.19	1.26	1.22
2	A	602	HEC	C3C-C4C	2.19	1.47	1.42
2	B	608	HEC	C4C-NC	-2.18	1.34	1.36
2	A	607	HEC	C1B-C2B	2.15	1.47	1.43
2	A	603	HEC	C1D-C2D	2.15	1.47	1.43
2	B	608	HEC	C1B-CHB	2.14	1.45	1.39
2	B	602	HEC	C4B-NB	-2.14	1.34	1.36
2	B	601	HEC	C3B-C4B	2.14	1.47	1.42
2	A	607	HEC	C1A-C2A	2.14	1.48	1.42
2	B	607	HEC	C1A-CHA	2.13	1.47	1.37
2	A	601	HEC	C4C-CHD	2.13	1.47	1.37
2	A	607	HEC	C4A-NA	-2.12	1.34	1.36
2	B	601	HEC	C3C-C4C	2.12	1.47	1.42

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEC	C1C-CHC	2.12	1.45	1.39
2	B	602	HEC	C4A-NA	-2.12	1.34	1.36
2	B	603	HEC	C4D-C3D	2.08	1.47	1.43
2	B	601	HEC	C4C-NC	-2.08	1.34	1.36
2	A	603	HEC	C4A-CHB	2.08	1.47	1.37
2	A	604	HEC	C1A-CHA	2.08	1.47	1.37
2	A	607	HEC	C3C-C4C	2.08	1.47	1.42
2	A	604	HEC	C3C-C4C	2.07	1.47	1.42
2	B	608	HEC	C4B-CHC	2.07	1.46	1.37
2	B	601	HEC	C4C-CHD	2.07	1.46	1.37
2	A	604	HEC	C1B-CHB	2.06	1.45	1.39
2	A	601	HEC	C4D-CHA	2.06	1.45	1.39
2	B	607	HEC	C4C-CHD	2.06	1.46	1.37
2	B	605	HEC	C4B-CHC	2.06	1.46	1.37
2	A	608	HEC	C4D-C3D	2.05	1.47	1.43
2	A	601	HEC	C1C-C2C	2.05	1.47	1.43
2	B	606	HEC	C4C-CHD	2.05	1.46	1.37
2	B	602	HEC	C1A-NA	-2.05	1.34	1.36
2	B	602	HEC	FE-ND	2.04	2.01	1.92
2	A	604	HEC	C4A-CHB	2.04	1.46	1.37
2	A	605	HEC	C1B-C2B	2.04	1.47	1.43
2	A	603	HEC	C4B-NB	-2.03	1.34	1.36
2	B	602	HEC	C1D-C2D	2.03	1.47	1.43
2	A	606	HEC	C4A-NA	-2.02	1.34	1.36
2	B	603	HEC	C3C-C4C	2.02	1.47	1.42
2	A	606	HEC	C1D-C2D	2.02	1.47	1.43
2	A	602	HEC	C1A-CHA	2.01	1.46	1.37
2	B	603	HEC	C4B-CHC	2.01	1.46	1.37
2	A	601	HEC	C4B-NB	-2.01	1.34	1.36
2	B	602	HEC	C4C-NC	-2.00	1.34	1.36

All (399) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	605	HEC	C2C-C1C-NC	11.52	117.19	109.50
2	A	606	HEC	C2D-C1D-ND	11.30	117.05	109.50
2	A	605	HEC	C2C-C1C-NC	11.05	116.88	109.50
2	B	606	HEC	C2D-C1D-ND	10.98	116.83	109.50
2	A	603	HEC	C2B-C1B-NB	10.94	116.81	109.50
2	B	601	HEC	C2C-C1C-NC	10.86	116.75	109.50
2	B	607	HEC	C2C-C1C-NC	10.78	116.70	109.50
2	A	603	HEC	C2C-C1C-NC	10.71	116.65	109.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	603	HEC	C2B-C1B-NB	10.63	116.60	109.50
2	B	608	HEC	C2B-C1B-NB	10.51	116.52	109.50
2	A	602	HEC	C2B-C1B-NB	10.30	116.38	109.50
2	B	603	HEC	C2D-C1D-ND	10.21	116.32	109.50
2	B	608	HEC	C2C-C1C-NC	10.17	116.29	109.50
2	A	603	HEC	C2D-C1D-ND	10.16	116.29	109.50
2	B	602	HEC	CBB-CAB-C3B	-10.13	105.22	127.36
2	A	608	HEC	C2B-C1B-NB	9.99	116.17	109.50
2	A	606	HEC	C2B-C1B-NB	9.98	116.17	109.50
2	A	608	HEC	C2C-C1C-NC	9.90	116.11	109.50
2	A	604	HEC	C2C-C1C-NC	9.85	116.08	109.50
2	B	601	HEC	C2B-C1B-NB	9.64	115.94	109.50
2	A	601	HEC	C2B-C1B-NB	9.61	115.92	109.50
2	B	607	HEC	C2B-C1B-NB	9.61	115.92	109.50
2	A	607	HEC	C2C-C1C-NC	9.59	115.91	109.50
2	B	608	HEC	C2D-C1D-ND	9.59	115.91	109.50
2	B	601	HEC	C2D-C1D-ND	9.30	115.71	109.50
