



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:33 AM GMT

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
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Deposited on : 2002-08-01
Resolution : 2.51 Å(reported)

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

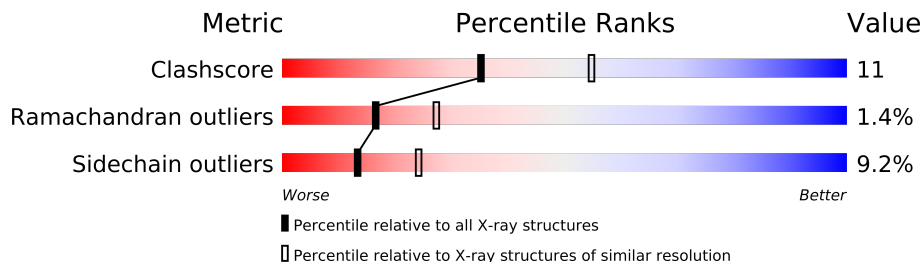
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (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 ≥ 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.

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

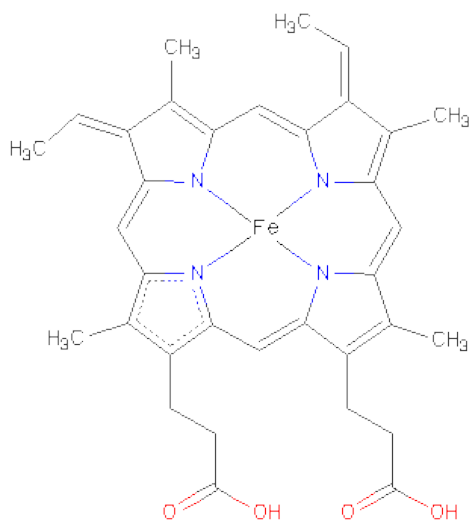
There are 3 unique types of molecules in this entry. The entry contains 18287 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HIGH-MOLECULAR-WEIGHTCYTOCHROME 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
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

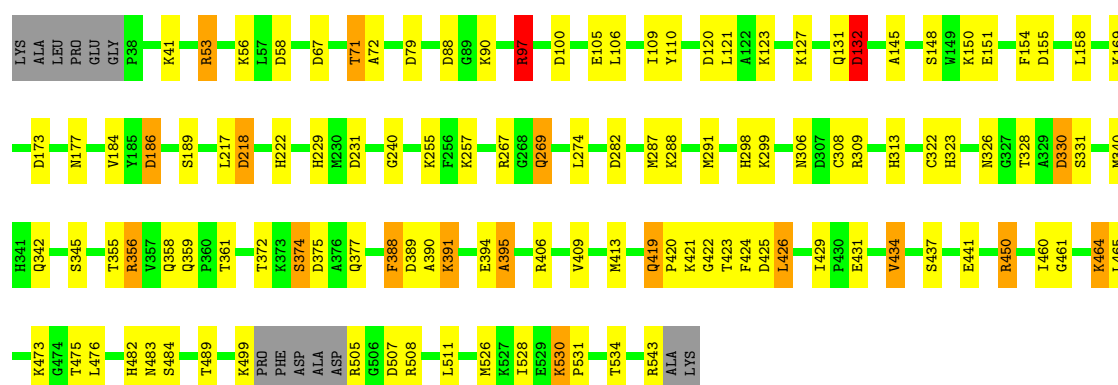
3 Residue-property plots

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

Note EDS was not executed.

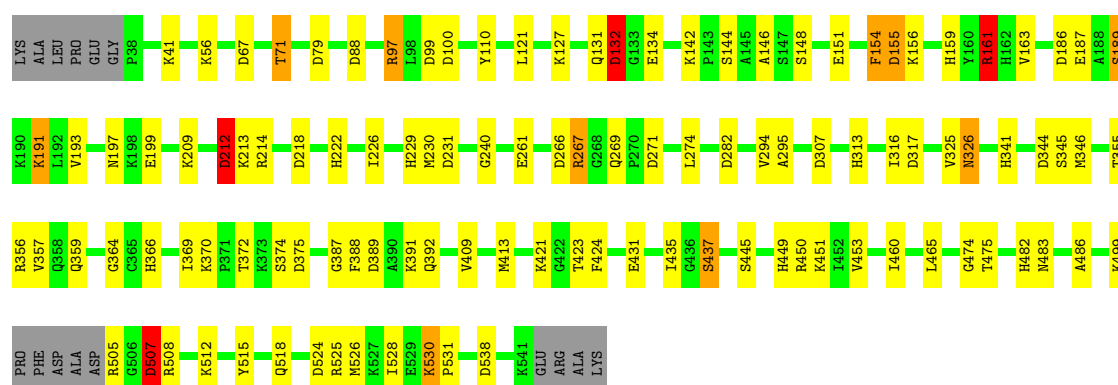
• Molecule 1: HIGH-MOLECULAR-WEIGHTCYTOCHROME C

Chain A:



