



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2017 – 03:40 PM EDT

PDB ID : 1H29  
Title : Sulfate respiration in *Desulfovibrio vulgaris* Hildenborough: Structure of the 16-heme Cytochrome c HmcA at 2.5 Å resolution and a view of its role in transmembrane electron transfer  
Authors : Matias, P.M.; Coelho, A.V.; Valente, F.M.A.; Placido, D.; Legall, J.; Xavier, A.V.; Pereira, I.A.C.; Carrondo, M.A.  
Deposited on : unknown  
Resolution : 2.51 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

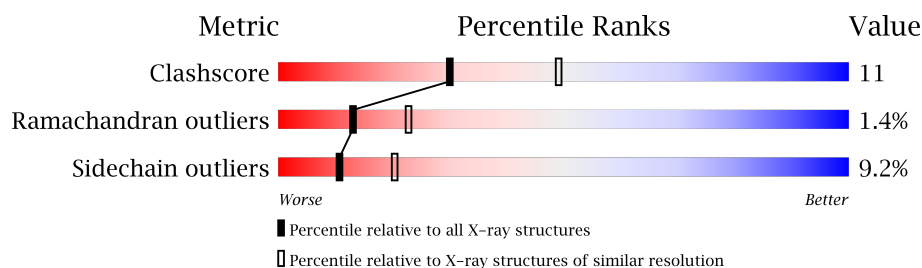
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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	514	
1	B	514	
1	C	514	
1	D	514	

## 2 Entry composition [i](#)

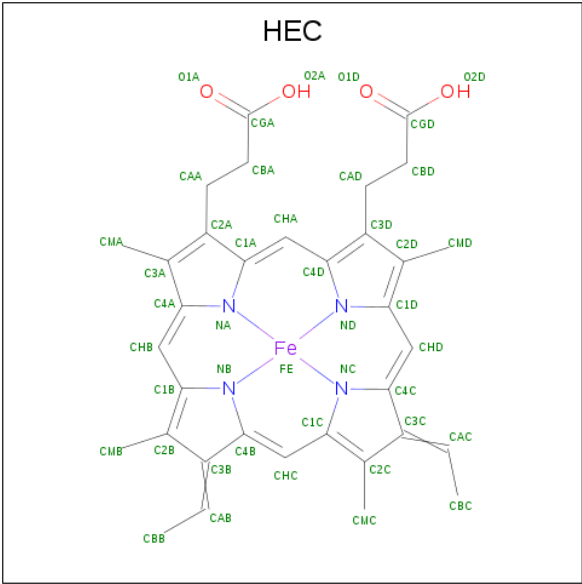
There are 3 unique types of molecules in this entry. The entry contains 18287 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HIGH-MOLECULAR-WEIGHT CYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	38	0	0
			3783	2323	717	699	44			
1	B	499	Total	C	N	O	S	75	0	0
			3763	2312	712	695	44			
1	C	501	Total	C	N	O	S	90	0	0
			3777	2320	714	699	44			
1	D	492	Total	C	N	O	S	70	0	0
			3715	2284	699	688	44			

- 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		

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

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

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

- Molecule 3 is water.

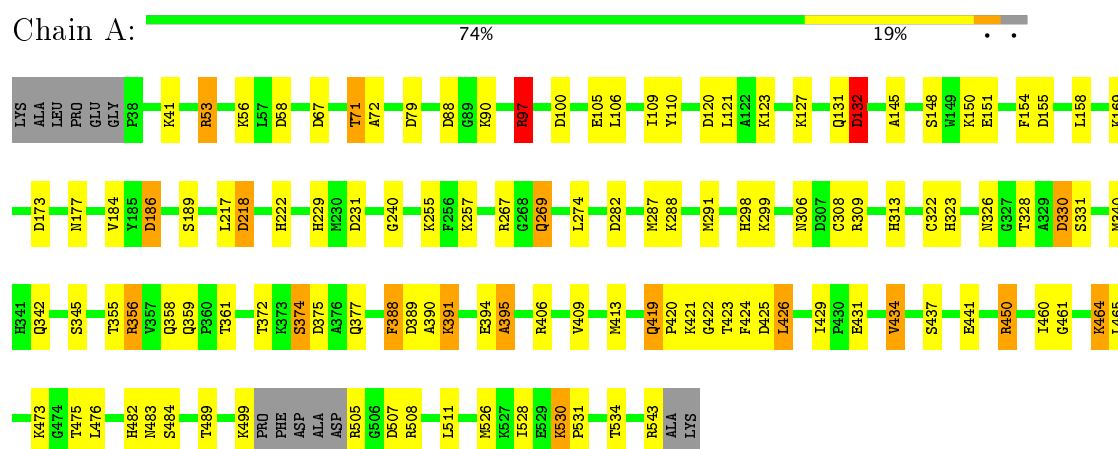
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total 123	O 123	0	0
3	B	126	Total 126	O 126	0	0
3	C	136	Total 136	O 136	0	0
3	D	112	Total 112	O 112	0	0

### 3 Residue-property plots

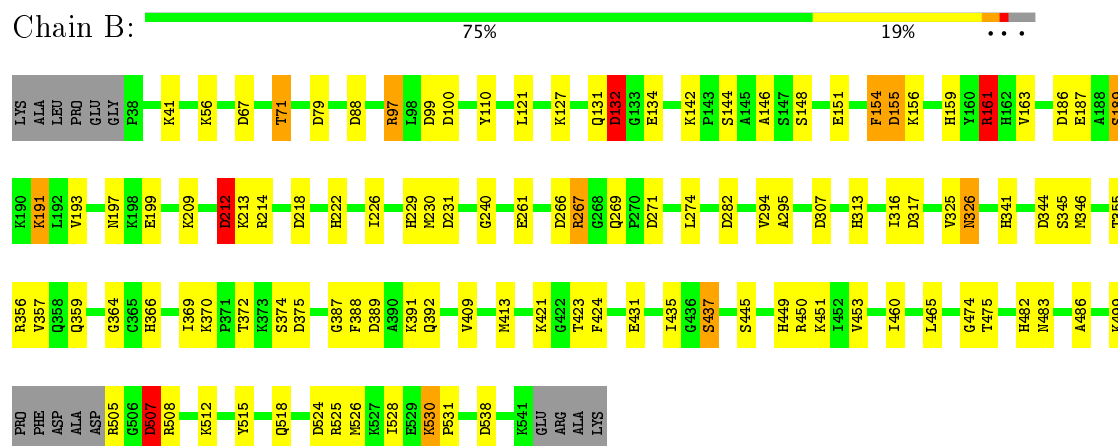
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

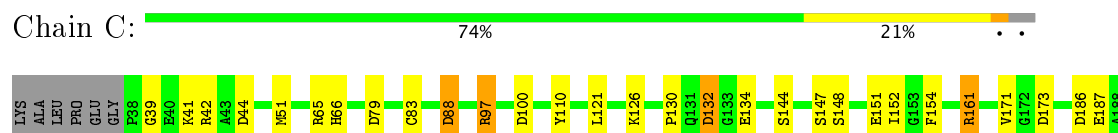
#### • Molecule 1: HIGH-MOLECULAR-WEIGHT CYTOCHROME C



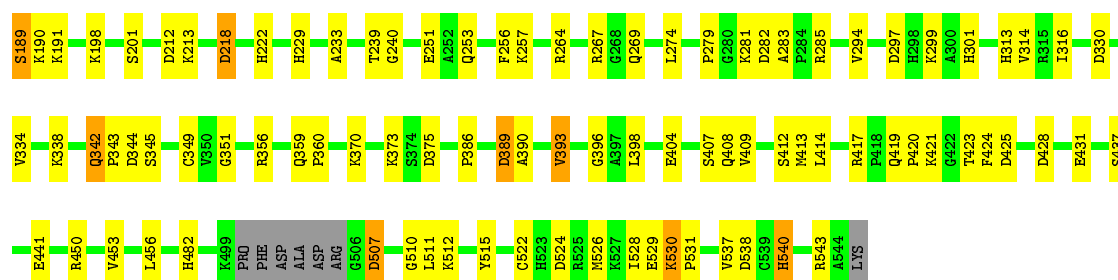
#### • Molecule 1: HIGH-MOLECULAR-WEIGHT CYTOCHROME C



#### • Molecule 1: HIGH-MOLECULAR-WEIGHT CYTOCHROME C

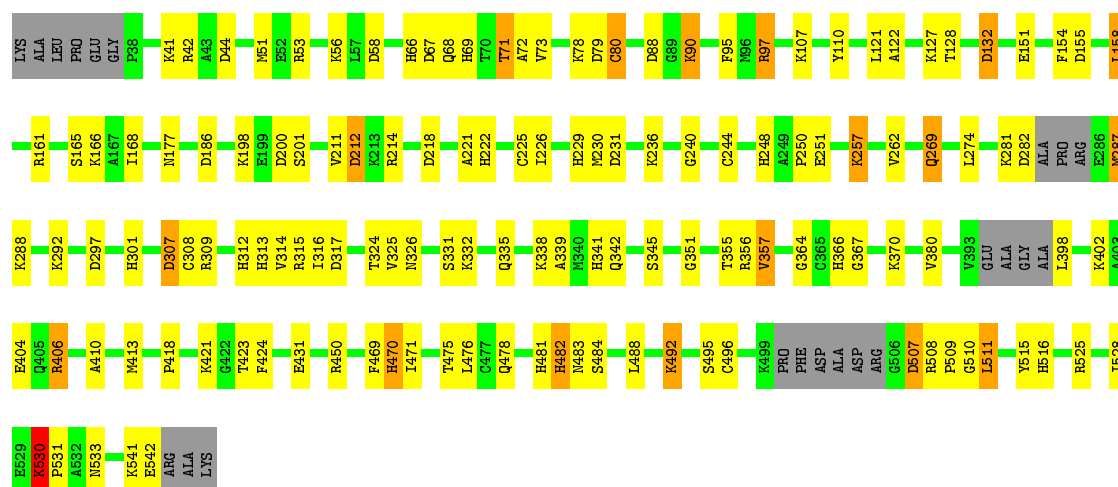






• Molecule 1: HIGH-MOLECULAR-WEIGHT CYTOCHROME C

Chain D: 69% 23%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.39Å 220.39Å 102.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.51	Depositor
% Data completeness (in resolution range)	92.1 (30.00-2.51)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.192 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18287	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.59	0/3864	0.83	17/5201 (0.3%)
1	B	0.59	1/3844 (0.0%)	0.83	21/5175 (0.4%)
1	C	0.57	0/3858	0.85	19/5194 (0.4%)
1	D	0.53	0/3793	0.83	15/5103 (0.3%)
All	All	0.57	1/15359 (0.0%)	0.84	72/20673 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	D	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	SER	CB-OG	7.80	1.52	1.42

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	ASP	CB-CG-OD2	10.44	127.69	118.30
1	A	132	ASP	CB-CG-OD2	8.26	125.73	118.30
1	D	79	ASP	CB-CG-OD2	8.20	125.68	118.30
1	C	97	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	C	428	ASP	CB-CG-OD2	7.37	124.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	ASP	CB-CG-OD2	7.15	124.73	118.30
1	B	132	ASP	CB-CG-OD2	7.08	124.68	118.30
1	B	79	ASP	CB-CG-OD2	6.94	124.55	118.30
1	C	100	ASP	CB-CG-OD2	6.93	124.53	118.30
1	D	507	ASP	CB-CG-OD2	6.93	124.53	118.30
1	A	97	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	D	58	ASP	CB-CG-OD2	6.72	124.35	118.30
1	B	271	ASP	CB-CG-OD2	6.71	124.34	118.30
1	D	97	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	425	ASP	CB-CG-OD2	6.56	124.20	118.30
1	A	186	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	58	ASP	CB-CG-OD2	6.48	124.13	118.30
1	A	120	ASP	CB-CG-OD2	6.43	124.08	118.30
1	D	231	ASP	CB-CG-OD2	6.43	124.08	118.30
1	C	330	ASP	CB-CG-OD2	6.33	123.99	118.30
1	C	88	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	79	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	100	ASP	CB-CG-OD2	6.13	123.82	118.30
1	D	282	ASP	CB-CG-OD2	6.11	123.80	118.30
1	D	186	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	266	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	218	ASP	CB-CG-OD2	5.92	123.63	118.30
1	C	297	ASP	CB-CG-OD2	5.86	123.58	118.30
1	D	218	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	212	ASP	CB-CG-OD2	5.83	123.55	118.30
1	C	524	ASP	CB-CG-OD2	5.76	123.48	118.30
1	D	297	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	100	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	186	ASP	CB-CG-OD2	5.67	123.41	118.30
1	C	44	ASP	CB-CG-OD2	5.65	123.39	118.30
1	C	173	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	507	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	282	ASP	CB-CG-OD2	5.53	123.27	118.30
1	B	99	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	173	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	330	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	344	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	200	ASP	CB-CG-OD2	5.46	123.21	118.30
1	C	396	GLY	N-CA-C	5.41	126.63	113.10
1	A	389	ASP	CB-CG-OD2	5.39	123.15	118.30
1	D	307	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	218	ASP	CB-CG-OD2	5.36	123.13	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	ASP	CB-CG-OD2	5.35	123.12	118.30
1	D	364	GLY	N-CA-C	-5.30	99.84	113.10
1	C	282	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	212	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	507	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	88	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	375	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	155	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	231	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	344	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	231	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	88	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	375	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	97	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	C	425	ASP	CB-CG-OD2	5.11	122.90	118.30
1	D	44	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	375	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	307	ASP	CB-CG-OD2	5.07	122.87	118.30
1	C	538	ASP	CB-CG-OD2	5.07	122.87	118.30
1	D	212	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	538	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	524	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	507	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	161	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	97	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	GLN	Peptide
1	A	217	LEU	Peptide
1	B	131	GLN	Peptide
1	B	154	PHE	Peptide
1	D	470	HIS	Peptide