2	A	601	HEC	C2D-C1D-ND	9.28	115.70	109.50
2	B	602	HEC	C2B-C1B-NB	9.23	115.66	109.50
2	A	604	HEC	C2B-C1B-NB	9.13	115.60	109.50
2	B	605	HEC	C2B-C1B-NB	9.10	115.58	109.50
2	A	602	HEC	C2D-C1D-ND	9.00	115.51	109.50
2	B	602	HEC	C2D-C1D-ND	8.99	115.51	109.50
2	A	602	HEC	C2C-C1C-NC	8.98	115.50	109.50
2	A	601	HEC	C2C-C1C-NC	8.81	115.38	109.50
2	B	606	HEC	C2C-C1C-NC	8.80	115.38	109.50
2	B	606	HEC	C2B-C1B-NB	8.73	115.33	109.50
2	A	606	HEC	C2C-C1C-NC	8.67	115.29	109.50
2	B	603	HEC	C2C-C1C-NC	8.65	115.28	109.50
2	B	603	HEC	CBB-CAB-C3B	-8.45	108.88	127.36
2	B	601	HEC	CBB-CAB-C3B	-8.27	109.28	127.36
2	A	607	HEC	C2B-C1B-NB	8.26	115.01	109.50
2	A	604	HEC	C2D-C1D-ND	8.20	114.98	109.50
2	A	605	HEC	C2B-C1B-NB	8.09	114.90	109.50
2	A	604	HEC	CBB-CAB-C3B	-8.03	109.80	127.36
2	A	608	HEC	C2D-C1D-ND	7.97	114.82	109.50
2	B	602	HEC	C2C-C1C-NC	7.90	114.78	109.50
2	A	602	HEC	CBB-CAB-C3B	-7.83	110.24	127.36
2	B	605	HEC	CMB-C2B-C3B	7.83	133.52	126.22
2	A	607	HEC	CBB-CAB-C3B	-7.78	110.35	127.36
2	A	608	HEC	CMC-C2C-C3C	7.76	133.47	126.22
2	A	604	HEC	CBA-CAA-C2A	-7.72	99.78	112.63

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	608	HEC	CBB-CAB-C3B	-7.63	110.67	127.36
2	B	601	HEC	C1D-C2D-C3D	-7.55	101.74	107.00
2	A	607	HEC	C2D-C1D-ND	7.42	114.45	109.50
2	A	603	HEC	CBB-CAB-C3B	-7.40	111.18	127.36
2	B	605	HEC	CBA-CAA-C2A	-7.34	100.41	112.63
2	A	602	HEC	C1D-C2D-C3D	-7.24	101.96	107.00
2	A	601	HEC	CBB-CAB-C3B	-7.24	111.54	127.36
2	B	608	HEC	CMC-C2C-C3C	7.21	132.95	126.22
2	B	602	HEC	C1D-C2D-C3D	-7.13	102.03	107.00
2	A	605	HEC	CMB-C2B-C3B	7.07	132.82	126.22
2	B	607	HEC	CBB-CAB-C3B	-7.04	111.97	127.36
2	B	603	HEC	C1D-C2D-C3D	-7.00	102.12	107.00
2	B	603	HEC	CBC-CAC-C3C	-6.88	112.32	127.36
2	B	603	HEC	CMB-C2B-C3B	6.71	132.48	126.22
2	B	606	HEC	C1D-C2D-C3D	-6.65	102.37	107.00
2	A	606	HEC	C1D-C2D-C3D	-6.60	102.40	107.00
2	B	607	HEC	C2D-C1D-ND	6.54	113.87	109.50
2	A	605	HEC	CBA-CAA-C2A	-6.53	101.76	112.63
2	B	607	HEC	C3C-C2C-C1C	-6.51	100.25	107.11
2	B	603	HEC	CMC-C2C-C3C	6.49	132.28	126.22
2	A	608	HEC	C1D-C2D-C3D	-6.47	102.49	107.00
2	A	608	HEC	CBC-CAC-C3C	-6.46	113.25	127.36
2	B	605	HEC	C3C-C2C-C1C	-6.45	100.32	107.11
2	B	608	HEC	C1D-C2D-C3D	-6.32	102.60	107.00
2	A	603	HEC	CMC-C2C-C3C	6.24	132.04	126.22
2	A	606	HEC	CBC-CAC-C3C	-6.09	114.04	127.36
2	A	606	HEC	CMC-C2C-C3C	6.06	131.88	126.22
2	A	606	HEC	CBB-CAB-C3B	-6.03	114.17	127.36
2	A	607	HEC	CBA-CAA-C2A	-6.02	102.61	112.63
2	A	603	HEC	C3B-C2B-C1B	-6.01	100.78	107.11
2	B	606	HEC	CBB-CAB-C3B	-5.92	114.42	127.36
2	B	605	HEC	C3B-C2B-C1B	-5.92	100.88	107.11
2	A	603	HEC	CBC-CAC-C3C	-5.91	114.44	127.36
2	B	601	HEC	C3B-C2B-C1B	-5.89	100.90	107.11
2	B	601	HEC	C3C-C2C-C1C	-5.88	100.92	107.11