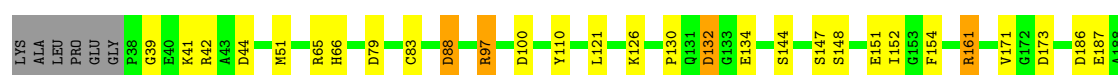
• Molecule 1: HIGH-MOLECULAR-WEIGHTCYTOCHROME C

Chain B:



• Molecule 1: HIGH-MOLECULAR-WEIGHTCYTOCHROME C

Chain C:



E529	E404	K288		LYS
K530	Q405	K292	R161	ALA
P531	R406		K165	LEU
A532		D297	S166	PRO
N533	A410		A187	GLU
	K413	H301	I188	GLY
K541	P418	D307	M177	P38
E542		C308		K41
ARG	K421	R309	D186	K42
ALA	G422			K43
LYS	T423	H312	K198	D44
	F424	H313	E199	
		V314	D200	M51
	E431	R315	S201	E52
		I316		B53
	R450	D317	V211	
			D212	K56
F469	F469	T324	K213	L57
H470	H470	V325	R214	D58
L471	L471	N326		
			D218	H66
T475	T475	S331		D67
L476	L476	K332	A221	Q68
C477	C477		H222	H69
Q478	Q478	Q335		T71
			C225	A72
H481	H481	K338	L226	V73
H482	H482	A339		
I483	I483	P340	H229	K78
S484	S484	H341	M230	D79
		Q342	D231	C80
L488	L488			
	K492	S345	K236	D88
			G240	G89
S495	S495	G351		K90
C496	C496	T355	C244	P95
		R356		N96
K499	K499	V357	H248	B97
	PRO		A249	
PHE	PHE	G364	P250	K107
ASP	ASP	C365	E251	
ALA	ALA	H366		Y110
ASP	ASP	G367	K257	
ARG	ARG			L121
G566	G566	K370	V282	A122
D507	D507			
R508	R508	V380	Q289	K127
P509	P509			T128
G510	G510	V393	L274	
L511	L511	GLU		D132
		ALA	K281	E151
		GLY	D282	
		ALA	ALA	F154
		L398	PRO	D155
R525	R525		ARG	
		K402	E286	K159
		K403	M237	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	31.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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

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 11.