## 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	3783	0	3716	68	0
1	B	3763	0	3697	67	0
1	C	3777	0	3708	80	0
1	D	3715	0	3644	81	0
2	A	688	0	480	38	0
2	B	688	0	480	36	0
2	C	688	0	480	39	0
2	D	688	0	480	44	0
3	A	123	0	0	1	0
3	B	126	0	0	2	0
3	C	136	0	0	3	0
3	D	112	0	0	1	0
All	All	18287	0	16685	357	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 (357) 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:D:530:LYS:HB3	1:D:531:PRO:CD	1.85	1.07
1:B:530:LYS:HB2	1:B:531:PRO:HD3	1.34	1.06
1:D:530:LYS:HB3	1:D:531:PRO:HD3	1.29	1.06
1:C:522:CYS:SG	1:C:526:MET:HE2	1.97	1.03
1:B:530:LYS:CB	1:B:531:PRO:HD3	1.89	1.03
1:C:522:CYS:SG	1:C:526:MET:CE	2.54	0.96
1:C:409:VAL:HG12	1:C:413:MET:CE	1.97	0.95
1:C:409:VAL:HG12	1:C:413:MET:HE2	1.46	0.94
1:B:530:LYS:HB2	1:B:531:PRO:CD	1.99	0.92
1:C:161:ARG:HH11	1:C:161:ARG:HG2	1.40	0.87
1:D:528:ILE:CG2	1:D:530:LYS:HB2	2.06	0.85
1:D:410:ALA:HA	1:D:413:MET:HE2	1.57	0.84
1:D:530:LYS:CB	1:D:531:PRO:CD	2.55	0.83
1:A:530:LYS:HB3	1:A:531:PRO:HD3	1.60	0.82
1:A:186:ASP:HB3	1:A:189:SER:HB2	1.62	0.80
1:B:530:LYS:CB	1:B:531:PRO:CD	2.58	0.80
1:A:429:ILE:HD11	2:A:1113:HEC:HMB2	1.63	0.79
1:B:189:SER:HB2	1:B:191:LYS:HD3	1.67	0.76
1:B:526:MET:HE1	2:B:1115:HEC:HHD	1.67	0.76
1:A:429:ILE:CD1	2:A:1113:HEC:HMB2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:ASP:O	1:D:71:THR:HG23	1.84	0.76
1:B:356:ARG:O	1:B:359:GLN:HG2	1.86	0.75
1:C:526:MET:HE1	2:C:1115:HEC:CAC	2.16	0.75
2:A:1102:HEC:HMC1	2:A:1102:HEC:HBC3	1.69	0.75
1:A:356:ARG:O	1:A:359:GLN:HG2	1.87	0.74
1:B:526:MET:CE	2:B:1115:HEC:HMD3	2.18	0.74
1:A:426:LEU:O	1:A:429:ILE:HB	1.88	0.74
2:B:1106:HEC:HBC3	2:B:1106:HEC:HMC1	1.70	0.73
2:C:1106:HEC:HBC3	2:C:1106:HEC:HMC1	1.71	0.73
1:A:274:LEU:HD23	1:A:406:ARG:HG2	1.70	0.72
1:B:526:MET:HE3	2:B:1115:HEC:HMD3	1.72	0.72
1:C:522:CYS:SG	1:C:526:MET:HE1	2.30	0.71
1:D:410:ALA:HA	1:D:413:MET:CE	2.20	0.70
1:C:39:GLY:HA3	1:C:144:SER:O	1.92	0.70
1:D:341:HIS:HE1	2:D:1112:HEC:NA	1.90	0.70
1:A:419:GLN:HG3	1:A:420:PRO:HD2	1.74	0.69
1:C:356:ARG:O	1:C:359:GLN:HG2	1.92	0.69
1:A:41:LYS:HB3	1:A:148:SER:HB3	1.73	0.69
1:D:528:ILE:HG22	1:D:530:LYS:HB2	1.75	0.69
1:A:388:PHE:N	1:A:388:PHE:CD1	2.60	0.69
1:D:269:GLN:HG2	2:D:1108:HEC:HMB2	1.74	0.68
1:C:414:LEU:HA	1:C:417:ARG:HE	1.58	0.68
1:D:51:MET:HE1	1:D:107:LYS:HB2	1.75	0.68
2:A:1110:HEC:HMC1	2:A:1110:HEC:HBC3	1.76	0.67
1:A:409:VAL:HG12	1:A:413:MET:CE	2.25	0.67
2:D:1110:HEC:HMC1	2:D:1110:HEC:HBC3	1.76	0.67
1:C:393:VAL:HG22	1:C:398:LEU:HD12	1.77	0.66
1:A:530:LYS:HB3	1:A:531:PRO:CD	2.25	0.66
2:D:1104:HEC:CMD	2:D:1106:HEC:HBB2	2.25	0.66
2:B:1102:HEC:HMC1	2:B:1102:HEC:HBC3	1.77	0.66
1:A:67:ASP:O	1:A:71:THR:HG23	1.96	0.66
1:C:154:PHE:HB2	2:C:1104:HEC:HBD2	1.77	0.65
2:D:1110:HEC:HMB1	2:D:1110:HEC:HBB3	1.77	0.65
1:B:530:LYS:HB3	1:B:531:PRO:HD3	1.78	0.65
1:C:510:GLY:HA3	3:C:2118:HOH:O	1.95	0.65
1:D:165:SER:HB3	1:D:168:ILE:HD12	1.78	0.65
1:B:423:THR:HG22	1:B:424:PHE:H	1.62	0.65
1:B:121:LEU:HD13	2:B:1102:HEC:HMD3	1.80	0.64
1:C:423:THR:HG22	1:C:424:PHE:H	1.62	0.64
1:D:211:VAL:HG23	1:D:212:ASP:H	1.61	0.64
2:D:1102:HEC:HMC1	2:D:1102:HEC:HBC3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LYS:HB3	1:B:148:SER:HB3	1.81	0.63
1:D:511:LEU:HD13	1:D:515:TYR:CE1	2.34	0.62
1:B:326:ASN:HD22	1:B:326:ASN:H	1.46	0.62
1:D:423:THR:HG22	1:D:424:PHE:N	2.14	0.62
2:D:1111:HEC:HBB3	2:D:1111:HEC:HMB1	1.80	0.62
1:A:409:VAL:HG12	1:A:413:MET:HE2	1.80	0.62
1:C:423:THR:HG22	1:C:424:PHE:N	2.15	0.61
1:D:211:VAL:HG21	1:D:214:ARG:CZ	2.29	0.61
1:B:526:MET:CE	2:B:1115:HEC:HHD	2.30	0.61
1:A:530:LYS:CB	1:A:531:PRO:CD	2.78	0.61
1:B:372:THR:CG2	1:B:374:SER:HB3	2.31	0.61
1:D:511:LEU:HD13	1:D:515:TYR:HE1	1.65	0.61
1:A:328:THR:HG22	1:A:330:ASP:H	1.66	0.60
1:A:356:ARG:HG2	1:A:465:LEU:HD12	1.82	0.60
1:B:356:ARG:O	1:B:359:GLN:CG	2.49	0.60
2:C:1115:HEC:HMC1	2:C:1115:HEC:HBC3	1.83	0.60
2:B:1115:HEC:HMC1	2:B:1115:HEC:HBC3	1.84	0.60
1:B:372:THR:HG22	1:B:374:SER:HB3	1.84	0.60
2:C:1108:HEC:HBC1	2:C:1110:HEC:HMC2	1.83	0.59
1:B:474:GLY:HA3	1:B:486:ALA:HB1	1.84	0.59
2:C:1102:HEC:HBC3	2:C:1102:HEC:HMC1	1.84	0.59
1:A:355:THR:HA	1:A:358:GLN:HG3	1.85	0.58
1:C:526:MET:HE3	2:C:1115:HEC:HHD	1.84	0.58
2:B:1101:HEC:HBB3	2:B:1101:HEC:HMB1	1.86	0.58
1:C:274:LEU:HD13	1:C:413:MET:CE	2.34	0.57
1:C:274:LEU:HD13	1:C:413:MET:HE3	1.86	0.57
1:C:41:LYS:HB3	1:C:148:SER:HB3	1.85	0.57
1:C:409:VAL:HG12	1:C:413:MET:HE1	1.82	0.57
1:D:229:HIS:CE1	1:D:240:GLY:HA3	2.39	0.57
1:A:374:SER:HB3	1:A:377:GLN:H	1.70	0.56
2:D:1112:HEC:HBC3	2:D:1112:HEC:HMC1	1.87	0.56
2:A:1108:HEC:HMB1	2:A:1108:HEC:HBB3	1.86	0.56
1:C:251:GLU:CD	1:C:251:GLU:H	2.09	0.56
1:B:97:ARG:NH2	1:B:110:TYR:OH	2.39	0.56
1:C:389:ASP:CG	1:C:390:ALA:H	2.08	0.56
1:C:414:LEU:HB3	1:C:417:ARG:HH21	1.71	0.56
2:A:1115:HEC:HBC3	2:A:1115:HEC:HMC1	1.88	0.56
1:D:496:CYS:O	1:D:508:ARG:HD3	2.04	0.56
1:A:431:GLU:HA	1:A:450:ARG:HB3	1.88	0.56
1:D:225:CYS:HB3	2:D:1106:HEC:C4B	2.36	0.56
2:A:1109:HEC:HBA2	2:A:1109:HEC:HMA2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:HIS:CE1	1:D:314:VAL:HG23	2.41	0.55
1:B:161:ARG:NH1	1:B:161:ARG:HG2	2.21	0.55
1:B:409:VAL:HG12	1:B:413:MET:CE	2.36	0.55
1:C:526:MET:CE	2:C:1115:HEC:HHD	2.36	0.55
2:D:1115:HEC:HMC1	2:D:1115:HEC:HBC3	1.88	0.55
1:D:68:GLN:HE22	2:D:1102:HEC:HBA2	1.71	0.55
1:B:294:VAL:HG11	2:B:1112:HEC:HMD3	1.88	0.55
1:D:154:PHE:CD1	1:D:158:LEU:HD13	2.42	0.55
1:D:80:CYS:HB3	2:D:1101:HEC:CHC	2.37	0.55
1:A:394:GLU:O	1:A:395:ALA:CB	2.54	0.55
2:B:1110:HEC:HMC1	2:B:1110:HEC:HBC3	1.87	0.55
2:C:1115:HEC:HBB3	2:C:1115:HEC:HMB1	1.87	0.55
1:B:161:ARG:HG2	1:B:161:ARG:HH11	1.72	0.55
1:B:189:SER:CB	1:B:191:LYS:HD3	2.35	0.54
1:D:301:HIS:CD2	2:D:1110:HEC:NC	2.75	0.54
2:C:1102:HEC:HMC1	2:C:1102:HEC:CBC	2.38	0.54
1:A:298:HIS:HE1	2:A:1108:HEC:NB	2.06	0.54
2:B:1102:HEC:HBB3	2:B:1102:HEC:HMB1	1.88	0.54
2:D:1113:HEC:HBB3	2:D:1113:HEC:HMB1	1.89	0.54
1:D:470:HIS:HA	1:D:475:THR:HG21	1.89	0.54
1:A:374:SER:HB2	1:A:377:GLN:HB2	1.89	0.54
1:C:264:ARG:NH1	1:C:299:LYS:HD2	2.23	0.54
1:C:393:VAL:HG22	1:C:398:LEU:CD1	2.37	0.54
2:C:1109:HEC:HMC1	2:C:1109:HEC:HBC3	1.88	0.53
1:B:409:VAL:HG12	1:B:413:MET:HE3	1.91	0.53
1:B:483:ASN:HD22	2:B:1114:HEC:C1D	2.22	0.53
2:B:1104:HEC:HBB3	2:B:1104:HEC:HMB1	1.91	0.53
1:C:537:VAL:HA	1:C:540:HIS:O	2.08	0.53
2:A:1113:HEC:HBC3	2:A:1113:HEC:HMC1	1.91	0.53
1:A:322:CYS:HB3	1:A:331:SER:HB3	1.91	0.53
2:C:1110:HEC:HMC1	2:C:1110:HEC:HBC3	1.89	0.53
1:C:360:PRO:O	1:C:526:MET:HG2	2.08	0.53
1:D:274:LEU:HD13	1:D:413:MET:CE	2.39	0.53
1:B:526:MET:HE1	2:B:1115:HEC:HMD3	1.88	0.53
1:D:66:HIS:HE1	2:D:1101:HEC:NB	2.04	0.53
1:C:419:GLN:NE2	1:C:420:PRO:HD2	2.24	0.52
2:D:1106:HEC:HBC3	2:D:1106:HEC:HMC1	1.90	0.52
1:D:222:HIS:HA	1:D:226:ILE:HD12	1.90	0.52
1:B:460:ILE:HD11	2:B:1111:HEC:HMC2	1.90	0.52
1:B:316:ILE:HD13	2:B:1108:HEC:HMB3	1.91	0.52
2:A:1110:HEC:HMB1	2:A:1110:HEC:HBB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:HIS:CD2	2:D:1102:HEC:NC	2.78	0.52
1:A:464:LYS:HB2	2:A:1110:HEC:CGD	2.39	0.52
1:C:97:ARG:NH2	1:C:110:TYR:CZ	2.78	0.52
1:D:80:CYS:HB3	2:D:1101:HEC:C4B	2.38	0.52
1:D:423:THR:HG22	1:D:424:PHE:H	1.73	0.52
1:A:423:THR:HG23	1:A:473:LYS:O	2.10	0.52
1:B:341:HIS:HE1	2:B:1112:HEC:C1A	2.23	0.52
1:C:294:VAL:HG11	2:C:1112:HEC:HMD3	1.92	0.52
1:C:186:ASP:OD2	1:C:189:SER:HB2	2.09	0.52
2:A:1112:HEC:HMC1	2:A:1112:HEC:HBC3	1.92	0.52
1:A:388:PHE:HD1	1:A:388:PHE:H	1.52	0.52
1:D:431:GLU:HA	1:D:450:ARG:HB2	1.92	0.52
1:D:530:LYS:CB	1:D:531:PRO:HD2	2.38	0.51
1:A:528:ILE:CG2	1:A:530:LYS:HB2	2.39	0.51
1:A:340:MET:HG3	2:A:1112:HEC:C3D	2.41	0.51
1:B:154:PHE:HB2	2:B:1104:HEC:HBD2	1.92	0.51
1:D:168:ILE:HG22	1:D:177:ASN:HB2	1.93	0.51
1:D:367:GLY:HA3	1:D:525:ARG:HD3	1.93	0.50
1:D:510:GLY:HA3	3:D:2100:HOH:O	2.11	0.50
1:D:541:LYS:O	1:D:542:GLU:HB2	2.11	0.50
1:C:316:ILE:HD12	2:C:1108:HEC:HMB3	1.93	0.50
1:C:66:HIS:CE1	2:C:1101:HEC:NB	2.80	0.50
1:A:464:LYS:HD3	2:A:1110:HEC:O1D	2.11	0.50
1:A:154:PHE:HB2	2:A:1104:HEC:HBD2	1.94	0.50
1:A:186:ASP:OD2	1:A:189:SER:N	2.45	0.50
1:B:507:ASP:OD2	1:B:507:ASP:N	2.45	0.50
1:B:199:GLU:OE1	1:B:267:ARG:HG3	2.12	0.50
2:A:1106:HEC:HBB3	2:A:1106:HEC:HMB1	1.95	0.49
1:A:394:GLU:O	1:A:395:ALA:HB2	2.13	0.49
1:B:295:ALA:HB2	1:B:413:MET:SD	2.52	0.49
2:D:1101:HEC:HBC1	2:D:1102:HEC:HMC2	1.93	0.49
1:B:134:GLU:OE2	1:D:533:ASN:ND2	2.25	0.49
1:C:233:ALA:HB2	1:C:239:THR:HG21	1.94	0.49
1:C:97:ARG:NH2	1:C:110:TYR:OH	2.39	0.49
1:C:161:ARG:HG2	1:C:161:ARG:NH1	2.16	0.49
1:C:386:PRO:HG3	1:C:412:SER:OG	2.13	0.49
1:C:530:LYS:HB2	1:C:531:PRO:CD	2.43	0.49
1:D:121:LEU:HD13	2:D:1102:HEC:HMD3	1.95	0.49
1:D:287:MET:SD	1:D:325:VAL:HG12	2.52	0.49
1:A:423:THR:HG22	1:A:424:PHE:H	1.77	0.49
2:A:1102:HEC:HMC1	2:A:1102:HEC:CBC	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:LEU:HD13	1:D:413:MET:HE1	1.94	0.48
1:C:431:GLU:HA	1:C:450:ARG:HB2	1.95	0.48
1:D:73:VAL:HG13	1:D:78:LYS:HB2	1.93	0.48
1:A:229:HIS:CE1	1:A:240:GLY:HA3	2.48	0.48
1:D:250:PRO:HD2	1:D:251:GLU:OE2	2.14	0.48
1:B:132:ASP:CG	1:D:516:HIS:HD1	2.17	0.48
1:B:41:LYS:HA	1:B:146:ALA:O	2.13	0.48
2:C:1111:HEC:HBB3	2:C:1111:HEC:HMB1	1.94	0.48
1:A:530:LYS:HB3	2:A:1115:HEC:HBA1	1.96	0.48
1:C:338:LYS:HE2	1:C:342:GLN:OE1	2.14	0.48
1:D:221:ALA:O	1:D:225:CYS:SG	2.71	0.48
2:A:1109:HEC:HBA2	2:A:1109:HEC:CMA	2.43	0.48
1:B:67:ASP:O	1:B:71:THR:HG23	2.13	0.48
1:A:222:HIS:HB3	2:A:1101:HEC:HMA3	1.95	0.48
1:B:274:LEU:HD13	1:B:413:MET:HE3	1.96	0.48
1:C:370:LYS:HG3	2:C:1114:HEC:O2D	2.14	0.47
1:A:526:MET:HB2	1:A:528:ILE:HG12	1.95	0.47
1:B:121:LEU:CD1	2:B:1102:HEC:HMD3	2.43	0.47
2:B:1106:HEC:CBC	2:B:1106:HEC:HMC1	2.44	0.47
1:C:530:LYS:CB	1:C:531:PRO:CD	2.92	0.47
1:D:211:VAL:CG2	1:D:214:ARG:HB2	2.45	0.47
1:D:248:HIS:CD2	2:D:1107:HEC:NB	2.83	0.47
2:D:1112:HEC:O2D	2:D:1112:HEC:HBA2	2.14	0.47
2:C:1101:HEC:HBB3	2:C:1101:HEC:HMB1	1.97	0.47
1:D:274:LEU:HB3	1:D:406:ARG:HG2	1.97	0.47
1:D:380:VAL:HG11	1:D:469:PHE:CE2	2.50	0.47
1:D:345:SER:O	1:D:351:GLY:HA3	2.15	0.47
1:A:475:THR:O	2:A:1111:HEC:HMD2	2.14	0.47
2:B:1111:HEC:HMC1	2:B:1111:HEC:HBC3	1.97	0.47
1:A:342:GLN:HG2	1:A:345:SER:HB2	1.96	0.46
1:A:530:LYS:CB	1:A:531:PRO:HD3	2.36	0.46
2:C:1105:HEC:HMC1	2:C:1105:HEC:HBC3	1.96	0.46
1:B:229:HIS:CE1	1:B:240:GLY:HA3	2.51	0.46
1:B:431:GLU:HA	1:B:450:ARG:HB2	1.97	0.46
1:C:51:MET:HG3	2:C:1103:HEC:O1D	2.15	0.46
2:D:1111:HEC:HMC1	2:D:1111:HEC:HBC3	1.98	0.46
1:D:483:ASN:HD22	2:D:1114:HEC:C1D	2.28	0.46
1:A:423:THR:OG1	1:A:476:LEU:HD12	2.14	0.46
2:C:1102:HEC:HBB3	2:C:1102:HEC:HMB1	1.97	0.46
1:C:389:ASP:OD1	1:C:390:ALA:N	2.46	0.46
1:D:211:VAL:HG23	1:D:212:ASP:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:ILE:HG22	1:D:230:MET:CE	2.45	0.46
1:C:313:HIS:HE1	2:C:1109:HEC:ND	2.11	0.46
1:A:422:GLY:O	1:A:473:LYS:HA	2.15	0.46
2:A:1103:HEC:HMC1	2:A:1103:HEC:HBC3	1.97	0.46
1:C:186:ASP:HB3	1:C:191:LYS:O	2.16	0.46
1:D:357:VAL:HG13	1:D:366:HIS:HB3	1.98	0.46
1:C:130:PRO:HA	1:C:134:GLU:OE1	2.16	0.45
1:C:313:HIS:HE1	2:C:1109:HEC:C1D	2.29	0.45
1:D:307:ASP:HB2	2:D:1104:HEC:O1A	2.16	0.45
1:D:66:HIS:HB3	1:D:244:CYS:SG	2.56	0.45
1:A:308:CYS:SG	2:A:1104:HEC:HBA1	2.56	0.45
1:B:222:HIS:CD2	2:B:1107:HEC:NC	2.83	0.45
1:B:226:ILE:HG22	1:B:230:MET:CE	2.47	0.45
2:A:1115:HEC:HMB1	2:A:1115:HEC:HBB3	1.98	0.45
1:C:152:ILE:O	2:C:1107:HEC:O1D	2.34	0.45
1:C:161:ARG:CG	1:C:161:ARG:HH11	2.18	0.45
1:D:476:LEU:HB3	2:D:1111:HEC:HBC2	1.98	0.45
1:D:423:THR:CG2	1:D:424:PHE:N	2.80	0.45
1:D:508:ARG:HA	1:D:509:PRO:HD2	1.85	0.45
1:D:331:SER:HA	2:D:1109:HEC:HMD3	1.98	0.45
1:D:201:SER:HA	2:D:1104:HEC:HAD2	1.99	0.45
1:C:313:HIS:CE1	1:C:314:VAL:HG23	2.51	0.45
2:A:1112:HEC:O1A	2:A:1112:HEC:HMA3	2.17	0.45
2:B:1107:HEC:CMA	2:B:1107:HEC:HBA2	2.46	0.45
1:A:97:ARG:NH2	1:A:110:TYR:OH	2.50	0.44
1:B:212:ASP:O	1:B:213:LYS:HB2	2.17	0.44
1:A:372:THR:HG21	3:A:2088:HOH:O	2.17	0.44
1:B:528:ILE:HG23	1:B:530:LYS:HG2	1.98	0.44
2:C:1108:HEC:HBC1	2:C:1110:HEC:CMC	2.48	0.44
1:C:301:HIS:CE1	2:C:1110:HEC:NA	2.85	0.44
1:A:460:ILE:HG12	2:A:1111:HEC:HBB2	2.00	0.44
1:B:435:ILE:O	2:B:1116:HEC:HBD1	2.18	0.44
1:D:492:LYS:HD3	2:D:1113:HEC:O1A	2.17	0.44
1:C:342:GLN:NE2	2:C:1109:HEC:O2A	2.49	0.44
1:D:72:ALA:HB1	2:D:1102:HEC:HMD2	2.00	0.44
2:B:1111:HEC:HBB3	2:B:1111:HEC:HMB1	2.00	0.44
1:B:346:MET:CE	1:B:355:THR:OG1	2.66	0.44
1:C:511:LEU:HG	1:C:515:TYR:CE1	2.52	0.44
1:D:161:ARG:NH1	1:D:257:LYS:O	2.46	0.44
1:B:465:LEU:HD13	2:B:1110:HEC:CHA	2.48	0.44
1:C:152:ILE:HG23	2:C:1107:HEC:HMD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1111:HEC:CHA	2:C:1111:HEC:HBA2	2.48	0.43
1:C:349:CYS:HA	2:C:1110:HEC:CHC	2.48	0.43
1:A:121:LEU:CD1	2:A:1102:HEC:HMD3	2.48	0.43
2:D:1108:HEC:HBC1	2:D:1110:HEC:C2C	2.48	0.43
1:B:346:MET:HE1	1:B:355:THR:HB	2.00	0.43
1:C:342:GLN:HG2	1:C:345:SER:HB2	2.00	0.43
1:D:313:HIS:HE1	2:D:1109:HEC:C1D	2.32	0.43
1:D:316:ILE:HD11	2:D:1104:HEC:HAA2	1.99	0.43
1:A:323:HIS:CE1	2:A:1109:HEC:ND	2.86	0.43
1:C:83:CYS:HB2	2:C:1101:HEC:C2C	2.48	0.43
1:C:161:ARG:CG	1:C:161:ARG:NH1	2.79	0.43
2:C:1111:HEC:HMC1	2:C:1111:HEC:HBC3	1.99	0.43
1:C:423:THR:CG2	1:C:424:PHE:H	2.29	0.43
1:C:528:ILE:CG2	1:C:530:LYS:HB2	2.48	0.43
1:A:72:ALA:HB1	2:A:1102:HEC:HMD2	2.00	0.43
2:B:1106:HEC:HBB3	2:B:1106:HEC:HMB1	2.01	0.43
2:D:1108:HEC:HBC1	2:D:1110:HEC:HMC2	1.99	0.43
1:D:308:CYS:SG	2:D:1104:HEC:HBA1	2.58	0.43
1:C:453:VAL:HG22	2:C:1113:HEC:HMC2	2.00	0.43
1:D:211:VAL:HG22	1:D:214:ARG:HB2	1.99	0.43
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.74	0.42
1:C:253:GLN:HA	1:C:256:PHE:CE2	2.54	0.42
1:B:475:THR:O	2:B:1111:HEC:HMD2	2.19	0.42
1:B:214:ARG:HD3	2:B:1105:HEC:HMD3	2.01	0.42
1:C:274:LEU:HD21	1:C:398:LEU:HD22	2.00	0.42
1:C:423:THR:CG2	1:C:424:PHE:N	2.81	0.42
1:D:88:ASP:C	1:D:90:LYS:H	2.22	0.42
2:B:1102:HEC:HMC1	2:B:1102:HEC:CBC	2.48	0.42
1:A:105:GLU:HG2	1:A:109:ILE:HD12	2.01	0.42
1:A:328:THR:HG22	1:A:330:ASP:N	2.34	0.42
1:B:387:GLY:O	1:B:388:PHE:C	2.57	0.42
1:C:334:VAL:HG13	1:C:338:LYS:HD3	2.01	0.42
1:D:122:ALA:HB2	1:D:128:THR:HG21	2.02	0.42
1:B:357:VAL:HG13	1:B:366:HIS:HB3	2.01	0.42
1:D:211:VAL:HG21	1:D:214:ARG:NH2	2.35	0.42
1:D:482:HIS:HE1	2:D:1114:HEC:CHA	2.33	0.42
1:A:483:ASN:HD22	2:A:1114:HEC:C1D	2.33	0.42
1:B:453:VAL:HG22	2:B:1113:HEC:HMC2	2.01	0.42
1:B:161:ARG:HG3	3:B:2113:HOH:O	2.19	0.42
1:C:42:ARG:HE	1:C:65:ARG:HG2	1.84	0.42
1:D:478:GLN:HA	1:D:481:HIS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:GLN:CD	2:B:1114:HEC:HMB2	2.40	0.42
1:A:269:GLN:HG2	2:A:1108:HEC:HMB2	2.02	0.42
1:A:53:ARG:HG2	1:A:53:ARG:H	1.66	0.42
1:C:222:HIS:CD2	2:C:1107:HEC:NC	2.87	0.42
1:C:404:GLU:CD	1:C:404:GLU:H	2.23	0.41
2:D:1101:HEC:HBC3	2:D:1101:HEC:HMC1	2.02	0.41
1:B:226:ILE:HG22	1:B:230:MET:HE2	2.01	0.41
1:C:121:LEU:CD1	2:C:1102:HEC:HMD3	2.50	0.41
1:D:66:HIS:ND1	2:D:1107:HEC:HBB1	2.35	0.41
1:C:229:HIS:CE1	1:C:240:GLY:HA3	2.56	0.41
2:D:1108:HEC:HBC1	2:D:1110:HEC:CMC	2.50	0.41
2:D:1104:HEC:HBC1	2:D:1106:HEC:C2C	2.50	0.41
2:C:1103:HEC:HBB3	2:C:1103:HEC:HMB1	2.02	0.41
1:D:339:ALA:HA	2:D:1109:HEC:CMA	2.51	0.41
1:A:429:ILE:HD12	2:A:1113:HEC:HMB2	1.97	0.41
1:A:291:MET:HG3	2:A:1112:HEC:CHB	2.51	0.41
1:B:313:HIS:HE1	2:B:1109:HEC:ND	2.17	0.41
1:C:345:SER:O	1:C:351:GLY:HA3	2.21	0.41
1:C:342:GLN:HA	1:C:343:PRO:HD3	1.93	0.41
1:A:309:ARG:NH1	2:A:1104:HEC:CGD	2.84	0.41
2:B:1112:HEC:HBC3	2:B:1112:HEC:HMC1	2.01	0.41
1:B:515:TYR:OH	2:B:1113:HEC:O1D	2.31	0.41
1:A:340:MET:HE3	2:A:1112:HEC:HAD2	2.03	0.41
1:C:420:PRO:HG3	3:C:2100:HOH:O	2.21	0.41
1:C:456:LEU:HD22	2:C:1111:HEC:HMC1	2.02	0.41
1:A:429:ILE:HD11	2:A:1113:HEC:CMB	2.41	0.41
1:A:423:THR:HA	1:A:473:LYS:O	2.20	0.41
1:B:372:THR:HG21	1:B:374:SER:HB3	2.01	0.41
1:C:279:PRO:HB2	1:C:283:ALA:CB	2.50	0.41
1:C:389:ASP:CG	1:C:390:ALA:N	2.74	0.41
1:D:95:PHE:CD1	2:D:1101:HEC:HMD3	2.56	0.41
1:A:313:HIS:H	1:A:313:HIS:CD2	2.39	0.40
1:B:159:HIS:O	1:B:163:VAL:HG23	2.21	0.40
1:C:201:SER:O	2:C:1105:HEC:HMC3	2.21	0.40
1:D:313:HIS:CE1	2:D:1109:HEC:C1D	3.04	0.40
1:D:97:ARG:NH2	1:D:110:TYR:OH	2.52	0.40
1:D:326:ASN:HA	1:D:335:GLN:HE21	1.85	0.40
1:B:364:GLY:O	1:B:525:ARG:NH1	2.54	0.40
1:A:177:ASN:O	2:A:1104:HEC:HMC3	2.21	0.40
1:A:434:VAL:O	1:A:434:VAL:HG22	2.21	0.40
1:B:346:MET:CE	1:B:355:THR:CB	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1106:HEC:HMB1	2:C:1106:HEC:HBB3	2.04	0.40
2:D:1110:HEC:CBC	2:D:1110:HEC:HMC1	2.48	0.40
1:B:197:ASN:HA	1:B:267:ARG:HG2	2.02	0.40
1:C:299:LYS:NZ	3:C:2075:HOH:O	2.55	0.40
1:D:312:HIS:HB3	1:D:315:ARG:O	2.21	0.40
1:A:121:LEU:HD13	2:A:1102:HEC:HMD3	2.02	0.40
1:A:287:MET:SD	1:A:326:ASN:HA	2.62	0.40
1:A:528:ILE:HG22	1:A:530:LYS:HB2	2.04	0.40
1:B:71:THR:HG22	3:B:2059:HOH:O	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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	497/514 (97%)	463 (93%)	25 (5%)	9 (2%)	10	17
1	B	495/514 (96%)	460 (93%)	28 (6%)	7 (1%)	13	23
1	C	497/514 (97%)	468 (94%)	24 (5%)	5 (1%)	18	32
1	D	484/514 (94%)	451 (93%)	26 (5%)	7 (1%)	13	23
All	All	1973/2056 (96%)	1842 (93%)	103 (5%)	28 (1%)	13	23