2	A	604	HEC	C1D-C2D-C3D	-5.86	102.92	107.00
2	A	603	HEC	C1D-C2D-C3D	-5.85	102.92	107.00
2	B	608	HEC	C3C-C2C-C1C	-5.84	100.96	107.11
2	A	601	HEC	C1D-C2D-C3D	-5.84	102.94	107.00
2	B	608	HEC	CBD-CAD-C3D	-5.83	102.92	112.63
2	A	602	HEC	C3B-C2B-C1B	-5.77	101.03	107.11
2	B	601	HEC	CMB-C2B-C3B	5.75	131.59	126.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEC	C4A-C3A-C2A	-5.73	100.33	106.69
2	B	602	HEC	C3B-C2B-C1B	-5.72	101.08	107.11
2	B	603	HEC	C3B-C2B-C1B	-5.66	101.15	107.11
2	A	608	HEC	CBB-CAB-C3B	-5.66	114.98	127.36
2	A	604	HEC	C3C-C2C-C1C	-5.65	101.16	107.11
2	A	604	HEC	C3B-C2B-C1B	-5.63	101.18	107.11
2	A	601	HEC	C3B-C2B-C1B	-5.62	101.19	107.11
2	A	605	HEC	C2D-C1D-ND	5.62	113.59	109.00
2	A	605	HEC	C3B-C2B-C1B	-5.60	101.21	107.11
2	A	605	HEC	CBB-CAB-C3B	-5.53	115.27	127.36
2	B	608	HEC	CBA-CAA-C2A	-5.52	103.44	112.63
2	A	604	HEC	CBD-CAD-C3D	-5.52	103.44	112.63
2	A	605	HEC	C3C-C2C-C1C	-5.50	101.32	107.11
2	B	605	HEC	CBC-CAC-C3C	-5.47	115.41	127.36
2	B	605	HEC	CMC-C2C-C3C	5.46	131.32	126.22
2	A	603	HEC	C3C-C2C-C1C	-5.45	101.37	107.11
2	A	605	HEC	C3A-C4A-NA	5.45	116.92	109.32
2	B	608	HEC	CBC-CAC-C3C	-5.42	115.51	127.36
2	B	605	HEC	C2D-C1D-ND	5.41	113.11	109.50
2	B	607	HEC	CBA-CAA-C2A	-5.36	103.70	112.63
2	A	603	HEC	CBA-CAA-C2A	-5.36	103.71	112.63
2	B	602	HEC	CMC-C2C-C3C	5.36	131.22	126.22
2	B	606	HEC	CMC-C2C-C3C	5.35	131.21	126.22
2	A	607	HEC	C1D-C2D-C3D	-5.32	103.30	107.00
2	B	605	HEC	C3A-C4A-NA	5.32	116.74	109.32
2	A	608	HEC	C3C-C2C-C1C	-5.31	101.52	107.11
2	B	603	HEC	C3A-C4A-NA	5.26	116.66	109.32
2	B	608	HEC	C3B-C2B-C1B	-5.25	101.58	107.11
2	B	605	HEC	C4A-C3A-C2A	-5.22	100.90	106.69
2	B	608	HEC	CMB-C2B-C3B	5.17	131.04	126.22
2	A	604	HEC	CMB-C2B-C3B	5.14	131.02	126.22
2	B	603	HEC	CBA-CAA-C2A	-5.13	104.09	112.63
2	A	606	HEC	C3C-C2C-C1C	-5.10	101.73	107.11
2	B	607	HEC	CMC-C2C-C3C	5.10	130.98	126.22
2	A	606	HEC	C4D-ND-C1D	-5.10	102.21	107.12
2	A	603	HEC	CMB-C2B-C3B	5.06	130.94	126.22
2	A	605	HEC	CMC-C2C-C3C	5.06	130.94	126.22
2	A	602	HEC	C1A-C2A-C3A	-5.05	102.63	106.70
2	A	602	HEC	C3A-C4A-NA	5.04	116.35	109.32
2	B	606	HEC	C4D-ND-C1D	-5.02	102.28	107.12
2	A	606	HEC	CMB-C2B-C3B	5.01	130.89	126.22
2	A	602	HEC	CBC-CAC-C3C	-4.97	116.49	127.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	606	HEC	C1A-C2A-C3A	-4.97	102.70	106.70
2	B	603	HEC	CBD-CAD-C3D	-4.93	104.42	112.63
2	B	602	HEC	C3A-C4A-NA	4.93	116.19	109.32
2	B	602	HEC	CMB-C2B-C3B	4.92	130.81	126.22
2	B	605	HEC	CBB-CAB-C3B	-4.92	116.61	127.36
2	B	605	HEC	C4D-C3D-C2D	-4.88	102.03	107.04
2	B	602	HEC	C1A-C2A-C3A	-4.81	102.82	106.70
2	B	603	HEC	C4A-C3A-C2A	-4.81	101.36	106.69
2	B	606	HEC	CBC-CAC-C3C	-4.79	116.90	127.36
2	B	606	HEC	C3D-C4D-ND	4.78	116.37	109.73
2	A	607	HEC	C3B-C2B-C1B	-4.77	102.08	107.11