All (357) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(Å)
1:D:67:ASP:O	1:D:71:THR:HG23	1.84	0.76
1:C:526:MET:HE1	2:C:1115:HEC:CAC	2.16	0.75
1:B:356:ARG:O	1:B:359:GLN:HG2	1.86	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:D:341:HIS:HE1	2:D:1112:HEC:NA	1.90	0.70
1:C:39:GLY:HA3	1:C:144:SER:O	1.92	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:D:528:ILE:HG22	1:D:530:LYS:HB2	1.75	0.69
1:A:41:LYS:HB3	1:A:148:SER:HB3	1.73	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
2:D:1110:HEC:HMB1	2:D:1110:HEC:HBB3	1.77	0.65
1:C:154:PHE:HB2	2:C:1104:HEC:HBD2	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
1:B:41:LYS:HB3	1:B:148:SER:HB3	1.81	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:511:LEU:HD13	1:D:515:TYR:CE1	2.34	0.62
1:D:423:THR:HG22	1:D:424:PHE:N	2.14	0.62
1:B:326:ASN:HD22	1:B:326:ASN:H	1.46	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:409:VAL:HG12	1:C:413:MET:HE1	1.82	0.57
1:C:41:LYS:HB3	1:C:148:SER:HB3	1.85	0.57
1:D:229:HIS:CE1	1:D:240:GLY:HA3	2.39	0.57
2:D:1112:HEC:HBC3	2:D:1112:HEC:HMC1	1.87	0.56
1:A:374:SER:HB3	1:A:377:GLN:H	1.70	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:C:414:LEU:HB3	1:C:417:ARG:HH21	1.71	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
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
1:D:313:HIS:CE1	1:D:314:VAL:HG23	2.41	0.55
1:C:526:MET:CE	2:C:1115:HEC:HHD	2.36	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:409:VAL:HG12	1:B:413:MET:CE	2.36	0.55
1:B:161:ARG:NH1	1:B:161:ARG:HG2	2.21	0.55
1:D:68:GLN:HE22	2:D:1102:HEC:HBA2	1.71	0.55
2:D:1115:HEC:HMC1	2:D:1115:HEC:HBC3	1.88	0.55
1:D:80:CYS:HB3	2:D:1101:HEC:CHC	2.37	0.55
1:D:154:PHE:CD1	1:D:158:LEU:HD13	2.42	0.55
1:B:294:VAL:HG11	2:B:1112:HEC:HMD3	1.88	0.55
2:C:1115:HEC:HBB3	2:C:1115:HEC:HMB1	1.87	0.55
2:B:1110:HEC:HMC1	2:B:1110:HEC:HBC3	1.87	0.55
1:A:394:GLU:O	1:A:395:ALA:CB	2.54	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
2:B:1102:HEC:HBB3	2:B:1102:HEC:HMB1	1.88	0.54
1:A:298:HIS:HE1	2:A:1108:HEC:NB	2.06	0.54
1:D:470:HIS:HA	1:D:475:THR:HG21	1.89	0.54
2:D:1113:HEC:HBB3	2:D:1113:HEC:HMB1	1.89	0.54
1:A:374:SER:HB2	1:A:377:GLN:HB2	1.89	0.54
1:C:393:VAL:HG22	1:C:398:LEU:CD1	2.37	0.54
1:C:264:ARG:NH1	1:C:299:LYS:HD2	2.23	0.54
2:C:1109:HEC:HBC3	2:C:1109:HEC:HMC1	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
1:C:537:VAL:HA	1:C:540:HIS:O	2.08	0.53
2:B:1104:HEC:HBB3	2:B:1104:HEC:HMB1	1.91	0.53
2:A:1113:HEC:HBC3	2:A:1113:HEC:HMC1	1.91	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
2:C:1110:HEC:HMC1	2:C:1110:HEC:HBC3	1.89	0.53
1:A:322:CYS:HB3	1:A:331:SER:HB3	1.91	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
2:D:1106:HEC:HBC3	2:D:1106:HEC:HMC1	1.90	0.52
1:C:419:GLN:NE2	1:C:420:PRO:HD2	2.24	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
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:D:80:CYS:HB3	2:D:1101:HEC:C4B	2.38	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:423:THR:HG22	1:D:424:PHE:H	1.73	0.52
1:C:97:ARG:NH2	1:C:110:TYR:CZ	2.78	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:186:ASP:OD2	1:C:189:SER:HB2	2.09	0.52
1:C:294:VAL:HG11	2:C:1112:HEC:HMD3	1.92	0.52
1:A:388:PHE:HD1	1:A:388:PHE:H	1.52	0.52
2:A:1112:HEC:HMC1	2:A:1112:HEC:HBC3	1.92	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:D:168:ILE:HG22	1:D:177:ASN:HB2	1.93	0.51