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ASP
1	A	218	ASP
1	A	390	ALA
1	A	395	ALA
1	B	132	ASP
1	B	530	LYS

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Mol	Chain	Res	Type
1	C	132	ASP
1	C	218	ASP
1	D	530	LYS
1	A	530	LYS
1	B	212	ASP
1	B	317	ASP
1	C	507	ASP
1	D	132	ASP
1	D	495	SER
1	A	391	LYS
1	B	155	ASP
1	B	437	SER
1	C	530	LYS
1	D	317	ASP
1	D	507	ASP
1	A	145	ALA
1	A	437	SER
1	A	461	GLY
1	B	449	HIS
1	C	393	VAL
1	D	418	PRO
1	D	309	ARG

### 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	405/414 (98%)	363 (90%)	42 (10%)	8	15
1	B	403/414 (97%)	368 (91%)	35 (9%)	12	23
1	C	404/414 (98%)	374 (93%)	30 (7%)	16	30
1	D	400/414 (97%)	359 (90%)	41 (10%)	8	16
All	All	1612/1656 (97%)	1464 (91%)	148 (9%)	11	20

All (148) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	53	ARG
1	A	56	LYS
1	A	71	THR
1	A	90	LYS
1	A	97	ARG
1	A	123	LYS
1	A	127	LYS
1	A	132	ASP
1	A	150	LYS
1	A	151	GLU
1	A	155	ASP
1	A	158	LEU
1	A	169	LYS
1	A	184	VAL
1	A	255	LYS
1	A	257	LYS
1	A	267	ARG
1	A	269	GLN
1	A	288	LYS
1	A	299	LYS
1	A	306	ASN
1	A	356	ARG
1	A	361	THR
1	A	374	SER
1	A	388	PHE
1	A	391	LYS
1	A	419	GLN
1	A	421	LYS
1	A	426	LEU
1	A	434	VAL
1	A	441	GLU
1	A	450	ARG
1	A	464	LYS
1	A	482	HIS
1	A	484	SER
1	A	489	THR
1	A	499	LYS
1	A	505	ARG
1	A	508	ARG
1	A	511	LEU
1	A	534	THR
1	A	543	ARG
1	B	56	LYS

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Mol	Chain	Res	Type
1	B	71	THR
1	B	127	LYS
1	B	132	ASP
1	B	142	LYS
1	B	144	SER
1	B	151	GLU
1	B	155	ASP
1	B	156	LYS
1	B	161	ARG
1	B	187	GLU
1	B	191	LYS
1	B	193	VAL
1	B	209	LYS
1	B	261	GLU
1	B	267	ARG
1	B	269	GLN
1	B	325	VAL
1	B	326	ASN
1	B	345	SER
1	B	369	ILE
1	B	370	LYS
1	B	389	ASP
1	B	391	LYS
1	B	392	GLN
1	B	421	LYS
1	B	437	SER
1	B	445	SER
1	B	451	LYS
1	B	482	HIS
1	B	499	LYS
1	B	505	ARG
1	B	507	ASP
1	B	508	ARG
1	B	512	LYS
1	C	88	ASP
1	C	126	LYS
1	C	132	ASP
1	C	147	SER
1	C	151	GLU
1	C	161	ARG
1	C	171	VAL
1	C	187	GLU

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Mol	Chain	Res	Type
1	C	189	SER
1	C	190	LYS
1	C	198	LYS
1	C	213	LYS
1	C	257	LYS
1	C	267	ARG
1	C	269	GLN
1	C	281	LYS
1	C	285	ARG
1	C	342	GLN
1	C	373	LYS
1	C	389	ASP
1	C	407	SER
1	C	408	GLN
1	C	421	LYS
1	C	437	SER
1	C	441	GLU
1	C	482	HIS
1	C	512	LYS
1	C	529	GLU
1	C	540	HIS
1	C	543	ARG
1	D	41	LYS
1	D	42	ARG
1	D	53	ARG
1	D	56	LYS
1	D	71	THR
1	D	80	CYS
1	D	90	LYS
1	D	127	LYS
1	D	132	ASP
1	D	151	GLU
1	D	158	LEU
1	D	166	LYS
1	D	198	LYS
1	D	236	LYS
1	D	257	LYS
1	D	262	VAL
1	D	269	GLN
1	D	281	LYS
1	D	287	MET
1	D	288	LYS

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Mol	Chain	Res	Type
1	D	292	LYS
1	D	324	THR
1	D	332	LYS
1	D	338	LYS
1	D	342	GLN
1	D	355	THR
1	D	356	ARG
1	D	357	VAL
1	D	370	LYS
1	D	398	LEU
1	D	402	LYS
1	D	404	GLU
1	D	406	ARG
1	D	421	LYS
1	D	471	ILE
1	D	482	HIS
1	D	484	SER
1	D	488	LEU
1	D	492	LYS
1	D	511	LEU
1	D	530	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	359	GLN
1	A	408	GLN
1	A	483	ASN
1	B	197	ASN
1	B	326	ASN
1	B	335	GLN
1	B	342	GLN
1	B	358	GLN
1	B	377	GLN
1	B	392	GLN
1	B	483	ASN
1	C	68	GLN
1	C	358	GLN
1	C	377	GLN
1	C	419	GLN
1	C	483	ASN

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Mol	Chain	Res	Type
1	D	68	GLN
1	D	335	GLN
1	D	342	GLN
1	D	354	ASN
1	D	358	GLN
1	D	377	GLN
1	D	443	GLN
1	D	483	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

64 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	1101	1	28,50,50	2.31	9 (32%)	16,82,82	1.51	3 (18%)
2	HEC	A	1102	1	28,50,50	2.35	6 (21%)	16,82,82	1.64	4 (25%)
2	HEC	A	1103	1	28,50,50	2.47	8 (28%)	16,82,82	2.24	4 (25%)
2	HEC	A	1104	1	28,50,50	2.46	6 (21%)	16,82,82	1.57	1 (6%)
2	HEC	A	1105	1	28,50,50	2.58	6 (21%)	16,82,82	1.64	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEC	A	1106	1	28,50,50	2.57	7 (25%)	16,82,82	1.61	4 (25%)
2	HEC	A	1107	1	28,50,50	2.30	7 (25%)	16,82,82	2.26	6 (37%)
2	HEC	A	1108	1	28,50,50	2.47	6 (21%)	16,82,82	1.98	7 (43%)
2	HEC	A	1109	1	28,50,50	2.49	6 (21%)	16,82,82	1.67	3 (18%)
2	HEC	A	1110	1	28,50,50	2.56	6 (21%)	16,82,82	1.68	3 (18%)
2	HEC	A	1111	1	28,50,50	2.60	6 (21%)	16,82,82	1.45	2 (12%)
2	HEC	A	1112	1	28,50,50	2.46	5 (17%)	16,82,82	1.46	4 (25%)
2	HEC	A	1113	1	28,50,50	2.46	5 (17%)	16,82,82	1.57	3 (18%)
2	HEC	A	1114	1	28,50,50	2.51	8 (28%)	16,82,82	1.34	1 (6%)
2	HEC	A	1115	1	28,50,50	2.35	6 (21%)	16,82,82	2.01	5 (31%)
2	HEC	A	1116	1	28,50,50	2.37	5 (17%)	16,82,82	2.03	4 (25%)
2	HEC	B	1101	1	28,50,50	2.33	8 (28%)	16,82,82	1.59	3 (18%)
2	HEC	B	1102	1	28,50,50	2.46	6 (21%)	16,82,82	1.70	5 (31%)
2	HEC	B	1103	1	28,50,50	2.46	8 (28%)	16,82,82	1.89	4 (25%)
2	HEC	B	1104	1	28,50,50	2.29	8 (28%)	16,82,82	1.90	3 (18%)
2	HEC	B	1105	1	28,50,50	2.59	9 (32%)	16,82,82	1.42	2 (12%)
2	HEC	B	1106	1	28,50,50	2.39	6 (21%)	16,82,82	1.92	5 (31%)
2	HEC	B	1107	1	28,50,50	2.43	5 (17%)	16,82,82	1.82	3 (18%)
2	HEC	B	1108	1	28,50,50	2.49	8 (28%)	16,82,82	1.52	3 (18%)
2	HEC	B	1109	1	28,50,50	2.66	10 (35%)	16,82,82	1.27	1 (6%)
2	HEC	B	1110	1	28,50,50	2.33	6 (21%)	16,82,82	2.12	5 (31%)
2	HEC	B	1111	1	28,50,50	2.66	5 (17%)	16,82,82	1.51	4 (25%)
2	HEC	B	1112	1	28,50,50	2.46	6 (21%)	16,82,82	1.82	5 (31%)
2	HEC	B	1113	1	28,50,50	2.66	7 (25%)	16,82,82	2.03	3 (18%)
2	HEC	B	1114	1	28,50,50	2.50	9 (32%)	16,82,82	1.52	3 (18%)
2	HEC	B	1115	1	28,50,50	2.42	6 (21%)	16,82,82	1.65	4 (25%)
2	HEC	B	1116	1	28,50,50	2.56	6 (21%)	16,82,82	1.92	4 (25%)
2	HEC	C	1101	1	28,50,50	2.30	5 (17%)	16,82,82	1.51	3 (18%)
2	HEC	C	1102	1	28,50,50	2.55	7 (25%)	16,82,82	1.77	5 (31%)
2	HEC	C	1103	1	28,50,50	2.45	8 (28%)	16,82,82	2.11	4 (25%)
2	HEC	C	1104	1	28,50,50	2.36	6 (21%)	16,82,82	1.78	4 (25%)
2	HEC	C	1105	1	28,50,50	2.58	7 (25%)	16,82,82	1.56	4 (25%)
2	HEC	C	1106	1	28,50,50	2.43	8 (28%)	16,82,82	2.01	5 (31%)
2	HEC	C	1107	1	28,50,50	2.31	6 (21%)	16,82,82	1.90	5 (31%)
2	HEC	C	1108	1	28,50,50	2.43	5 (17%)	16,82,82	1.69	5 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEC	C	1109	1	28,50,50	2.49	9 (32%)	16,82,82	1.76	3 (18%)
2	HEC	C	1110	1	28,50,50	2.35	5 (17%)	16,82,82	1.80	5 (31%)
2	HEC	C	1111	1	28,50,50	2.50	7 (25%)	16,82,82	1.53	3 (18%)
2	HEC	C	1112	1	28,50,50	2.60	8 (28%)	16,82,82	1.30	3 (18%)
2	HEC	C	1113	1	28,50,50	2.60	5 (17%)	16,82,82	2.00	6 (37%)
2	HEC	C	1114	1	28,50,50	2.59	8 (28%)	16,82,82	1.53	3 (18%)
2	HEC	C	1115	1	28,50,50	2.59	7 (25%)	16,82,82	2.04	6 (37%)
2	HEC	C	1116	1	28,50,50	2.44	6 (21%)	16,82,82	2.17	5 (31%)
2	HEC	D	1101	1	28,50,50	2.42	7 (25%)	16,82,82	1.40	2 (12%)
2	HEC	D	1102	1	28,50,50	2.40	7 (25%)	16,82,82	1.82	5 (31%)
2	HEC	D	1103	1	28,50,50	2.54	7 (25%)	16,82,82	1.97	5 (31%)
2	HEC	D	1104	1	28,50,50	2.39	7 (25%)	16,82,82	1.99	6 (37%)
2	HEC	D	1105	1	28,50,50	2.39	7 (25%)	16,82,82	1.80	4 (25%)
2	HEC	D	1106	1	28,50,50	2.40	6 (21%)	16,82,82	1.67	3 (18%)
2	HEC	D	1107	1	28,50,50	2.42	5 (17%)	16,82,82	1.63	5 (31%)
2	HEC	D	1108	1	28,50,50	2.57	5 (17%)	16,82,82	1.77	3 (18%)
2	HEC	D	1109	1	28,50,50	2.54	8 (28%)	16,82,82	1.38	3 (18%)
2	HEC	D	1110	1	28,50,50	2.46	7 (25%)	16,82,82	1.65	5 (31%)
2	HEC	D	1111	1	28,50,50	2.36	7 (25%)	16,82,82	1.68	4 (25%)
2	HEC	D	1112	1	28,50,50	2.45	6 (21%)	16,82,82	1.49	3 (18%)
2	HEC	D	1113	1	28,50,50	2.56	6 (21%)	16,82,82	1.57	4 (25%)
2	HEC	D	1114	1	28,50,50	2.47	6 (21%)	16,82,82	1.58	3 (18%)
2	HEC	D	1115	1	28,50,50	2.39	9 (32%)	16,82,82	1.65	4 (25%)
2	HEC	D	1116	1	28,50,50	2.67	7 (25%)	16,82,82	1.95	3 (18%)