2	B	601	HEC	CMC-C2C-C3C	4.75	130.65	126.22
2	A	608	HEC	C3B-C2B-C1B	-4.73	102.13	107.11
2	A	607	HEC	C1A-C2A-C3A	-4.71	102.90	106.70
2	A	601	HEC	C3A-C4A-NA	4.67	115.84	109.32
2	B	607	HEC	C1A-C2A-C3A	-4.66	102.95	106.70
2	A	601	HEC	C3C-C2C-C1C	-4.65	102.22	107.11
2	B	607	HEC	C1D-C2D-C3D	-4.65	103.76	107.00
2	B	606	HEC	C4D-C3D-C2D	-4.63	102.12	106.92
2	A	607	HEC	C3C-C2C-C1C	-4.63	102.24	107.11
2	B	607	HEC	C3B-C2B-C1B	-4.61	102.26	107.11
2	A	602	HEC	CMB-C2B-C3B	4.60	130.51	126.22
2	A	602	HEC	CMC-C2C-C3C	4.59	130.50	126.22
2	A	606	HEC	C3B-C2B-C1B	-4.56	102.31	107.11
2	A	603	HEC	C4D-C3D-C2D	-4.50	102.26	106.92
2	A	602	HEC	C3C-C2C-C1C	-4.50	102.37	107.11
2	B	606	HEC	C3B-C2B-C1B	-4.49	102.38	107.11
2	B	602	HEC	CBC-CAC-C3C	-4.48	117.56	127.36
2	A	605	HEC	CBC-CAC-C3C	-4.47	117.59	127.36
2	B	601	HEC	C1A-C2A-C3A	-4.47	103.10	106.70
2	A	601	HEC	CMC-C2C-C3C	4.43	130.35	126.22
2	A	606	HEC	CBA-CAA-C2A	-4.43	105.26	112.63
2	A	604	HEC	C4A-C3A-C2A	-4.43	101.78	106.69
2	B	606	HEC	CMB-C2B-C3B	4.42	130.35	126.22
2	B	608	HEC	C3A-C4A-NA	4.41	115.47	109.32
2	A	606	HEC	C3D-C4D-ND	4.40	115.85	109.73
2	A	601	HEC	C4D-C3D-C2D	-4.39	102.38	106.92
2	A	602	HEC	C2A-C1A-NA	4.38	115.82	109.73
2	A	607	HEC	CBC-CAC-C3C	-4.36	117.82	127.36
2	A	607	HEC	C3A-C4A-NA	4.36	115.40	109.32
2	A	604	HEC	C3A-C4A-NA	4.32	115.35	109.32
2	A	601	HEC	CBC-CAC-C3C	-4.31	117.95	127.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	606	HEC	C3C-C2C-C1C	-4.29	102.59	107.11
2	A	606	HEC	C4D-C3D-C2D	-4.29	102.48	106.92
2	A	608	HEC	CMB-C2B-C3B	4.28	130.22	126.22
2	A	604	HEC	C3D-C4D-ND	4.28	115.68	109.73
2	B	608	HEC	C1A-C2A-C3A	-4.28	103.25	106.70
2	A	606	HEC	C1A-C2A-C3A	-4.27	103.26	106.70
2	B	607	HEC	C3A-C4A-NA	4.27	115.27	109.32
2	B	603	HEC	C3C-C2C-C1C	-4.25	102.64	107.11
2	B	601	HEC	C3A-C4A-NA	4.25	115.24	109.32
2	A	603	HEC	CBD-CAD-C3D	-4.24	105.57	112.63
2	B	608	HEC	C4A-C3A-C2A	-4.23	102.00	106.69
2	B	603	HEC	C4D-ND-C1D	-4.19	103.08	107.12
2	A	603	HEC	C3A-C4A-NA	4.18	115.15	109.32
2	A	601	HEC	C4A-C3A-C2A	-4.15	102.09	106.69
2	A	602	HEC	C4A-C3A-C2A	-4.15	102.09	106.69
2	A	601	HEC	C3D-C4D-ND	4.14	115.49	109.73
2	A	603	HEC	C1A-C2A-C3A	-4.13	103.37	106.70
2	B	601	HEC	C3D-C4D-ND	4.13	115.47	109.73
2	B	608	HEC	C4D-C3D-C2D	-4.08	102.70	106.92
2	A	608	HEC	C4A-C3A-C2A	-4.06	102.19	106.69
2	B	605	HEC	C2B-C1B-CHB	-4.03	118.37	126.00
2	B	605	HEC	C2C-C1C-CHC	-4.01	118.39	126.00
2	A	604	HEC	C4D-C3D-C2D	-4.00	102.78	106.92
2	A	608	HEC	CBD-CAD-C3D	-3.96	106.03	112.63
2	B	607	HEC	CMB-C2B-C3B	3.94	129.89	126.22
2	A	603	HEC	C4D-ND-C1D	-3.93	103.34	107.12
2	B	608	HEC	C3D-C4D-ND	3.92	115.18	109.73
2	B	602	HEC	C4A-C3A-C2A	-3.91	102.35	106.69
2	B	607	HEC	C2A-C1A-NA	3.90	115.15	109.73
2	B	602	HEC	C3C-C2C-C1C	-3.90	103.00	107.11