1:B:154:PHE:HB2	2:B:1104:HEC:HBD2	1.92	0.51
1:A:340:MET:HG3	2:A:1112:HEC:C3D	2.41	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
1:A:394:GLU:O	1:A:395:ALA:HB2	2.13	0.49
2:A:1106:HEC:HMB1	2:A:1106:HEC:HBB3	1.95	0.49
2:D:1101:HEC:HBC1	2:D:1102:HEC:HMC2	1.93	0.49
1:B:295:ALA:HB2	1:B:413:MET:SD	2.52	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:D:121:LEU:HD13	2:D:1102:HEC:HMD3	1.95	0.49
1:C:530:LYS:HB2	1:C:531:PRO:CD	2.43	0.49
1:C:386:PRO:HG3	1:C:412:SER:OG	2.13	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
1:D:274:LEU:HD13	1:D:413:MET:HE1	1.94	0.48
2:A:1102:HEC:HMC1	2:A:1102:HEC:CBC	2.41	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:B:132:ASP:CG	1:D:516:HIS:HD1	2.17	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:250:PRO:HD2	1:D:251:GLU:OE2	2.14	0.48
1:A:229:HIS:CE1	1:A:240:GLY:HA3	2.48	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:D:221:ALA:O	1:D:225:CYS:SG	2.71	0.48
1:C:338:LYS:HE2	1:C:342:GLN:OE1	2.14	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
2:B:1106:HEC:CBC	2:B:1106:HEC:HMC1	2.44	0.47
1:B:121:LEU:CD1	2:B:1102:HEC:HMD3	2.43	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
1:C:530:LYS:CB	1:C:531:PRO:CD	2.92	0.47
2:D:1112:HEC:O2D	2:D:1112:HEC:HBA2	2.14	0.47
1:D:274:LEU:HB3	1:D:406:ARG:HG2	1.97	0.47
2:C:1101:HEC:HBB3	2:C:1101:HEC:HMB1	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
2:B:1111:HEC:HMC1	2:B:1111:HEC:HBC3	1.97	0.47
1:A:475:THR:O	2:A:1111:HEC:HMD2	2.14	0.47
1:A:530:LYS:CB	1:A:531:PRO:HD3	2.36	0.46
1:A:342:GLN:HG2	1:A:345:SER:HB2	1.96	0.46
2:C:1105:HEC:HMC1	2:C:1105:HEC:HBC3	1.96	0.46
2:D:1111:HEC:HMC1	2:D:1111:HEC:HBC3	1.98	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
1:B:229:HIS:CE1	1:B:240:GLY:HA3	2.51	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
1:D:211:VAL:HG23	1:D:212:ASP:N	2.30	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: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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:1103:HEC:HBC3	2:A:1103:HEC:HMC1	1.97	0.46
1:D:307:ASP:HB2	2:D:1104:HEC:O1A	2.16	0.45
1:C:313:HIS:HE1	2:C:1109:HEC:C1D	2.29	0.45
1:C:130:PRO:HA	1:C:134:GLU:OE1	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
1:C:161:ARG:CG	1:C:161:ARG:HH11	2.18	0.45
2:A:1115:HEC:HMB1	2:A:1115:HEC:HBB3	1.98	0.45
1:D:476:LEU:HB3	2:D:1111:HEC:HBC2	1.98	0.45
1:C:152:ILE:O	2:C:1107:HEC:O1D	2.34	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: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:372:THR:HG21	3:A:2088:HOH:O	2.17	0.44
1:D:492:LYS:HD3	2:D:1113:HEC:O1A	2.17	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: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
1:C:349:CYS:HA	2:C:1110:HEC:CHC	2.48	0.43
2:C:1111:HEC:CHA	2:C:1111:HEC:HBA2	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:D:316:ILE:HD11	2:D:1104:HEC:HAA2	1.99	0.43
1:D:313:HIS:HE1	2:D:1109:HEC:C1D	2.32	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:342:GLN:HG2	1:C:345:SER:HB2	2.00	0.43
1:B:346:MET:HE1	1:B:355:THR:HB	2.00	0.43
1:A:323:HIS:CE1	2:A:1109:HEC:ND	2.86	0.43
1:C:161:ARG:CG	1:C:161:ARG:NH1	2.79	0.43
1:C:83:CYS:HB2	2:C:1101:HEC:C2C	2.48	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