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	1101	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1102	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1103	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1104	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1105	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1106	1	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	1107	1	-	1/6/54/54	0/0/8/8
2	HEC	A	1108	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1109	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1110	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1111	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1112	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1113	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1114	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1115	1	-	0/6/54/54	0/0/8/8
2	HEC	A	1116	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1101	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1102	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1103	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1104	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1105	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1106	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1107	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1108	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1109	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1110	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1111	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1112	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1113	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1114	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1115	1	-	0/6/54/54	0/0/8/8
2	HEC	B	1116	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1101	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1102	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1103	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1104	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1105	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1106	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1107	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1108	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1109	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1110	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1111	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1112	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1113	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1114	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1115	1	-	0/6/54/54	0/0/8/8
2	HEC	C	1116	1	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	D	1101	1	-	0/6/54/54	0/0/8/8
2	HEC	D	1102	1	-	0/6/54/54	0/0/8/8
2	HEC	D	1103	1	-	0/6/54/54	0/0/8/8
2	HEC	D	1104	1	-	0/6/54/54	0/0/8/8
2	HEC	D	1105	1	-	0/6/54/54	0/0/8/8
2	HEC	D	1106	1	-	0/6/54/54	0/0/8/8
2	HEC	D	1107	1	-	0/6/54/54	0/0/8/8
2	HEC	D	1108	1	-	0/6/54/54	0/0/8/8
2	HEC	D	1109	1	-	0/6/54/54	0/0/8/8
2	HEC	D	1110	1	-	0/6/54/54	0/0/8/8
2	HEC	D	1111	1	-	0/6/54/54	0/0/8/8
2	HEC	D	1112	1	-	0/6/54/54	0/0/8/8
2	HEC	D	1113	1	-	0/6/54/54	0/0/8/8
2	HEC	D	1114	1	-	0/6/54/54	0/0/8/8
2	HEC	D	1115	1	-	0/6/54/54	0/0/8/8
2	HEC	D	1116	1	-	0/6/54/54	0/0/8/8