2	B	607	HEC	C3D-C4D-ND	3.89	115.14	109.73
2	B	602	HEC	C4D-ND-C1D	-3.88	103.38	107.12
2	A	608	HEC	C3D-C4D-ND	3.88	115.12	109.73
2	B	602	HEC	C2A-C1A-NA	3.88	115.12	109.73
2	B	608	HEC	C2A-C1A-NA	3.87	115.11	109.73
2	A	607	HEC	C2A-C1A-NA	3.87	115.11	109.73
2	A	608	HEC	C4D-C3D-C2D	-3.86	102.92	106.92
2	A	607	HEC	CBD-CAD-C3D	-3.86	106.20	112.63
2	A	603	HEC	C3D-C4D-ND	3.85	115.08	109.73
2	A	605	HEC	C2B-C1B-CHB	-3.84	118.71	126.00
2	B	607	HEC	C4D-C3D-C2D	-3.84	102.94	106.92
2	A	601	HEC	C4D-ND-C1D	-3.84	103.42	107.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	607	HEC	CMC-C2C-C3C	3.82	129.79	126.22
2	B	606	HEC	C2A-C1A-NA	3.80	115.01	109.73
2	B	602	HEC	C3D-C4D-ND	3.78	114.99	109.73
2	A	608	HEC	C3A-C4A-NA	3.77	114.58	109.32
2	A	602	HEC	CAD-CBD-CGD	-3.77	101.39	113.66
2	B	602	HEC	CMA-C3A-C2A	3.77	132.04	124.94
2	B	608	HEC	C4D-ND-C1D	-3.74	103.52	107.12
2	B	606	HEC	CBA-CAA-C2A	-3.74	106.41	112.63
2	B	603	HEC	C3D-C4D-ND	3.72	114.90	109.73
2	A	607	HEC	C3D-C4D-ND	3.70	114.87	109.73
2	B	602	HEC	C4C-C3C-C2C	-3.69	102.36	106.35
2	B	601	HEC	C4D-ND-C1D	-3.69	103.56	107.12
2	B	606	HEC	CAA-CBA-CGA	-3.69	101.66	113.66
2	A	601	HEC	C1A-C2A-C3A	-3.67	103.74	106.70
2	B	603	HEC	C2D-C1D-CHD	-3.65	119.09	126.00
2	A	604	HEC	C4D-ND-C1D	-3.62	103.64	107.12
2	A	604	HEC	CBC-CAC-C3C	-3.60	119.50	127.36
2	B	606	HEC	C3A-C4A-NA	3.56	114.28	109.32
2	A	607	HEC	CMB-C2B-C3B	3.55	129.53	126.22
2	B	605	HEC	C3D-C4D-ND	3.54	114.66	109.73
2	B	601	HEC	CBC-CAC-C3C	-3.53	119.63	127.36
2	B	605	HEC	C2A-C1A-NA	3.50	114.60	109.73
2	A	604	HEC	CMC-C2C-C3C	3.49	129.47	126.22
2	A	606	HEC	C4A-C3A-C2A	-3.47	102.84	106.69
2	B	601	HEC	C2A-C1A-NA	3.45	114.53	109.73
2	A	601	HEC	C2A-C1A-NA	3.45	114.53	109.73
2	A	607	HEC	C4D-ND-C1D	-3.44	103.80	107.12
2	A	607	HEC	C4A-C3A-C2A	-3.43	102.89	106.69
2	A	605	HEC	C2C-C1C-CHC	-3.43	119.49	126.00
2	A	606	HEC	C3A-C4A-NA	3.43	114.10	109.32
2	A	606	HEC	C2A-C1A-NA	3.39	114.44	109.73
2	A	606	HEC	C2C-C1C-CHC	-3.39	119.58	126.00
2	A	601	HEC	CBA-CAA-C2A	-3.38	107.00	112.63
2	A	602	HEC	C3D-C4D-ND	3.36	114.41	109.73
2	B	601	HEC	C4D-C3D-C2D	-3.35	103.45	106.92
2	A	601	HEC	CMB-C2B-C3B	3.33	129.33	126.22
2	A	608	HEC	C2C-C1C-CHC	-3.32	119.70	126.00
2	A	607	HEC	C4D-C3D-C2D	-3.31	103.49	106.92
2	A	603	HEC	C4A-C3A-C2A	-3.31	103.03	106.69
2	A	606	HEC	CAA-CBA-CGA	-3.30	102.93	113.66
2	B	603	HEC	CMA-C3A-C2A	3.28	131.13	124.94
2	B	603	HEC	C4D-C3D-C2D	-3.28	103.52	106.92

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	HEC	CMA-C3A-C2A	3.27	131.10	124.94
2	A	603	HEC	C2A-C1A-NA	3.27	114.27	109.73
2	B	601	HEC	C4A-C3A-C2A	-3.26	103.08	106.69
2	B	606	HEC	C2C-C1C-CHC	-3.24	119.86	126.00
2	B	601	HEC	CBD-CAD-C3D	-3.19	107.32	112.63
2	B	608	HEC	C2C-C1C-CHC	-3.17	119.99	126.00