2:C:1111:HEC:HMC1	2:C:1111:HEC:HBC3	1.99	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:D:211:VAL:HG22	1:D:214:ARG:HB2	1.99	0.43
1:C:453:VAL:HG22	2:C:1113:HEC:HMC2	2.00	0.43
1:C:253:GLN:HA	1:C:256:PHE:CE2	2.54	0.42
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.74	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: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: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:328:THR:HG22	1:A:330:ASP:N	2.34	0.42
1:C:334:VAL:HG13	1:C:338:LYS:HD3	2.01	0.42
1:A:105:GLU:HG2	1:A:109:ILE:HD12	2.01	0.42
1:B:387:GLY:O	1:B:388:PHE:C	2.57	0.42
1:D:122:ALA:HB2	1:D:128:THR:HG21	2.02	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:B:357:VAL:HG13	1:B:366:HIS:HB3	2.01	0.42
1:B:453:VAL:HG22	2:B:1113:HEC:HMC2	2.01	0.42
1:A:483:ASN:HD22	2:A:1114:HEC:C1D	2.33	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
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:C:222:HIS:CD2	2:C:1107:HEC:NC	2.87	0.42
1:A:53:ARG:HG2	1:A:53:ARG:H	1.66	0.42
2:D:1101:HEC:HBC3	2:D:1101:HEC:HMC1	2.02	0.41
1:C:404:GLU:CD	1:C:404:GLU:H	2.23	0.41
1:D:66:HIS:ND1	2:D:1107:HEC:HBB1	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:121:LEU:CD1	2:C:1102:HEC:HMD3	2.50	0.41
1:B:226:ILE:HG22	1:B:230:MET:HE2	2.01	0.41
2:D:1108:HEC:HBC1	2:D:1110:HEC:CMC	2.50	0.41
1:C:229:HIS:CE1	1:C:240:GLY:HA3	2.56	0.41
2:D:1104:HEC:HBC1	2:D:1106:HEC:C2C	2.50	0.41
1:D:339:ALA:HA	2:D:1109:HEC:CMA	2.51	0.41
2:C:1103:HEC:HBB3	2:C:1103:HEC:HMB1	2.02	0.41
1:A:429:ILE:HD12	2:A:1113:HEC:HMB2	1.97	0.41
1:C:345:SER:O	1:C:351:GLY:HA3	2.21	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:342:GLN:HA	1:C:343:PRO:HD3	1.93	0.41
2:B:1112:HEC:HBC3	2:B:1112:HEC:HMC1	2.01	0.41
1:A:309:ARG:NH1	2:A:1104:HEC:CGD	2.84	0.41
1:C:420:PRO:HG3	3:C:2100:HOH:O	2.21	0.41
1:A:340:MET:HE3	2:A:1112:HEC:HAD2	2.03	0.41
1:C:456:LEU:HD22	2:C:1111:HEC:HMC1	2.02	0.41
1:B:515:TYR:OH	2:B:1113:HEC:O1D	2.31	0.41
1:A:429:ILE:HD11	2:A:1113:HEC:CMB	2.41	0.41
1:D:95:PHE:CD1	2:D:1101:HEC:HMD3	2.56	0.41
1:B:372:THR:HG21	1:B:374:SER:HB3	2.01	0.41
1:C:389:ASP:CG	1:C:390:ALA:N	2.74	0.41
1:A:423:THR:HA	1:A:473:LYS:O	2.20	0.41
1:C:279:PRO:HB2	1:C:283:ALA:CB	2.50	0.41
1:D:313:HIS:CE1	2:D:1109:HEC:C1D	3.04	0.40
1:C:201:SER:O	2:C:1105:HEC:HMC3	2.21	0.40
1:A:313:HIS:H	1:A:313:HIS:CD2	2.39	0.40
1:D:97:ARG:NH2	1:D:110:TYR:OH	2.52	0.40
1:B:159:HIS:O	1:B:163:VAL:HG23	2.21	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
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:A:177:ASN:O	2:A:1104:HEC:HMC3	2.21	0.40
1:B:346:MET:CE	1:B:355:THR:CB	2.99	0.40
1:A:434:VAL:HG22	1:A:434:VAL:O	2.21	0.40
1:C:299:LYS:NZ	3:C:2075:HOH:O	2.55	0.40
1:B:197:ASN:HA	1:B:267:ARG:HG2	2.02	0.40
1:D:312:HIS:HB3	1:D:315:ARG:O	2.21	0.40
1:A:528:ILE:HG22	1:A:530:LYS:HB2	2.04	0.40
1:A:121:LEU:HD13	2:A:1102:HEC:HMD3	2.02	0.40
1:B:71:THR:HG22	3:B:2059:HOH:O	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:287:MET:SD	1:A:326:ASN:HA	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/514 (97%)	463 (93%)	25 (5%)	9 (2%)	13	20
1	B	495/514 (96%)	460 (93%)	28 (6%)	7 (1%)	16	27
1	C	497/514 (97%)	468 (94%)	24 (5%)	5 (1%)	22	38
1	D	484/514 (94%)	451 (93%)	26 (5%)	7 (1%)	16	27
All	All	1973/2056 (96%)	1842 (93%)	103 (5%)	28 (1%)	16	27