All (429) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1112	HEC	C3B-C2B	-7.96	1.32	1.40
2	D	1108	HEC	C3B-C2B	-7.85	1.32	1.40
2	D	1113	HEC	C3C-C2C	-7.76	1.32	1.40
2	C	1113	HEC	C3C-C2C	-7.70	1.32	1.40
2	B	1109	HEC	C3C-C2C	-7.54	1.32	1.40
2	D	1116	HEC	C3B-C2B	-7.51	1.32	1.40
2	B	1111	HEC	C3B-C2B	-7.42	1.32	1.40
2	A	1103	HEC	C3B-C2B	-7.35	1.33	1.40
2	B	1113	HEC	C3B-C2B	-7.33	1.33	1.40
2	A	1110	HEC	C3B-C2B	-7.25	1.33	1.40
2	D	1116	HEC	C3C-C2C	-7.14	1.33	1.40
2	A	1106	HEC	C3C-C2C	-7.11	1.33	1.40
2	A	1104	HEC	C3B-C2B	-7.10	1.33	1.40
2	A	1105	HEC	C3C-C2C	-7.04	1.33	1.40
2	C	1103	HEC	C3B-C2B	-7.02	1.33	1.40
2	C	1115	HEC	C3B-C2B	-7.00	1.33	1.40
2	B	1103	HEC	C3B-C2B	-6.99	1.33	1.40
2	C	1105	HEC	C3B-C2B	-6.93	1.33	1.40
2	C	1102	HEC	C3C-C2C	-6.88	1.33	1.40
2	C	1114	HEC	C3B-C2B	-6.84	1.33	1.40
2	A	1112	HEC	C3B-C2B	-6.81	1.33	1.40
2	B	1105	HEC	C3B-C2B	-6.80	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1112	HEC	C3B-C2B	-6.80	1.33	1.40
2	B	1107	HEC	C3C-C2C	-6.77	1.33	1.40
2	B	1113	HEC	C3C-C2C	-6.75	1.33	1.40
2	C	1111	HEC	C3C-C2C	-6.70	1.33	1.40
2	C	1105	HEC	C3C-C2C	-6.69	1.33	1.40
2	A	1111	HEC	C3C-C2C	-6.68	1.33	1.40
2	B	1102	HEC	C3B-C2B	-6.67	1.33	1.40
2	A	1111	HEC	C3B-C2B	-6.65	1.33	1.40
2	B	1116	HEC	C3B-C2B	-6.57	1.33	1.40
2	D	1112	HEC	C3B-C2B	-6.55	1.33	1.40
2	B	1108	HEC	C3B-C2B	-6.50	1.33	1.40
2	D	1113	HEC	C3B-C2B	-6.50	1.33	1.40
2	D	1108	HEC	C3C-C2C	-6.49	1.33	1.40
2	D	1115	HEC	C3B-C2B	-6.48	1.33	1.40
2	C	1115	HEC	C3C-C2C	-6.47	1.33	1.40
2	B	1111	HEC	C3C-C2C	-6.44	1.34	1.40
2	D	1103	HEC	C3B-C2B	-6.42	1.34	1.40
2	D	1103	HEC	C3C-C2C	-6.41	1.34	1.40
2	B	1116	HEC	C3C-C2C	-6.40	1.34	1.40
2	A	1114	HEC	C3B-C2B	-6.39	1.34	1.40
2	C	1113	HEC	C3B-C2B	-6.36	1.34	1.40
2	C	1106	HEC	C3C-C2C	-6.35	1.34	1.40
2	D	1109	HEC	C3C-C2C	-6.33	1.34	1.40
2	D	1101	HEC	C3B-C2B	-6.33	1.34	1.40
2	A	1113	HEC	C3B-C2B	-6.32	1.34	1.40
2	A	1105	HEC	C3B-C2B	-6.29	1.34	1.40
2	A	1113	HEC	C3C-C2C	-6.28	1.34	1.40
2	A	1106	HEC	C3B-C2B	-6.27	1.34	1.40
2	C	1109	HEC	C3B-C2B	-6.26	1.34	1.40
2	C	1110	HEC	C3B-C2B	-6.25	1.34	1.40
2	B	1108	HEC	C3C-C2C	-6.25	1.34	1.40
2	C	1102	HEC	C3B-C2B	-6.24	1.34	1.40
2	C	1116	HEC	C3C-C2C	-6.19	1.34	1.40
2	C	1104	HEC	C3C-C2C	-6.18	1.34	1.40
2	B	1115	HEC	C3B-C2B	-6.18	1.34	1.40
2	C	1114	HEC	C3C-C2C	-6.16	1.34	1.40
2	C	1108	HEC	C3C-C2C	-6.16	1.34	1.40
2	A	1115	HEC	C3B-C2B	-6.15	1.34	1.40
2	B	1109	HEC	C3B-C2B	-6.13	1.34	1.40
2	C	1108	HEC	C3B-C2B	-6.12	1.34	1.40
2	A	1109	HEC	C3C-C2C	-6.10	1.34	1.40
2	B	1107	HEC	C3B-C2B	-6.07	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1106	HEC	C3C-C2C	-6.06	1.34	1.40
2	D	1102	HEC	C3B-C2B	-6.03	1.34	1.40
2	D	1109	HEC	C3B-C2B	-6.01	1.34	1.40
2	A	1108	HEC	C3C-C2C	-6.00	1.34	1.40
2	D	1107	HEC	C3C-C2C	-5.99	1.34	1.40
2	A	1110	HEC	C3C-C2C	-5.98	1.34	1.40
2	C	1112	HEC	C3C-C2C	-5.97	1.34	1.40
2	A	1109	HEC	C3B-C2B	-5.96	1.34	1.40
2	C	1109	HEC	C3C-C2C	-5.94	1.34	1.40
2	D	1104	HEC	C3B-C2B	-5.93	1.34	1.40
2	B	1101	HEC	C3B-C2B	-5.91	1.34	1.40
2	C	1107	HEC	C3B-C2B	-5.91	1.34	1.40
2	A	1107	HEC	C3C-C2C	-5.86	1.34	1.40
2	A	1112	HEC	C3C-C2C	-5.86	1.34	1.40
2	D	1105	HEC	C3B-C2B	-5.85	1.34	1.40
2	B	1114	HEC	C3B-C2B	-5.82	1.34	1.40
2	C	1107	HEC	C3C-C2C	-5.79	1.34	1.40
2	C	1116	HEC	C3B-C2B	-5.78	1.34	1.40
2	A	1116	HEC	C3B-C2B	-5.77	1.34	1.40
2	A	1102	HEC	C3C-C2C	-5.76	1.34	1.40
2	A	1104	HEC	C3C-C2C	-5.74	1.34	1.40
2	B	1105	HEC	C3C-C2C	-5.73	1.34	1.40
2	B	1106	HEC	C3B-C2B	-5.73	1.34	1.40
2	C	1101	HEC	C3B-C2B	-5.72	1.34	1.40
2	D	1110	HEC	C3B-C2B	-5.71	1.34	1.40
2	A	1116	HEC	C3C-C2C	-5.70	1.34	1.40
2	D	1107	HEC	C3B-C2B	-5.69	1.34	1.40
2	A	1103	HEC	C3C-C2C	-5.67	1.34	1.40
2	B	1115	HEC	C3C-C2C	-5.67	1.34	1.40
2	D	1114	HEC	C3B-C2B	-5.65	1.34	1.40
2	D	1112	HEC	C3C-C2C	-5.65	1.34	1.40
2	A	1108	HEC	C3B-C2B	-5.64	1.34	1.40
2	B	1104	HEC	C3C-C2C	-5.61	1.34	1.40
2	C	1111	HEC	C3B-C2B	-5.59	1.34	1.40
2	D	1114	HEC	C3C-C2C	-5.54	1.34	1.40
2	C	1103	HEC	C3C-C2C	-5.50	1.34	1.40
2	D	1111	HEC	C3B-C2B	-5.49	1.35	1.40
2	B	1110	HEC	C3C-C2C	-5.47	1.35	1.40
2	B	1106	HEC	C3C-C2C	-5.46	1.35	1.40
2	B	1102	HEC	C3C-C2C	-5.45	1.35	1.40
2	B	1112	HEC	C3C-C2C	-5.43	1.35	1.40
2	A	1102	HEC	C3B-C2B	-5.43	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1111	HEC	C3C-C2C	-5.40	1.35	1.40
2	B	1114	HEC	C3C-C2C	-5.38	1.35	1.40
2	A	1115	HEC	C3C-C2C	-5.37	1.35	1.40
2	D	1106	HEC	C3B-C2B	-5.30	1.35	1.40
2	C	1106	HEC	C3B-C2B	-5.25	1.35	1.40
2	C	1110	HEC	C3C-C2C	-5.21	1.35	1.40
2	C	1101	HEC	C3C-C2C	-5.15	1.35	1.40
2	D	1104	HEC	C3C-C2C	-5.13	1.35	1.40
2	A	1101	HEC	C3C-C2C	-5.06	1.35	1.40
2	B	1110	HEC	C3B-C2B	-5.05	1.35	1.40
2	A	1107	HEC	C3B-C2B	-5.01	1.35	1.40
2	A	1101	HEC	C3B-C2B	-4.99	1.35	1.40
2	A	1114	HEC	C3C-C2C	-4.98	1.35	1.40
2	D	1115	HEC	C3C-C2C	-4.97	1.35	1.40
2	D	1110	HEC	C3C-C2C	-4.80	1.35	1.40
2	B	1101	HEC	C3C-C2C	-4.75	1.35	1.40
2	B	1104	HEC	C3B-C2B	-4.74	1.35	1.40
2	D	1102	HEC	C3C-C2C	-4.72	1.35	1.40
2	D	1105	HEC	C3C-C2C	-4.66	1.35	1.40
2	B	1103	HEC	C3C-C2C	-4.65	1.35	1.40
2	D	1101	HEC	C3C-C2C	-4.59	1.35	1.40
2	C	1104	HEC	C3B-C2B	-4.48	1.36	1.40
2	A	1106	HEC	CBC-CAC	-4.12	1.33	1.49
2	A	1105	HEC	CBC-CAC	-4.10	1.33	1.49
2	B	1112	HEC	CBC-CAC	-4.08	1.33	1.49
2	B	1116	HEC	CBC-CAC	-4.07	1.33	1.49
2	D	1107	HEC	CBB-CAB	-4.05	1.33	1.49
2	C	1116	HEC	CBC-CAC	-4.05	1.33	1.49
2	C	1110	HEC	CBB-CAB	-4.04	1.33	1.49
2	C	1113	HEC	CBC-CAC	-4.03	1.33	1.49
2	B	1111	HEC	CBB-CAB	-4.02	1.33	1.49
2	B	1108	HEC	CBC-CAC	-4.00	1.33	1.49
2	D	1114	HEC	CBB-CAB	-3.99	1.33	1.49
2	B	1116	HEC	CBB-CAB	-3.97	1.33	1.49
2	A	1114	HEC	CBB-CAB	-3.97	1.33	1.49
2	B	1106	HEC	CBB-CAB	-3.97	1.33	1.49
2	C	1109	HEC	CBC-CAC	-3.96	1.33	1.49
2	A	1115	HEC	CBC-CAC	-3.95	1.33	1.49
2	C	1116	HEC	CBB-CAB	-3.94	1.33	1.49
2	A	1111	HEC	CBC-CAC	-3.93	1.33	1.49
2	A	1112	HEC	CBB-CAB	-3.93	1.33	1.49
2	B	1110	HEC	CBB-CAB	-3.92	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1108	HEC	CBC-CAC	-3.92	1.33	1.49
2	D	1115	HEC	CBB-CAB	-3.91	1.33	1.49
2	A	1116	HEC	CBC-CAC	-3.91	1.33	1.49
2	C	1108	HEC	CBB-CAB	-3.91	1.34	1.49
2	B	1115	HEC	CBB-CAB	-3.90	1.34	1.49
2	D	1116	HEC	CBC-CAC	-3.89	1.34	1.49
2	A	1109	HEC	CBC-CAC	-3.89	1.34	1.49
2	C	1114	HEC	CBB-CAB	-3.88	1.34	1.49
2	D	1108	HEC	CBC-CAC	-3.88	1.34	1.49
2	C	1104	HEC	CBC-CAC	-3.87	1.34	1.49
2	D	1111	HEC	CBB-CAB	-3.87	1.34	1.49
2	B	1113	HEC	CBB-CAB	-3.87	1.34	1.49
2	B	1111	HEC	CBC-CAC	-3.87	1.34	1.49
2	D	1104	HEC	CBB-CAB	-3.87	1.34	1.49
2	C	1111	HEC	CBB-CAB	-3.87	1.34	1.49
2	B	1105	HEC	CBB-CAB	-3.86	1.34	1.49
2	C	1112	HEC	CBC-CAC	-3.85	1.34	1.49
2	A	1114	HEC	CBC-CAC	-3.84	1.34	1.49
2	B	1103	HEC	CBC-CAC	-3.84	1.34	1.49
2	B	1109	HEC	CBC-CAC	-3.83	1.34	1.49
2	D	1101	HEC	CBC-CAC	-3.83	1.34	1.49
2	D	1105	HEC	CBB-CAB	-3.83	1.34	1.49
2	B	1115	HEC	CBC-CAC	-3.82	1.34	1.49
2	B	1114	HEC	CBB-CAB	-3.82	1.34	1.49
2	D	1103	HEC	CBB-CAB	-3.81	1.34	1.49
2	A	1113	HEC	CBC-CAC	-3.81	1.34	1.49
2	D	1115	HEC	CBC-CAC	-3.81	1.34	1.49
2	D	1114	HEC	CBC-CAC	-3.80	1.34	1.49
2	D	1108	HEC	CBB-CAB	-3.79	1.34	1.49
2	B	1112	HEC	CBB-CAB	-3.79	1.34	1.49
2	C	1103	HEC	CBC-CAC	-3.78	1.34	1.49
2	B	1105	HEC	CBC-CAC	-3.78	1.34	1.49
2	C	1115	HEC	CBC-CAC	-3.77	1.34	1.49
2	C	1112	HEC	CBB-CAB	-3.76	1.34	1.49
2	D	1110	HEC	CBB-CAB	-3.76	1.34	1.49
2	D	1113	HEC	CBC-CAC	-3.76	1.34	1.49
2	A	1109	HEC	CBB-CAB	-3.75	1.34	1.49
2	D	1112	HEC	CBB-CAB	-3.75	1.34	1.49
2	D	1103	HEC	CBC-CAC	-3.74	1.34	1.49
2	D	1113	HEC	CBB-CAB	-3.74	1.34	1.49
2	D	1104	HEC	CBC-CAC	-3.74	1.34	1.49
2	D	1109	HEC	CBC-CAC	-3.73	1.34	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1116	HEC	CBB-CAB	-3.72	1.34	1.49
2	A	1102	HEC	CBC-CAC	-3.72	1.34	1.49
2	B	1101	HEC	CBC-CAC	-3.72	1.34	1.49
2	B	1109	HEC	CBB-CAB	-3.72	1.34	1.49
2	D	1106	HEC	CBC-CAC	-3.72	1.34	1.49
2	C	1105	HEC	CBC-CAC	-3.72	1.34	1.49
2	C	1115	HEC	CBB-CAB	-3.71	1.34	1.49
2	B	1106	HEC	CBC-CAC	-3.71	1.34	1.49
2	A	1115	HEC	CBB-CAB	-3.71	1.34	1.49
2	D	1107	HEC	CBC-CAC	-3.71	1.34	1.49
2	C	1107	HEC	CBC-CAC	-3.70	1.34	1.49
2	A	1108	HEC	CBB-CAB	-3.70	1.34	1.49
2	C	1105	HEC	CBB-CAB	-3.70	1.34	1.49
2	A	1106	HEC	CBB-CAB	-3.68	1.34	1.49
2	B	1108	HEC	CBB-CAB	-3.68	1.34	1.49
2	B	1103	HEC	CBB-CAB	-3.67	1.34	1.49
2	A	1104	HEC	CBC-CAC	-3.66	1.34	1.49
2	B	1107	HEC	CBC-CAC	-3.66	1.35	1.49
2	A	1107	HEC	CBC-CAC	-3.65	1.35	1.49
2	A	1110	HEC	CBC-CAC	-3.65	1.35	1.49
2	D	1116	HEC	CBB-CAB	-3.65	1.35	1.49