2	A	602	HEC	C4D-C3D-C2D	-3.14	103.66	106.92
2	A	602	HEC	C4C-C3C-C2C	-3.14	102.97	106.35
2	A	602	HEC	CMA-C3A-C2A	3.11	130.81	124.94
2	B	601	HEC	CBA-CAA-C2A	-3.08	107.50	112.63
2	A	603	HEC	C2C-C1C-CHC	-3.06	120.19	126.00
2	B	603	HEC	C1A-C2A-C3A	-3.05	104.25	106.70
2	B	608	HEC	C2B-C1B-CHB	-3.03	120.25	126.00
2	B	607	HEC	C4A-C3A-C2A	-3.02	103.34	106.69
2	A	606	HEC	CBD-CAD-C3D	-3.01	107.62	112.63
2	B	607	HEC	C4D-ND-C1D	-3.00	104.23	107.12
2	A	607	HEC	C4C-NC-C1C	-2.99	102.48	106.77
2	A	608	HEC	C1A-C2A-C3A	-2.99	104.29	106.70
2	B	601	HEC	C2D-C1D-CHD	-2.99	120.33	126.00
2	A	601	HEC	CBD-CAD-C3D	-2.98	107.66	112.63
2	B	603	HEC	C2B-C1B-CHB	-2.98	120.34	126.00
2	B	605	HEC	C1A-C2A-C3A	-2.96	104.31	106.70
2	B	608	HEC	CMA-C3A-C2A	2.96	130.52	124.94
2	B	607	HEC	C3D-C4D-CHA	-2.96	120.39	126.00
2	B	606	HEC	C2D-C1D-CHD	-2.90	120.51	126.00
2	B	607	HEC	C4C-NC-C1C	-2.89	102.63	106.77
2	A	602	HEC	C4D-ND-C1D	-2.88	104.34	107.12
2	B	606	HEC	C2B-C1B-CHB	-2.88	120.54	126.00
2	A	602	HEC	CMD-C2D-C3D	2.87	130.35	124.94
2	A	602	HEC	C4B-NB-C1B	-2.83	102.72	106.77
2	A	606	HEC	C4B-C3B-C2B	-2.83	103.30	106.35
2	B	606	HEC	C4C-C3C-C2C	-2.83	103.30	106.35
2	B	602	HEC	C4D-C3D-C2D	-2.83	103.99	106.92
2	B	602	HEC	C4B-NB-C1B	-2.82	102.73	106.77
2	A	606	HEC	C2B-C1B-CHB	-2.80	120.68	126.00
2	A	603	HEC	C4C-C3C-C2C	-2.80	103.33	106.35
2	B	607	HEC	C2B-C1B-CHB	-2.79	120.71	126.00
2	B	603	HEC	C2A-C1A-NA	2.79	113.61	109.73
2	B	601	HEC	CMD-C2D-C3D	2.78	130.18	124.94
2	B	607	HEC	C2C-C1C-CHC	-2.77	120.75	126.00
2	B	601	HEC	C3D-C4D-CHA	-2.75	120.78	126.00
2	A	607	HEC	C3D-C4D-CHA	-2.75	120.78	126.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	603	HEC	C2C-C1C-CHC	-2.75	120.79	126.00
2	A	607	HEC	CAD-CBD-CGD	-2.75	104.72	113.66
2	A	603	HEC	C4B-NB-C1B	-2.73	102.86	106.77
2	A	604	HEC	C2A-C1A-NA	2.73	113.53	109.73
2	B	607	HEC	CBC-CAC-C3C	-2.72	121.41	127.36
2	B	602	HEC	C3C-C4C-NC	2.71	116.06	110.94
2	A	604	HEC	C1A-C2A-C3A	-2.70	104.52	106.70
2	B	603	HEC	C4C-C3C-C2C	-2.70	103.44	106.35
2	A	608	HEC	C2A-C1A-NA	2.69	113.47	109.73
2	A	607	HEC	C4C-C3C-C2C	-2.67	103.47	106.35
2	A	608	HEC	C4B-NB-C1B	-2.67	102.95	106.77
2	A	601	HEC	C3D-C4D-CHA	-2.66	120.96	126.00
2	A	605	HEC	O1A-CGA-CBA	-2.63	114.16	123.06
2	A	608	HEC	C4D-ND-C1D	-2.62	104.59	107.12
2	B	607	HEC	CAD-CBD-CGD	-2.62	105.15	113.66
2	A	601	HEC	C4C-C3C-C2C	-2.61	103.54	106.35
2	A	608	HEC	C4B-C3B-C2B	-2.60	103.54	106.35
2	B	602	HEC	CAD-CBD-CGD	-2.60	105.19	113.66
2	A	608	HEC	CMA-C3A-C4A	2.59	131.28	126.16
2	A	607	HEC	C3C-C4C-NC	2.57	115.79	110.94
2	A	603	HEC	C2B-C1B-CHB	-2.55	121.16	126.00
2	A	601	HEC	C2D-C1D-CHD	-2.53	121.21	126.00
2	B	605	HEC	CMA-C3A-C4A	2.53	131.15	126.16
2	B	602	HEC	CAA-CBA-CGA	-2.52	105.45	113.66