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
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

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Mol	Chain	Res	Type
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%)	10	18
1	B	403/414 (97%)	368 (91%)	35 (9%)	15	27
1	C	404/414 (98%)	374 (93%)	30 (7%)	20	35
1	D	400/414 (97%)	359 (90%)	41 (10%)	10	19
All	All	1612/1656 (97%)	1464 (91%)	148 (9%)	13	24

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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 ⓘ

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	50,50,50	2.92	17 (34%)	56,82,82	1.48	10 (17%)
2	HEC	A	1102	1	50,50,50	2.76	16 (32%)	56,82,82	1.54	9 (16%)
2	HEC	A	1103	1	50,50,50	2.78	17 (34%)	56,82,82	1.80	13 (23%)
2	HEC	A	1104	1	50,50,50	2.72	14 (28%)	56,82,82	1.47	6 (10%)
2	HEC	A	1105	1	50,50,50	2.78	14 (28%)	56,82,82	1.52	11 (19%)
2	HEC	A	1106	1	50,50,50	2.72	16 (32%)	56,82,82	1.52	12 (21%)
2	HEC	A	1107	1	50,50,50	2.76	15 (30%)	56,82,82	1.89	14 (25%)
2	HEC	A	1108	1	50,50,50	2.82	15 (30%)	56,82,82	1.67	15 (26%)
2	HEC	A	1109	1	50,50,50	2.91	15 (30%)	56,82,82	1.52	10 (17%)
2	HEC	A	1110	1	50,50,50	2.76	16 (32%)	56,82,82	1.49	11 (19%)
2	HEC	A	1111	1	50,50,50	2.89	16 (32%)	56,82,82	1.42	7 (12%)
2	HEC	A	1112	1	50,50,50	2.79	16 (32%)	56,82,82	1.37	10 (17%)
2	HEC	A	1113	1	50,50,50	2.82	15 (30%)	56,82,82	1.45	8 (14%)
2	HEC	A	1114	1	50,50,50	2.97	16 (32%)	56,82,82	1.51	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	A	1115	1	50,50,50	2.86	16 (32%)	56,82,82	1.62	11 (19%)
2	HEC	A	1116	1	50,50,50	2.71	15 (30%)	56,82,82	1.65	12 (21%)
2	HEC	B	1101	1	50,50,50	2.83	15 (30%)	56,82,82	1.65	12 (21%)
2	HEC	B	1102	1	50,50,50	2.73	15 (30%)	56,82,82	1.46	10 (17%)
2	HEC	B	1103	1	50,50,50	2.86	16 (32%)	56,82,82	1.63	12 (21%)
2	HEC	B	1104	1	50,50,50	2.89	15 (30%)	56,82,82	1.52	8 (14%)
2	HEC	B	1105	1	50,50,50	2.95	18 (36%)	56,82,82	1.42	8 (14%)
2	HEC	B	1106	1	50,50,50	2.79	15 (30%)	56,82,82	1.52	12 (21%)
2	HEC	B	1107	1	50,50,50	2.73	14 (28%)	56,82,82	1.60	12 (21%)
2	HEC	B	1108	1	50,50,50	2.78	17 (34%)	56,82,82	1.49	7 (12%)
2	HEC	B	1109	1	50,50,50	2.91	18 (36%)	56,82,82	1.23	7 (12%)
2	HEC	B	1110	1	50,50,50	2.78	15 (30%)	56,82,82	1.79	13 (23%)
2	HEC	B	1111	1	50,50,50	2.83	16 (32%)	56,82,82	1.39	8 (14%)
2	HEC	B	1112	1	50,50,50	2.66	14 (28%)	56,82,82	1.71	14 (25%)
2	HEC	B	1113	1	50,50,50	2.81	16 (32%)	56,82,82	1.71	9 (16%)
2	HEC	B	1114	1	50,50,50	2.96	17 (34%)	56,82,82	1.42	8 (14%)
2	HEC	B	1115	1	50,50,50	2.91	16 (32%)	56,82,82	1.43	9 (16%)
2	HEC	B	1116	1	50,50,50	2.82	15 (30%)	56,82,82	1.65	11 (19%)
2	HEC	C	1101	1	50,50,50	2.67	14 (28%)	56,82,82	1.50	11 (19%)
2	HEC	C	1102	1	50,50,50	2.81	16 (32%)	56,82,82	1.50	10 (17%)
2	HEC	C	1103	1	50,50,50	2.76	16 (32%)	56,82,82	1.71	9 (16%)
2	HEC	C	1104	1	50,50,50	2.86	15 (30%)	56,82,82	1.45	11 (19%)
2	HEC	C	1105	1	50,50,50	2.80	15 (30%)	56,82,82	1.48	10 (17%)
2	HEC	C	1106	1	50,50,50	2.78	16 (32%)	56,82,82	1.68	15 (26%)
2	HEC	C	1107	1	50,50,50	2.73	13 (26%)	56,82,82	1.71	13 (23%)
2	HEC	C	1108	1	50,50,50	2.76	15 (30%)	56,82,82	1.43	11 (19%)
2	HEC	C	1109	1	50,50,50	2.73	16 (32%)	56,82,82	1.49	10 (17%)
2	HEC	C	1110	1	50,50,50	2.77	15 (30%)	56,82,82	1.65	12 (21%)
2	HEC	C	1111	1	50,50,50	2.77	15 (30%)	56,82,82	1.31	7 (12%)
2	HEC	C	1112	1	50,50,50	2.71	15 (30%)	56,82,82	1.39	7 (12%)
2	HEC	C	1113	1	50,50,50	2.79	14 (28%)	56,82,82	1.70	14 (25%)
2	HEC	C	1114	1	50,50,50	2.89	16 (32%)	56,82,82	1.47	7 (12%)
2	HEC	C	1115	1	50,50,50	2.91	15 (30%)	56,82,82	1.91	16 (28%)
2	HEC	C	1116	1	50,50,50	2.73	14 (28%)	56,82,82	1.66	13 (23%)
2	HEC	D	1101	1	50,50,50	2.91	15 (30%)	56,82,82	1.48	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	D	1102	1	50,50,50	2.84	17 (34%)	56,82,82	1.53	9 (16%)
2	HEC	D	1103	1	50,50,50	2.83	15 (30%)	56,82,82	1.79	15 (26%)
2	HEC	D	1104	1	50,50,50	2.81	15 (30%)	56,82,82	1.54	9 (16%)
2	HEC	D	1105	1	50,50,50	2.95	16 (32%)	56,82,82	1.45	8 (14%)
2	HEC	D	1106	1	50,50,50	2.80	16 (32%)	56,82,82	1.42	10 (17%)
2	HEC	D	1107	1	50,50,50	2.89	15 (30%)	56,82,82	1.51	10 (17%)
2	HEC	D	1108	1	50,50,50	2.88	16 (32%)	56,82,82	1.64	11 (19%)
2	HEC	D	1109	1	50,50,50	2.92	16 (32%)	56,82,82	1.37	11 (19%)
2	HEC	D	1110	1	50,50,50	2.94	17 (34%)	56,82,82	1.49	12 (21%)
2	HEC	D	1111	1	50,50,50	2.80	15 (30%)	56,82,82	1.51	10 (17%)
2	HEC	D	1112	1	50,50,50	2.78	14 (28%)	56,82,82	1.48	8 (14%)
2	HEC	D	1113	1	50,50,50	2.70	13 (26%)	56,82,82	1.63	12 (21%)
2	HEC	D	1114	1	50,50,50	2.82	17 (34%)	56,82,82	1.64	12 (21%)
2	HEC	D	1115	1	50,50,50	2.91	15 (30%)	56,82,82	1.53	8 (14%)
2	HEC	D	1116	1	50,50,50	2.72	14 (28%)	56,82,82	1.67	8 (14%)

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	-	0/10/54/54	0/0/8/8
2	HEC	A	1102	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1103	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1104	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1105	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1106	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1107	1	-	1/10/54/54	0/0/8/8
2	HEC	A	1108	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1109	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1110	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1111	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1112	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1113	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1114	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1115	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1116	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1101	1	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	B	1102	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1103	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1104	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1105	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1106	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1107	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1108	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1109	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1110	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1111	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1112	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1113	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1114	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1115	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1116	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1101	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1102	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1103	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1104	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1105	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1106	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1107	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1108	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1109	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1110	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1111	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1112	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1113	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1114	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1115	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1116	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1101	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1102	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1103	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1104	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1105	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1106	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1107	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1108	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1109	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1110	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1111	1	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	D	1112	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1113	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1114	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1115	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1116	1	-	0/10/54/54	0/0/8/8