2	C	1108	HEC	CBC-CAC	-3.65	1.35	1.49
2	A	1112	HEC	CBC-CAC	-3.65	1.35	1.49
2	A	1110	HEC	CBB-CAB	-3.65	1.35	1.49
2	C	1104	HEC	CBB-CAB	-3.65	1.35	1.49
2	D	1102	HEC	CBC-CAC	-3.64	1.35	1.49
2	A	1104	HEC	CBB-CAB	-3.64	1.35	1.49
2	A	1111	HEC	CBB-CAB	-3.63	1.35	1.49
2	B	1114	HEC	CBC-CAC	-3.63	1.35	1.49
2	C	1102	HEC	CBB-CAB	-3.63	1.35	1.49
2	B	1104	HEC	CBC-CAC	-3.63	1.35	1.49
2	C	1106	HEC	CBC-CAC	-3.62	1.35	1.49
2	A	1105	HEC	CBB-CAB	-3.62	1.35	1.49
2	C	1106	HEC	CBB-CAB	-3.61	1.35	1.49
2	B	1107	HEC	CBB-CAB	-3.61	1.35	1.49
2	D	1109	HEC	CBB-CAB	-3.61	1.35	1.49
2	C	1113	HEC	CBB-CAB	-3.60	1.35	1.49
2	D	1112	HEC	CBC-CAC	-3.58	1.35	1.49
2	A	1101	HEC	CBB-CAB	-3.58	1.35	1.49
2	D	1110	HEC	CBC-CAC	-3.57	1.35	1.49
2	B	1113	HEC	CBC-CAC	-3.57	1.35	1.49
2	C	1110	HEC	CBC-CAC	-3.56	1.35	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1103	HEC	CBC-CAC	-3.56	1.35	1.49
2	B	1102	HEC	CBC-CAC	-3.56	1.35	1.49
2	B	1101	HEC	CBB-CAB	-3.55	1.35	1.49
2	D	1106	HEC	CBB-CAB	-3.53	1.35	1.49
2	A	1107	HEC	CBB-CAB	-3.53	1.35	1.49
2	C	1114	HEC	CBC-CAC	-3.52	1.35	1.49
2	D	1101	HEC	CBB-CAB	-3.52	1.35	1.49
2	D	1105	HEC	CBC-CAC	-3.51	1.35	1.49
2	C	1102	HEC	CBC-CAC	-3.50	1.35	1.49
2	A	1113	HEC	CBB-CAB	-3.50	1.35	1.49
2	C	1103	HEC	CBB-CAB	-3.48	1.35	1.49
2	D	1102	HEC	CBB-CAB	-3.48	1.35	1.49
2	C	1109	HEC	CBB-CAB	-3.48	1.35	1.49
2	C	1101	HEC	CBB-CAB	-3.48	1.35	1.49
2	A	1101	HEC	CBC-CAC	-3.46	1.35	1.49
2	B	1104	HEC	CBB-CAB	-3.46	1.35	1.49
2	B	1110	HEC	CBC-CAC	-3.46	1.35	1.49
2	C	1111	HEC	CBC-CAC	-3.44	1.35	1.49
2	A	1102	HEC	CBB-CAB	-3.42	1.35	1.49
2	A	1103	HEC	CBB-CAB	-3.42	1.35	1.49
2	B	1102	HEC	CBB-CAB	-3.42	1.35	1.49
2	C	1101	HEC	CBC-CAC	-3.40	1.36	1.49
2	D	1111	HEC	CBC-CAC	-3.38	1.36	1.49
2	C	1107	HEC	CBB-CAB	-3.30	1.36	1.49
2	A	1101	HEC	CAA-C2A	2.00	1.56	1.52
2	D	1103	HEC	CAD-C3D	2.00	1.55	1.52
2	B	1104	HEC	CAA-C2A	2.00	1.56	1.52
2	C	1103	HEC	CMB-C2B	2.00	1.55	1.51
2	D	1115	HEC	CMB-C2B	2.01	1.55	1.51
2	D	1113	HEC	CAA-C2A	2.01	1.56	1.52
2	C	1105	HEC	CAD-C3D	2.01	1.55	1.52
2	D	1111	HEC	CMB-C2B	2.02	1.55	1.51
2	C	1107	HEC	C4A-NA	2.02	1.39	1.36
2	B	1108	HEC	C4D-ND	2.03	1.40	1.36
2	B	1101	HEC	CMC-C2C	2.03	1.55	1.51
2	D	1116	HEC	C4A-NA	2.03	1.39	1.36
2	C	1116	HEC	CMC-C2C	2.03	1.55	1.51
2	C	1115	HEC	CMB-C2B	2.03	1.55	1.51
2	D	1115	HEC	CMD-C2D	2.03	1.55	1.51
2	C	1112	HEC	CAA-C2A	2.05	1.56	1.52
2	D	1104	HEC	C4A-NA	2.05	1.39	1.36
2	D	1114	HEC	C4D-ND	2.05	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1104	HEC	C4B-NB	2.05	1.39	1.36
2	A	1103	HEC	CMB-C2B	2.06	1.56	1.51
2	C	1111	HEC	CAD-C3D	2.06	1.55	1.52
2	B	1113	HEC	C4B-NB	2.06	1.39	1.36
2	C	1109	HEC	C4B-NB	2.07	1.39	1.36
2	D	1105	HEC	C4C-NC	2.07	1.39	1.36
2	D	1115	HEC	CAA-C2A	2.07	1.56	1.52
2	C	1115	HEC	CMA-C3A	2.08	1.56	1.51
2	B	1102	HEC	CAD-C3D	2.09	1.55	1.52
2	D	1102	HEC	CMA-C3A	2.09	1.56	1.51
2	B	1116	HEC	C4B-NB	2.09	1.39	1.36
2	C	1112	HEC	C4B-NB	2.10	1.39	1.36
2	A	1114	HEC	C3C-C4C	2.10	1.46	1.43
2	C	1106	HEC	CMD-C2D	2.10	1.55	1.51
2	C	1105	HEC	C4B-NB	2.11	1.39	1.36
2	A	1102	HEC	CMD-C2D	2.11	1.55	1.51
2	B	1105	HEC	CMB-C2B	2.11	1.56	1.51
2	B	1109	HEC	CMB-C2B	2.12	1.56	1.51
2	D	1109	HEC	C4B-NB	2.12	1.39	1.36
2	D	1111	HEC	C4A-NA	2.12	1.39	1.36
2	B	1106	HEC	CMB-C2B	2.12	1.56	1.51
2	C	1112	HEC	CMA-C3A	2.12	1.56	1.51
2	A	1101	HEC	C3C-C4C	2.13	1.47	1.43
2	D	1104	HEC	CMB-C2B	2.13	1.56	1.51
2	B	1114	HEC	CMD-C2D	2.14	1.56	1.51
2	C	1109	HEC	C4C-NC	2.14	1.39	1.36
2	D	1109	HEC	CMD-C2D	2.14	1.56	1.51
2	C	1114	HEC	C4C-NC	2.15	1.39	1.36
2	B	1105	HEC	C4D-ND	2.15	1.40	1.36
2	A	1110	HEC	CMC-C2C	2.15	1.56	1.51
2	B	1115	HEC	C4B-NB	2.15	1.39	1.36
2	D	1102	HEC	C1D-ND	2.15	1.40	1.36
2	A	1115	HEC	C3B-C4B	2.16	1.47	1.43
2	A	1106	HEC	CMC-C2C	2.17	1.56	1.51
2	C	1102	HEC	CAD-C3D	2.17	1.55	1.52
2	B	1113	HEC	CMD-C2D	2.18	1.56	1.51
2	D	1115	HEC	C4A-NA	2.19	1.39	1.36
2	C	1114	HEC	CMD-C2D	2.19	1.56	1.51
2	B	1110	HEC	CMB-C2B	2.20	1.56	1.51
2	A	1104	HEC	CMC-C2C	2.20	1.56	1.51
2	A	1106	HEC	CAD-C3D	2.21	1.55	1.52
2	B	1108	HEC	CAA-C2A	2.21	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1109	HEC	CAA-C2A	2.22	1.56	1.52
2	C	1102	HEC	C3C-C4C	2.22	1.47	1.43
2	B	1101	HEC	CMA-C3A	2.22	1.56	1.51
2	B	1104	HEC	C4A-NA	2.23	1.39	1.36
2	B	1114	HEC	C4C-NC	2.25	1.39	1.36
2	A	1101	HEC	CMC-C2C	2.26	1.56	1.51
2	D	1103	HEC	CMB-C2B	2.28	1.56	1.51
2	C	1106	HEC	CAA-C2A	2.29	1.56	1.52
2	A	1114	HEC	C4B-NB	2.29	1.39	1.36
2	A	1107	HEC	CAA-C2A	2.30	1.56	1.52
2	A	1108	HEC	C4D-ND	2.30	1.41	1.36
2	D	1106	HEC	CAD-C3D	2.30	1.55	1.52
2	D	1101	HEC	C1A-NA	2.30	1.39	1.36
2	B	1103	HEC	CAD-C3D	2.31	1.55	1.52
2	D	1109	HEC	C1A-NA	2.31	1.39	1.36
2	B	1112	HEC	CMA-C3A	2.31	1.56	1.51
2	B	1105	HEC	CAD-C3D	2.32	1.55	1.52
2	B	1108	HEC	C4C-NC	2.32	1.39	1.36
2	D	1110	HEC	CMC-C2C	2.32	1.56	1.51
2	D	1116	HEC	CMA-C3A	2.32	1.56	1.51
2	B	1114	HEC	C3C-C4C	2.33	1.47	1.43
2	B	1114	HEC	CAD-C3D	2.38	1.56	1.52
2	A	1109	HEC	CAD-C3D	2.38	1.56	1.52
2	C	1103	HEC	C4C-NC	2.39	1.39	1.36
2	C	1109	HEC	CAD-C3D	2.40	1.56	1.52
2	B	1101	HEC	C4C-NC	2.41	1.39	1.36
2	D	1101	HEC	CMC-C2C	2.41	1.56	1.51
2	A	1105	HEC	C4C-NC	2.42	1.39	1.36
2	B	1109	HEC	C3C-C4C	2.42	1.47	1.43
2	B	1105	HEC	C4C-NC	2.43	1.39	1.36
2	C	1114	HEC	C4B-NB	2.45	1.39	1.36
2	A	1114	HEC	C4D-ND	2.45	1.41	1.36
2	A	1103	HEC	CAD-C3D	2.46	1.56	1.52
2	B	1109	HEC	CAD-C3D	2.46	1.56	1.52
2	A	1111	HEC	CAA-C2A	2.47	1.57	1.52
2	B	1103	HEC	CMB-C2B	2.48	1.56	1.51
2	C	1106	HEC	C4B-NB	2.49	1.39	1.36
2	A	1103	HEC	C4C-NC	2.49	1.39	1.36
2	A	1101	HEC	CAD-C3D	2.50	1.56	1.52
2	C	1111	HEC	C4B-NB	2.55	1.39	1.36
2	C	1109	HEC	CMA-C3A	2.59	1.57	1.51
2	D	1112	HEC	C4C-NC	2.60	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1110	HEC	CAD-C3D	2.63	1.56	1.52
2	A	1107	HEC	C4B-NB	2.66	1.39	1.36
2	D	1105	HEC	CAD-C3D	2.67	1.56	1.52
2	C	1103	HEC	CAD-C3D	2.78	1.56	1.52
2	B	1103	HEC	C4C-NC	2.85	1.40	1.36
2	B	1109	HEC	C4A-NA	2.95	1.40	1.36
2	C	1104	HEC	C4A-NA	3.00	1.40	1.36
2	D	1113	HEC	C3D-C2D	4.70	1.51	1.37
2	A	1103	HEC	C3D-C2D	4.72	1.51	1.37
2	A	1115	HEC	C3D-C2D	4.72	1.51	1.37
2	B	1104	HEC	C3D-C2D	4.75	1.51	1.37
2	D	1108	HEC	C3D-C2D	4.81	1.51	1.37
2	C	1104	HEC	C3D-C2D	4.83	1.52	1.37
2	B	1103	HEC	C3D-C2D	4.85	1.52	1.37
2	D	1115	HEC	C3D-C2D	4.88	1.52	1.37
2	C	1112	HEC	C3D-C2D	4.91	1.52	1.37
2	B	1107	HEC	C3D-C2D	4.93	1.52	1.37
2	B	1106	HEC	C3D-C2D	4.94	1.52	1.37
2	C	1107	HEC	C3D-C2D	4.95	1.52	1.37
2	A	1116	HEC	C3D-C2D	4.98	1.52	1.37
2	B	1112	HEC	C3D-C2D	4.98	1.52	1.37
2	C	1110	HEC	C3D-C2D	5.01	1.52	1.37
2	C	1103	HEC	C3D-C2D	5.03	1.52	1.37
2	D	1116	HEC	C3D-C2D	5.03	1.52	1.37
2	B	1109	HEC	C3D-C2D	5.03	1.52	1.37
2	C	1109	HEC	C3D-C2D	5.06	1.52	1.37
2	D	1112	HEC	C3D-C2D	5.07	1.52	1.37
2	C	1113	HEC	C3D-C2D	5.07	1.52	1.37
2	C	1106	HEC	C3D-C2D	5.10	1.52	1.37
2	A	1105	HEC	C3D-C2D	5.15	1.52	1.37
2	A	1104	HEC	C3D-C2D	5.15	1.52	1.37
2	A	1107	HEC	C3D-C2D	5.16	1.53	1.37
2	C	1108	HEC	C3D-C2D	5.16	1.53	1.37
2	C	1101	HEC	C3D-C2D	5.17	1.53	1.37
2	B	1110	HEC	C3D-C2D	5.19	1.53	1.37
2	B	1116	HEC	C3D-C2D	5.23	1.53	1.37
2	A	1112	HEC	C3D-C2D	5.25	1.53	1.37
2	B	1105	HEC	C3D-C2D	5.25	1.53	1.37
2	D	1107	HEC	C3D-C2D	5.25	1.53	1.37
2	B	1101	HEC	C3D-C2D	5.26	1.53	1.37
2	A	1101	HEC	C3D-C2D	5.27	1.53	1.37
2	B	1108	HEC	C3D-C2D	5.28	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1106	HEC	C3D-C2D	5.28	1.53	1.37
2	A	1113	HEC	C3D-C2D	5.29	1.53	1.37
2	C	1105	HEC	C3D-C2D	5.29	1.53	1.37
2	D	1104	HEC	C3D-C2D	5.30	1.53	1.37
2	B	1115	HEC	C3D-C2D	5.30	1.53	1.37
2	D	1103	HEC	C3D-C2D	5.36	1.53	1.37
2	A	1109	HEC	C3D-C2D	5.36	1.53	1.37
2	C	1115	HEC	C3D-C2D	5.40	1.53	1.37
2	A	1110	HEC	C3D-C2D	5.40	1.53	1.37
2	D	1101	HEC	C3D-C2D	5.42	1.53	1.37
2	B	1113	HEC	C3D-C2D	5.42	1.53	1.37
2	D	1106	HEC	C3D-C2D	5.43	1.53	1.37
2	A	1111	HEC	C3D-C2D	5.45	1.53	1.37
2	C	1111	HEC	C3D-C2D	5.46	1.53	1.37
2	C	1116	HEC	C3D-C2D	5.47	1.53	1.37
2	D	1102	HEC	C3D-C2D	5.48	1.53	1.37
2	D	1111	HEC	C3D-C2D	5.49	1.53	1.37
2	A	1102	HEC	C3D-C2D	5.54	1.54	1.37
2	C	1102	HEC	C3D-C2D	5.57	1.54	1.37
2	C	1114	HEC	C3D-C2D	5.58	1.54	1.37
2	B	1102	HEC	C3D-C2D	5.60	1.54	1.37
2	B	1111	HEC	C3D-C2D	5.60	1.54	1.37
2	D	1109	HEC	C3D-C2D	5.62	1.54	1.37
2	A	1114	HEC	C3D-C2D	5.68	1.54	1.37
2	D	1114	HEC	C3D-C2D	5.68	1.54	1.37
2	D	1105	HEC	C3D-C2D	5.79	1.54	1.37
2	B	1114	HEC	C3D-C2D	5.79	1.54	1.37
2	A	1108	HEC	C3D-C2D	5.88	1.55	1.37
2	D	1110	HEC	C3D-C2D	5.95	1.55	1.37