2	A	608	HEC	CAD-CBD-CGD	-2.52	105.47	113.66
2	B	606	HEC	C4B-C3B-C2B	-2.51	103.64	106.35
2	B	606	HEC	C4A-C3A-C2A	-2.51	103.91	106.69
2	A	602	HEC	CAA-CBA-CGA	-2.50	105.53	113.66
2	A	605	HEC	CMA-C3A-C2A	2.49	129.63	124.94
2	A	604	HEC	C2C-C1C-CHC	-2.48	121.29	126.00
2	B	606	HEC	CBD-CAD-C3D	-2.48	108.50	112.63
2	B	602	HEC	C3D-C4D-CHA	-2.48	121.31	126.00
2	A	602	HEC	C2C-C1C-CHC	-2.48	121.31	126.00
2	B	602	HEC	C2D-C1D-CHD	-2.47	121.32	126.00
2	A	608	HEC	C2B-C1B-CHB	-2.45	121.35	126.00
2	A	606	HEC	C2D-C1D-CHD	-2.45	121.35	126.00
2	A	601	HEC	CAA-C2A-C1A	2.45	129.09	124.67
2	A	608	HEC	CBA-CAA-C2A	-2.45	108.56	112.63
2	B	603	HEC	C4B-NB-C1B	-2.44	103.28	106.77
2	A	603	HEC	C2D-C1D-CHD	-2.43	121.40	126.00
2	B	601	HEC	C4C-NC-C1C	-2.43	103.30	106.77
2	A	607	HEC	CAA-C2A-C1A	2.42	129.03	124.67

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	606	HEC	C4C-C3C-C2C	-2.41	103.75	106.35
2	B	602	HEC	C2B-C1B-CHB	-2.41	121.43	126.00
2	A	605	HEC	C2A-C1A-NA	2.40	113.07	109.73
2	B	608	HEC	C4B-NB-C1B	-2.40	103.34	106.77
2	B	602	HEC	C2C-C1C-CHC	-2.39	121.48	126.00
2	A	608	HEC	C3D-C4D-CHA	-2.38	121.48	126.00
2	A	602	HEC	C3C-C4C-NC	2.36	115.41	110.94
2	A	602	HEC	C4C-NC-C1C	-2.35	103.40	106.77
2	B	605	HEC	O1A-CGA-CBA	-2.34	115.14	123.06
2	B	602	HEC	C3B-C4B-NB	2.34	115.36	110.94
2	B	602	HEC	C4C-NC-C1C	-2.33	103.43	106.77
2	B	603	HEC	CMD-C2D-C3D	2.33	129.34	124.94
2	A	607	HEC	C2B-C1B-CHB	-2.31	121.62	126.00
2	A	602	HEC	C3D-C4D-CHA	-2.31	121.62	126.00
2	B	607	HEC	C4B-C3B-C2B	-2.28	103.89	106.35
2	A	608	HEC	C4C-C3C-C2C	-2.28	103.89	106.35
2	A	606	HEC	C4B-NB-C1B	-2.27	103.51	106.77
2	A	608	HEC	CAA-CBA-CGA	-2.27	106.28	113.66
2	B	601	HEC	C2C-C1C-CHC	-2.27	121.70	126.00
2	B	608	HEC	C4B-C3B-C2B	-2.26	103.91	106.35
2	A	603	HEC	CMD-C2D-C3D	2.26	129.21	124.94
2	A	608	HEC	C2D-C1D-CHD	-2.26	121.71	126.00
2	B	605	HEC	C3D-C2D-C1D	-2.25	104.20	106.69
2	A	608	HEC	CMC-C2C-C1C	-2.25	125.01	128.46
2	A	607	HEC	CMA-C3A-C2A	2.24	129.16	124.94
2	A	608	HEC	C3B-C4B-NB	2.23	115.16	110.94
2	A	602	HEC	C2B-C1B-CHB	-2.23	121.78	126.00
2	A	602	HEC	C3B-C4B-NB	2.23	115.15	110.94
2	B	608	HEC	C2D-C1D-CHD	-2.23	121.78	126.00
2	A	604	HEC	C3B-C4B-NB	2.21	115.13	110.94
2	A	603	HEC	C4C-NC-C1C	-2.21	103.61	106.77
2	B	603	HEC	CMC-C2C-C1C	-2.20	125.08	128.46
2	B	606	HEC	CAA-C2A-C1A	2.20	128.63	124.67
2	B	606	HEC	C3D-C4D-CHA	-2.19	121.84	126.00
2	B	602	HEC	CBD-CAD-C3D	-2.19	108.98	112.63
2	B	608	HEC	C4C-C3C-C2C	-2.19	103.99	106.35
2	B	605	HEC	CMD-C2D-C3D	2.19	129.07	124.94
2	B	606	HEC	CMA-C3A-C2A	2.17	129.04	124.94
2	A	604	HEC	C4C-C3C-C2C	-2.15	104.03	106.35
2	A	606	HEC	CMA-C3A-C4A	2.13	130.37	126.16
2	A	602	HEC	C2D-C1D-CHD	-2.12	121.97	126.00