All (987) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1103	HEC	C3C-CAC	10.72	1.57	1.35
2	D	1105	HEC	C3C-CAC	10.70	1.57	1.35
2	A	1101	HEC	C3C-CAC	10.60	1.57	1.35
2	B	1110	HEC	C3C-CAC	10.57	1.57	1.35
2	A	1107	HEC	C3C-CAC	10.56	1.57	1.35
2	C	1103	HEC	C3C-CAC	10.55	1.57	1.35
2	A	1114	HEC	C3C-CAC	10.46	1.56	1.35
2	B	1104	HEC	C3C-CAC	10.36	1.56	1.35
2	B	1114	HEC	C3C-CAC	10.33	1.56	1.35
2	D	1115	HEC	C3C-CAC	10.30	1.56	1.35
2	D	1103	HEC	C3C-CAC	10.30	1.56	1.35
2	B	1115	HEC	C3C-CAC	10.27	1.56	1.35
2	C	1114	HEC	C3C-CAC	10.25	1.56	1.35
2	A	1103	HEC	C3C-CAC	10.25	1.56	1.35
2	C	1110	HEC	C3C-CAC	10.25	1.56	1.35
2	B	1105	HEC	C3C-CAC	10.24	1.56	1.35
2	C	1106	HEC	C3B-CAB	10.20	1.56	1.35
2	A	1108	HEC	C3B-CAB	10.17	1.56	1.35
2	D	1110	HEC	C3C-CAC	10.17	1.56	1.35
2	D	1104	HEC	C3C-CAC	10.14	1.56	1.35
2	D	1107	HEC	C3C-CAC	10.14	1.56	1.35
2	A	1112	HEC	C3C-CAC	10.12	1.56	1.35
2	A	1113	HEC	C3C-CAC	10.11	1.56	1.35
2	B	1106	HEC	C3C-CAC	10.11	1.56	1.35
2	C	1105	HEC	C3C-CAC	10.11	1.56	1.35
2	C	1104	HEC	C3B-CAB	10.08	1.56	1.35
2	C	1107	HEC	C3C-CAC	10.07	1.56	1.35
2	B	1101	HEC	C3C-CAC	10.07	1.56	1.35
2	D	1109	HEC	C3B-CAB	10.04	1.56	1.35
2	C	1107	HEC	C3B-CAB	10.00	1.56	1.35
2	D	1108	HEC	C3B-CAB	10.00	1.56	1.35
2	B	1104	HEC	C3B-CAB	10.00	1.56	1.35
2	A	1108	HEC	C3C-CAC	9.99	1.56	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1106	HEC	C3C-CAC	9.97	1.55	1.35
2	C	1104	HEC	C3C-CAC	9.96	1.55	1.35
2	C	1116	HEC	C3B-CAB	9.95	1.55	1.35
2	B	1109	HEC	C3C-CAC	9.91	1.55	1.35
2	B	1113	HEC	C3C-CAC	9.91	1.55	1.35
2	D	1111	HEC	C3C-CAC	9.88	1.55	1.35
2	C	1112	HEC	C3C-CAC	9.88	1.55	1.35
2	D	1101	HEC	C3C-CAC	9.87	1.55	1.35
2	C	1102	HEC	C3C-CAC	9.85	1.55	1.35
2	D	1105	HEC	C3B-CAB	9.83	1.55	1.35
2	C	1115	HEC	C3C-CAC	9.82	1.55	1.35
2	A	1107	HEC	C3B-CAB	9.82	1.55	1.35
2	B	1102	HEC	C3C-CAC	9.82	1.55	1.35
2	D	1106	HEC	C3B-CAB	9.81	1.55	1.35
2	B	1116	HEC	C3C-CAC	9.81	1.55	1.35
2	C	1108	HEC	C3B-CAB	9.80	1.55	1.35
2	D	1116	HEC	C3B-CAB	9.78	1.55	1.35
2	B	1107	HEC	C3C-CAC	9.74	1.55	1.35
2	D	1101	HEC	C3B-CAB	9.74	1.55	1.35
2	C	1101	HEC	C3C-CAC	9.73	1.55	1.35
2	A	1115	HEC	C3C-CAC	9.73	1.55	1.35
2	B	1108	HEC	C3C-CAC	9.72	1.55	1.35
2	D	1107	HEC	C3B-CAB	9.70	1.55	1.35
2	B	1108	HEC	C3B-CAB	9.70	1.55	1.35
2	C	1102	HEC	C3B-CAB	9.69	1.55	1.35
2	D	1102	HEC	C3B-CAB	9.68	1.55	1.35
2	A	1102	HEC	C3C-CAC	9.68	1.55	1.35
2	D	1108	HEC	C3C-CAC	9.67	1.55	1.35
2	A	1102	HEC	C3B-CAB	9.67	1.55	1.35