All (245) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1103	HEC	CBD-CAD-C3D	-6.75	99.57	112.48
2	C	1103	HEC	CBD-CAD-C3D	-6.07	100.89	112.48
2	B	1113	HEC	CBD-CAD-C3D	-5.45	102.07	112.48
2	A	1116	HEC	CBD-CAD-C3D	-5.44	102.07	112.48
2	C	1116	HEC	CBD-CAD-C3D	-5.27	102.40	112.48
2	B	1104	HEC	CAD-CBD-CGD	-4.85	104.37	112.66
2	A	1107	HEC	CMB-C2B-C1B	-4.59	121.41	128.46
2	D	1116	HEC	CBD-CAD-C3D	-4.55	103.79	112.48
2	B	1107	HEC	CAD-CBD-CGD	-4.50	104.97	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1103	HEC	CBD-CAD-C3D	-4.48	103.92	112.48
2	A	1104	HEC	CBA-CAA-C2A	-4.35	104.18	112.47
2	D	1103	HEC	CBD-CAD-C3D	-4.34	104.18	112.48
2	D	1116	HEC	C1D-C2D-C3D	-4.30	104.00	107.00
2	B	1116	HEC	C1D-C2D-C3D	-4.27	104.02	107.00
2	C	1113	HEC	CBA-CAA-C2A	-4.06	104.71	112.47
2	B	1105	HEC	CMC-C2C-C1C	-3.96	122.38	128.46
2	D	1104	HEC	CBA-CAA-C2A	-3.95	104.93	112.47
2	B	1101	HEC	CMB-C2B-C1B	-3.95	122.40	128.46
2	D	1105	HEC	CAA-CBA-CGA	-3.93	105.94	112.66
2	C	1104	HEC	CBA-CAA-C2A	-3.91	105.02	112.47
2	C	1109	HEC	CBA-CAA-C2A	-3.86	105.10	112.47
2	B	1110	HEC	CMC-C2C-C1C	-3.84	122.56	128.46
2	A	1115	HEC	CBD-CAD-C3D	-3.78	105.26	112.48
2	D	1108	HEC	C1D-C2D-C3D	-3.75	104.39	107.00
2	B	1113	HEC	C1D-C2D-C3D	-3.74	104.39	107.00
2	B	1106	HEC	CAD-CBD-CGD	-3.73	106.28	112.66
2	D	1115	HEC	C1D-C2D-C3D	-3.68	104.44	107.00
2	C	1104	HEC	CAD-CBD-CGD	-3.66	106.41	112.66
2	D	1104	HEC	C1D-C2D-C3D	-3.65	104.46	107.00
2	C	1106	HEC	C1D-C2D-C3D	-3.65	104.46	107.00
2	A	1108	HEC	CMC-C2C-C1C	-3.56	122.99	128.46
2	C	1107	HEC	C1D-C2D-C3D	-3.56	104.52	107.00
2	B	1110	HEC	CBD-CAD-C3D	-3.56	105.68	112.48
2	D	1106	HEC	CMC-C2C-C1C	-3.54	123.02	128.46
2	B	1110	HEC	CMB-C2B-C1B	-3.53	123.04	128.46
2	C	1102	HEC	CMC-C2C-C1C	-3.53	123.04	128.46
2	D	1112	HEC	CMC-C2C-C1C	-3.51	123.07	128.46
2	B	1102	HEC	CBA-CAA-C2A	-3.51	105.78	112.47
2	B	1116	HEC	CBD-CAD-C3D	-3.50	105.79	112.48
2	A	1108	HEC	CBD-CAD-C3D	-3.50	105.79	112.48
2	A	1102	HEC	CMC-C2C-C1C	-3.50	123.09	128.46
2	C	1106	HEC	CMB-C2B-C1B	-3.49	123.09	128.46
2	D	1102	HEC	C1D-C2D-C3D	-3.47	104.58	107.00
2	B	1112	HEC	C1D-C2D-C3D	-3.46	104.59	107.00
2	B	1115	HEC	C1D-C2D-C3D	-3.45	104.59	107.00
2	D	1102	HEC	CBA-CAA-C2A	-3.45	105.89	112.47
2	A	1116	HEC	C1D-C2D-C3D	-3.45	104.60	107.00
2	B	1110	HEC	C1D-C2D-C3D	-3.41	104.62	107.00
2	C	1106	HEC	CMC-C2C-C1C	-3.41	123.22	128.46
2	A	1101	HEC	CMC-C2C-C1C	-3.40	123.23	128.46
2	C	1110	HEC	CMC-C2C-C1C	-3.40	123.24	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1105	HEC	CMB-C2B-C1B	-3.38	123.27	128.46
2	D	1109	HEC	C1D-C2D-C3D	-3.37	104.65	107.00
2	B	1104	HEC	CMB-C2B-C1B	-3.37	123.29	128.46
2	C	1108	HEC	CMC-C2C-C1C	-3.35	123.31	128.46
2	C	1115	HEC	CMB-C2B-C1B	-3.35	123.31	128.46
2	A	1109	HEC	C1D-C2D-C3D	-3.31	104.70	107.00
2	B	1101	HEC	CMC-C2C-C1C	-3.30	123.39	128.46
2	A	1103	HEC	CMB-C2B-C1B	-3.28	123.43	128.46
2	C	1115	HEC	CAA-CBA-CGA	-3.27	107.08	112.66
2	B	1106	HEC	CBD-CAD-C3D	-3.23	106.30	112.48
2	B	1102	HEC	C1D-C2D-C3D	-3.23	104.75	107.00
2	A	1107	HEC	C1D-C2D-C3D	-3.23	104.75	107.00
2	C	1106	HEC	CBD-CAD-C3D	-3.22	106.32	112.48
2	C	1109	HEC	CMB-C2B-C1B	-3.19	123.56	128.46
2	B	1116	HEC	CMB-C2B-C1B	-3.18	123.57	128.46
2	C	1102	HEC	CBA-CAA-C2A	-3.17	106.42	112.47
2	C	1116	HEC	CMB-C2B-C1B	-3.13	123.65	128.46
2	A	1113	HEC	CBA-CAA-C2A	-3.11	106.53	112.47
2	B	1108	HEC	CMB-C2B-C1B	-3.11	123.69	128.46
2	D	1108	HEC	CAD-CBD-CGD	-3.09	107.38	112.66
2	D	1111	HEC	C1D-C2D-C3D	-3.07	104.86	107.00
2	D	1108	HEC	CBD-CAD-C3D	-3.04	106.66	112.48
2	C	1101	HEC	CMB-C2B-C1B	-3.04	123.79	128.46
2	B	1103	HEC	CMB-C2B-C1B	-3.03	123.80	128.46
2	C	1114	HEC	CBA-CAA-C2A	-3.02	106.70	112.47
2	D	1101	HEC	CMC-C2C-C1C	-3.02	123.82	128.46
2	A	1115	HEC	C1D-C2D-C3D	-3.02	104.90	107.00
2	B	1109	HEC	CMB-C2B-C1B	-3.01	123.83	128.46
2	C	1116	HEC	C1D-C2D-C3D	-3.01	104.90	107.00
2	A	1101	HEC	CMB-C2B-C1B	-2.99	123.87	128.46
2	A	1105	HEC	C1D-C2D-C3D	-2.98	104.92	107.00
2	C	1111	HEC	CAA-CBA-CGA	-2.98	107.56	112.66
2	D	1114	HEC	CBA-CAA-C2A	-2.98	106.78	112.47
2	C	1103	HEC	CMB-C2B-C1B	-2.98	123.89	128.46
2	B	1103	HEC	C1D-C2D-C3D	-2.98	104.92	107.00
2	B	1107	HEC	C1D-C2D-C3D	-2.98	104.93	107.00
2	A	1115	HEC	CMC-C2C-C1C	-2.97	123.89	128.46
2	D	1103	HEC	CMB-C2B-C1B	-2.95	123.92	128.46
2	C	1101	HEC	CMC-C2C-C1C	-2.95	123.93	128.46
2	C	1115	HEC	CMC-C2C-C1C	-2.94	123.94	128.46
2	A	1112	HEC	CBD-CAD-C3D	-2.94	106.87	112.48
2	B	1114	HEC	C1D-C2D-C3D	-2.93	104.96	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1106	HEC	CMB-C2B-C1B	-2.93	123.96	128.46
2	C	1107	HEC	CMB-C2B-C1B	-2.93	123.97	128.46
2	A	1109	HEC	CAA-CBA-CGA	-2.92	107.67	112.66
2	A	1115	HEC	CBA-CAA-C2A	-2.92	106.89	112.47
2	C	1105	HEC	CMB-C2B-C1B	-2.91	123.99	128.46
2	B	1116	HEC	CMC-C2C-C1C	-2.90	124.01	128.46
2	C	1115	HEC	C1D-C2D-C3D	-2.88	104.99	107.00
2	C	1104	HEC	CMB-C2B-C1B	-2.88	124.04	128.46
2	B	1106	HEC	C1D-C2D-C3D	-2.87	105.00	107.00
2	D	1112	HEC	CMB-C2B-C1B	-2.87	124.05	128.46
2	B	1115	HEC	CAA-CBA-CGA	-2.87	107.76	112.66
2	B	1112	HEC	CMC-C2C-C1C	-2.87	124.06	128.46
2	C	1102	HEC	CAA-CBA-CGA	-2.85	107.78	112.66
2	C	1110	HEC	CAD-CBD-CGD	-2.85	107.79	112.66
2	A	1115	HEC	CMB-C2B-C1B	-2.85	124.08	128.46
2	C	1113	HEC	CMB-C2B-C1B	-2.85	124.09	128.46
2	C	1108	HEC	CAA-CBA-CGA	-2.83	107.83	112.66
2	A	1102	HEC	CMB-C2B-C1B	-2.83	124.12	128.46
2	A	1102	HEC	CBD-CAD-C3D	-2.83	107.08	112.48
2	B	1104	HEC	CMC-C2C-C1C	-2.82	124.13	128.46
2	D	1104	HEC	CMC-C2C-C1C	-2.80	124.17	128.46
2	C	1112	HEC	CMB-C2B-C1B	-2.79	124.18	128.46
2	D	1106	HEC	CMB-C2B-C1B	-2.78	124.19	128.46
2	C	1108	HEC	C1D-C2D-C3D	-2.78	105.06	107.00
2	A	1108	HEC	C1D-C2D-C3D	-2.76	105.08	107.00
2	B	1103	HEC	CMC-C2C-C1C	-2.75	124.23	128.46
2	C	1116	HEC	CMC-C2C-C1C	-2.74	124.25	128.46
2	D	1102	HEC	CMB-C2B-C1B	-2.74	124.26	128.46
2	B	1111	HEC	CMB-C2B-C1B	-2.73	124.26	128.46
2	D	1111	HEC	CMC-C2C-C1C	-2.73	124.27	128.46
2	D	1101	HEC	C1D-C2D-C3D	-2.73	105.10	107.00
2	D	1107	HEC	CBD-CAD-C3D	-2.72	107.28	112.48
2	C	1101	HEC	CBA-CAA-C2A	-2.71	107.29	112.47
2	C	1107	HEC	CAA-CBA-CGA	-2.71	108.03	112.66
2	B	1111	HEC	CMC-C2C-C1C	-2.70	124.31	128.46
2	D	1107	HEC	CMB-C2B-C1B	-2.70	124.32	128.46
2	A	1114	HEC	CMC-C2C-C1C	-2.70	124.32	128.46
2	D	1105	HEC	CMC-C2C-C1C	-2.70	124.32	128.46
2	A	1106	HEC	CMB-C2B-C1B	-2.70	124.32	128.46
2	B	1111	HEC	CAD-CBD-CGD	-2.68	108.08	112.66
2	C	1113	HEC	C1D-C2D-C3D	-2.68	105.13	107.00
2	D	1113	HEC	CBA-CAA-C2A	-2.65	107.42	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1111	HEC	C1D-C2D-C3D	-2.64	105.16	107.00
2	A	1110	HEC	CMB-C2B-C1B	-2.64	124.41	128.46
2	C	1107	HEC	CBD-CAD-C3D	-2.62	107.47	112.48
2	C	1107	HEC	CMC-C2C-C1C	-2.61	124.45	128.46
2	D	1102	HEC	CBD-CAD-C3D	-2.60	107.50	112.48
2	D	1115	HEC	CBD-CAD-C3D	-2.59	107.53	112.48
2	A	1106	HEC	CBD-CAD-C3D	-2.59	107.54	112.48
2	B	1112	HEC	CMB-C2B-C1B	-2.56	124.52	128.46
2	C	1102	HEC	CBD-CAD-C3D	-2.56	107.59	112.48
2	A	1110	HEC	C1D-C2D-C3D	-2.56	105.22	107.00
2	D	1103	HEC	C1D-C2D-C3D	-2.56	105.22	107.00
2	C	1110	HEC	CBD-CAD-C3D	-2.55	107.61	112.48
2	D	1110	HEC	CBA-CAA-C2A	-2.55	107.61	112.47
2	B	1102	HEC	CMC-C2C-C1C	-2.53	124.58	128.46
2	D	1110	HEC	CMB-C2B-C1B	-2.53	124.58	128.46
2	C	1113	HEC	CAA-CBA-CGA	-2.52	108.35	112.66
2	D	1115	HEC	CMC-C2C-C1C	-2.51	124.61	128.46
2	A	1116	HEC	CMC-C2C-C1C	-2.48	124.65	128.46
2	C	1112	HEC	CBD-CAD-C3D	-2.48	107.74	112.48
2	A	1102	HEC	C1D-C2D-C3D	-2.47	105.28	107.00
2	C	1105	HEC	CBD-CAD-C3D	-2.46	107.78	112.48
2	D	1111	HEC	CAA-CBA-CGA	-2.45	108.47	112.66
2	D	1112	HEC	C1D-C2D-C3D	-2.45	105.29	107.00
2	C	1113	HEC	CBD-CAD-C3D	-2.45	107.80	112.48
2	D	1104	HEC	CAD-CBD-CGD	-2.45	108.48	112.66
2	A	1116	HEC	CMB-C2B-C1B	-2.45	124.70	128.46
2	A	1101	HEC	CBA-CAA-C2A	-2.45	107.80	112.47
2	B	1111	HEC	CBA-CAA-C2A	-2.45	107.80	112.47
2	C	1106	HEC	CAD-CBD-CGD	-2.43	108.51	112.66
2	D	1113	HEC	CBD-CAD-C3D	-2.43	107.84	112.48
2	C	1109	HEC	C1D-C2D-C3D	-2.43	105.31	107.00
2	B	1108	HEC	CBD-CAD-C3D	-2.43	107.85	112.48
2	A	1113	HEC	CMC-C2C-C1C	-2.39	124.78	128.46
2	D	1107	HEC	C1D-C2D-C3D	-2.39	105.33	107.00
2	B	1115	HEC	CMC-C2C-C1C	-2.38	124.81	128.46
2	D	1113	HEC	C1D-C2D-C3D	-2.37	105.35	107.00
2	D	1106	HEC	CAD-CBD-CGD	-2.36	108.62	112.66
2	B	1112	HEC	CAD-CBD-CGD	-2.33	108.68	112.66
2	B	1106	HEC	CMC-C2C-C1C	-2.33	124.89	128.46
2	C	1115	HEC	CBD-CAD-C3D	-2.32	108.05	112.48
2	D	1107	HEC	CAD-CBD-CGD	-2.31	108.70	112.66
2	B	1102	HEC	CMB-C2B-C1B	-2.31	124.91	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1113	HEC	CBD-CAD-C3D	-2.30	108.08	112.48
2	D	1113	HEC	CMB-C2B-C1B	-2.29	124.94	128.46
2	C	1103	HEC	CMC-C2C-C1C	-2.27	124.97	128.46
2	A	1112	HEC	CMB-C2B-C1B	-2.27	124.97	128.46
2	C	1102	HEC	CMB-C2B-C1B	-2.26	124.99	128.46
2	C	1114	HEC	CMB-C2B-C1B	-2.26	125.00	128.46
2	D	1107	HEC	CAA-CBA-CGA	-2.25	108.82	112.66
2	D	1114	HEC	CMB-C2B-C1B	-2.22	125.05	128.46
2	D	1110	HEC	CMD-C2D-C1D	-2.22	125.05	128.46
2	D	1102	HEC	CMC-C2C-C1C	-2.20	125.08	128.46
2	A	1108	HEC	CAA-CBA-CGA	-2.20	108.90	112.66
2	A	1108	HEC	CMB-C2B-C1B	-2.20	125.09	128.46
2	C	1108	HEC	CBD-CAD-C3D	-2.19	108.30	112.48
2	C	1108	HEC	CMB-C2B-C1B	-2.19	125.10	128.46
2	A	1112	HEC	CBA-CAA-C2A	-2.19	108.30	112.47
2	D	1109	HEC	CMB-C2B-C1B	-2.18	125.11	128.46
2	B	1108	HEC	CMC-C2C-C1C	-2.18	125.12	128.46
2	D	1109	HEC	CMC-C2C-C1C	-2.18	125.12	128.46
2	B	1114	HEC	CMB-C2B-C1B	-2.17	125.12	128.46
2	B	1102	HEC	CBD-CAD-C3D	-2.16	108.36	112.48
2	A	1112	HEC	CMC-C2C-C1C	-2.14	125.17	128.46
2	D	1104	HEC	CMB-C2B-C1B	-2.14	125.18	128.46
2	C	1111	HEC	CMB-C2B-C1B	-2.13	125.19	128.46
2	A	1106	HEC	C1D-C2D-C3D	-2.11	105.53	107.00
2	A	1107	HEC	CAA-CBA-CGA	-2.11	109.06	112.66
2	A	1111	HEC	C1D-C2D-C3D	-2.09	105.54	107.00
2	D	1114	HEC	CBD-CAD-C3D	-2.08	108.50	112.48
2	C	1104	HEC	C1D-C2D-C3D	-2.08	105.55	107.00
2	B	1115	HEC	CMB-C2B-C1B	-2.08	125.27	128.46
2	B	1105	HEC	CAA-CBA-CGA	-2.07	109.12	112.66
2	C	1114	HEC	CAA-CBA-CGA	-2.06	109.13	112.66
2	B	1110	HEC	CBA-CAA-C2A	-2.06	108.53	112.47
2	C	1110	HEC	CMB-C2B-C1B	-2.06	125.30	128.46
2	C	1112	HEC	CMC-C2C-C1C	-2.04	125.33	128.46
2	D	1110	HEC	CAA-CBA-CGA	-2.03	109.19	112.66
2	D	1105	HEC	CMB-C2B-C1B	-2.03	125.35	128.46
2	A	1107	HEC	CMC-C2C-C1C	-2.03	125.35	128.46
2	D	1111	HEC	CMB-C2B-C1B	-2.02	125.35	128.46
2	C	1105	HEC	CAA-CBA-CGA	-2.01	109.22	112.66
2	A	1107	HEC	CBD-CAD-C3D	-2.00	108.65	112.48
2	B	1101	HEC	CBD-CAD-C3D	-2.00	108.65	112.48
2	A	1108	HEC	CAD-CBD-CGD	2.00	116.08	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1115	HEC	CMD-C2D-C3D	2.02	128.75	124.94
2	C	1110	HEC	CMA-C3A-C2A	2.04	128.78	124.94
2	D	1104	HEC	CMA-C3A-C2A	2.05	128.80	124.94
2	D	1110	HEC	CMD-C2D-C3D	2.11	128.92	124.94
2	C	1113	HEC	CMD-C2D-C3D	2.11	128.92	124.94
2	D	1115	HEC	C4B-C3B-C2B	2.15	108.67	106.35
2	A	1108	HEC	CMD-C2D-C3D	2.19	129.08	124.94
2	A	1110	HEC	CMD-C2D-C3D	2.19	129.08	124.94
2	B	1107	HEC	C4B-C3B-C2B	2.20	108.73	106.35
2	A	1105	HEC	CMA-C3A-C2A	2.21	129.11	124.94
2	A	1103	HEC	CMA-C3A-C2A	2.25	129.19	124.94
2	C	1103	HEC	CAD-CBD-CGD	2.26	116.52	112.66
2	D	1116	HEC	CMA-C3A-C2A	2.28	129.24	124.94
2	D	1103	HEC	C4B-C3B-C2B	2.28	108.81	106.35
2	A	1109	HEC	C4C-C3C-C2C	2.30	108.84	106.35
2	B	1113	HEC	CMD-C2D-C3D	2.31	129.29	124.94
2	A	1103	HEC	CAD-CBD-CGD	2.33	116.64	112.66
2	A	1106	HEC	CMA-C3A-C2A	2.38	129.43	124.94
2	D	1103	HEC	CMA-C3A-C2A	2.41	129.48	124.94
2	C	1105	HEC	CMA-C3A-C2A	2.48	129.61	124.94
2	C	1116	HEC	CAD-CBD-CGD	2.61	117.12	112.66
2	B	1112	HEC	CMA-C3A-C2A	2.73	130.09	124.94
2	B	1114	HEC	CAD-CBD-CGD	2.75	117.36	112.66
2	D	1105	HEC	CBA-CAA-C2A	2.83	117.86	112.47
2	A	1111	HEC	CBA-CAA-C2A	3.28	118.73	112.47
2	A	1107	HEC	CBA-CAA-C2A	4.97	121.94	112.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1107	HEC	C1A-C2A-CAA-CBA