2	A	601	HEC	C3C-C4C-NC	2.12	114.94	110.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	604	HEC	CMA-C3A-C2A	2.09	128.88	124.94
2	A	604	HEC	C4B-C3B-C2B	-2.09	104.10	106.35
2	A	603	HEC	C3C-C4C-NC	2.09	114.88	110.94
2	B	601	HEC	CHC-C1C-NC	-2.08	121.17	124.70
2	B	607	HEC	C2D-C1D-CHD	-2.08	122.07	126.00
2	B	601	HEC	CMA-C3A-C2A	2.06	128.82	124.94
2	A	603	HEC	C3B-C4B-NB	2.05	114.82	110.94
2	A	601	HEC	C4C-NC-C1C	-2.05	103.84	106.77
2	B	607	HEC	C4B-NB-C1B	-2.05	103.84	106.77
2	A	604	HEC	C4C-NC-C1C	-2.05	103.84	106.77
2	B	607	HEC	O1A-CGA-CBA	-2.04	116.16	123.06
2	B	601	HEC	CHB-C1B-NB	-2.03	121.25	124.70
2	A	603	HEC	CAA-C2A-C1A	2.01	128.29	124.67

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	520/520 (100%)	-0.52	2 (0%) 90 94	10, 15, 29, 55	1 (0%)
1	B	520/520 (100%)	-0.57	3 (0%) 86 92	8, 13, 27, 50	0
All	All	1040/1040 (100%)	-0.55	5 (0%) 86 94	8, 14, 28, 55	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	524	VAL	4.3
1	A	524	VAL	3.7
1	A	523	ALA	2.8
1	B	523	ALA	2.5
1	B	463[A]	ASP	2.2

### 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( $\text{\AA}^2$ )	Q<0.9
6	GOL	A	615[A]	1/6	0.30	23.60	36,36,36,36	1
6	GOL	A	615[B]	1/6	0.30	18.53	37,37,37,37	1
6	GOL	B	613[A]	1/6	0.10	12.87	12,12,12,12	1
6	GOL	A	614	6/6	0.13	8.14	20,25,26,28	0
6	GOL	A	613[B]	1/6	0.10	7.11	17,17,17,17	1
6	GOL	A	613[A]	1/6	0.10	7.11	14,14,14,14	1
7	SO4	A	616	5/5	0.19	7.02	26,27,29,30	5
7	SO4	B	615	5/5	0.16	6.54	21,21,22,23	5
5	MPD	A	612	8/8	0.16	6.19	21,26,27,28	0
6	GOL	B	614	6/6	0.11	4.91	19,23,24,28	0
6	GOL	B	613[B]	1/6	0.10	4.78	17,17,17,17	1
3	NO2	A	609	2/3	0.17	3.91	13,13,13,14	2
2	HEC	B	605	39/43	0.13	2.31	19,26,44,50	0
2	HEC	B	604[A]	4/43	0.08	2.22	8,9,9,9	4
5	MPD	B	612	8/8	0.10	2.13	18,21,22,22	0
2	HEC	A	605	38/43	0.14	2.13	21,29,44,47	0
2	HEC	B	604[B]	4/43	0.08	1.32	10,12,12,13	4
2	HEC	A	604	43/43	0.08	1.31	9,10,13,19	0
2	HEC	B	602	43/43	0.09	1.00	8,9,16,21	0
2	HEC	B	607	43/43	0.10	0.85	9,10,22,29	0
2	HEC	A	607	43/43	0.09	0.80	9,11,23,34	0
2	HEC	A	601	43/43	0.10	0.77	9,11,12,13	0
2	HEC	B	601	43/43	0.09	0.62	7,9,10,11	0
3	NO2	B	609	2/3	0.10	0.54	10,10,10,10	2
2	HEC	A	603	43/43	0.09	0.50	8,9,10,12	0
2	HEC	B	603	43/43	0.09	0.43	7,7,9,11	0
2	HEC	A	602	43/43	0.08	0.38	9,11,17,21	0
2	HEC	B	606	43/43	0.08	0.37	9,11,13,14	0
2	HEC	A	606	43/43	0.07	0.08	11,12,14,14	0
3	NO2	B	616	3/3	0.07	-0.27	21,21,22,23	3
2	HEC	A	608	43/43	0.06	-0.38	11,13,17,22	0
2	HEC	B	608	43/43	0.07	-0.49	12,16,18,22	0
3	NO2	A	618	3/3	0.06	-0.76	17,17,17,18	3
3	NO2	A	617	3/3	0.05	-0.82	23,23,24,25	3
3	NO2	B	617	3/3	0.04	-0.91	13,13,13,14	3
4	CA	B	611	1/1	0.05	-1.57	12,12,12,12	1
4	CA	A	611	1/1	0.04	-2.18	14,14,14,14	1
4	CA	A	610	1/1	0.03	-2.33	17,17,17,17	0
4	CA	B	610	1/1	0.02	-3.26	16,16,16,16	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.