There are no ring outliers.

56 monomers are involved in 157 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	HEC	1	0
2	A	1102	HEC	5	0
2	A	1103	HEC	1	0
2	A	1104	HEC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1106	HEC	1	0
2	A	1108	HEC	3	0
2	A	1109	HEC	3	0
2	A	1110	HEC	4	0
2	A	1111	HEC	2	0
2	A	1112	HEC	5	0
2	A	1113	HEC	5	0
2	A	1114	HEC	1	0
2	A	1115	HEC	3	0
2	B	1101	HEC	1	0
2	B	1102	HEC	5	0
2	B	1104	HEC	2	0
2	B	1105	HEC	1	0
2	B	1106	HEC	3	0
2	B	1107	HEC	2	0
2	B	1108	HEC	1	0
2	B	1109	HEC	1	0
2	B	1110	HEC	2	0
2	B	1111	HEC	4	0
2	B	1112	HEC	3	0
2	B	1113	HEC	2	0
2	B	1114	HEC	2	0
2	B	1115	HEC	6	0
2	B	1116	HEC	1	0
2	C	1101	HEC	3	0
2	C	1102	HEC	4	0
2	C	1103	HEC	2	0
2	C	1104	HEC	1	0
2	C	1105	HEC	2	0
2	C	1106	HEC	2	0
2	C	1107	HEC	3	0
2	C	1108	HEC	3	0
2	C	1109	HEC	4	0
2	C	1110	HEC	5	0
2	C	1111	HEC	4	0
2	C	1112	HEC	1	0
2	C	1113	HEC	1	0
2	C	1114	HEC	1	0
2	C	1115	HEC	5	0
2	D	1101	HEC	6	0
2	D	1102	HEC	6	0
2	D	1104	HEC	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1106	HEC	4	0
2	D	1107	HEC	2	0
2	D	1108	HEC	4	0
2	D	1109	HEC	4	0
2	D	1110	HEC	7	0
2	D	1111	HEC	3	0
2	D	1112	HEC	3	0
2	D	1113	HEC	2	0
2	D	1114	HEC	2	0
2	D	1115	HEC	1	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.