2	B	1111	HEC	C3C-CAC	9.66	1.55	1.35
2	B	1101	HEC	C3B-CAB	9.65	1.55	1.35
2	B	1109	HEC	C3B-CAB	9.65	1.55	1.35
2	A	1111	HEC	C3C-CAC	9.62	1.55	1.35
2	D	1112	HEC	C3B-CAB	9.61	1.55	1.35
2	D	1102	HEC	C3C-CAC	9.60	1.55	1.35
2	A	1103	HEC	C3B-CAB	9.60	1.55	1.35
2	A	1113	HEC	C3B-CAB	9.59	1.55	1.35
2	B	1115	HEC	C3B-CAB	9.58	1.55	1.35
2	B	1102	HEC	C3B-CAB	9.58	1.55	1.35
2	A	1101	HEC	C3B-CAB	9.57	1.55	1.35
2	B	1103	HEC	C3B-CAB	9.56	1.55	1.35
2	B	1106	HEC	C3B-CAB	9.56	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1116	HEC	C3C-CAC	9.56	1.55	1.35
2	A	1105	HEC	C3B-CAB	9.55	1.55	1.35
2	A	1104	HEC	C3B-CAB	9.55	1.55	1.35
2	C	1115	HEC	C3B-CAB	9.54	1.55	1.35
2	D	1109	HEC	C3C-CAC	9.54	1.55	1.35
2	C	1111	HEC	C3C-CAC	9.54	1.55	1.35
2	D	1114	HEC	C3C-CAC	9.52	1.55	1.35
2	D	1115	HEC	C3B-CAB	9.47	1.54	1.35
2	A	1110	HEC	C3C-CAC	9.47	1.54	1.35
2	B	1107	HEC	C3B-CAB	9.45	1.54	1.35
2	A	1105	HEC	C3C-CAC	9.44	1.54	1.35
2	A	1116	HEC	C3B-CAB	9.44	1.54	1.35
2	C	1109	HEC	C3C-CAC	9.43	1.54	1.35
2	A	1114	HEC	C3B-CAB	9.42	1.54	1.35
2	B	1114	HEC	C3B-CAB	9.42	1.54	1.35
2	C	1113	HEC	C3B-CAB	9.41	1.54	1.35
2	D	1111	HEC	C3B-CAB	9.41	1.54	1.35
2	C	1109	HEC	C3B-CAB	9.40	1.54	1.35
2	C	1116	HEC	C3C-CAC	9.39	1.54	1.35
2	C	1111	HEC	C3B-CAB	9.39	1.54	1.35
2	A	1115	HEC	C3B-CAB	9.38	1.54	1.35
2	D	1116	HEC	C3C-CAC	9.37	1.54	1.35
2	D	1110	HEC	C3B-CAB	9.36	1.54	1.35
2	C	1101	HEC	C3B-CAB	9.35	1.54	1.35
2	B	1116	HEC	C3B-CAB	9.34	1.54	1.35
2	D	1112	HEC	C3C-CAC	9.34	1.54	1.35
2	D	1104	HEC	C3B-CAB	9.33	1.54	1.35
2	A	1111	HEC	C3B-CAB	9.32	1.54	1.35
2	A	1106	HEC	C3C-CAC	9.31	1.54	1.35
2	A	1104	HEC	C3C-CAC	9.30	1.54	1.35
2	C	1108	HEC	C3C-CAC	9.27	1.54	1.35
2	A	1112	HEC	C3B-CAB	9.23	1.54	1.35
2	B	1111	HEC	C3B-CAB	9.20	1.54	1.35
2	A	1110	HEC	C3B-CAB	9.20	1.54	1.35
2	A	1109	HEC	C3B-CAB	9.18	1.54	1.35
2	A	1109	HEC	C3C-CAC	9.15	1.54	1.35
2	B	1110	HEC	C3B-CAB	9.12	1.54	1.35
2	C	1112	HEC	C3B-CAB	9.12	1.54	1.35
2	C	1114	HEC	C3B-CAB	9.09	1.54	1.35
2	C	1103	HEC	C3B-CAB	9.09	1.54	1.35
2	A	1106	HEC	C3B-CAB	9.07	1.54	1.35
2	D	1103	HEC	C3B-CAB	9.05	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1113	HEC	C3B-CAB	9.05	1.54	1.35
2	B	1112	HEC	C3C-CAC	9.04	1.54	1.35
2	C	1113	HEC	C3C-CAC	9.02	1.54	1.35
2	B	1105	HEC	C3B-CAB	9.01	1.54	1.35
2	D	1114	HEC	C3B-CAB	8.99	1.53	1.35
2	C	1106	HEC	C3C-CAC	8.99	1.53	1.35
2	C	1110	HEC	C3B-CAB	8.91	1.53	1.35
2	B	1112	HEC	C3B-CAB	8.89	1.53	1.35
2	C	1105	HEC	C3B-CAB	8.82	1.53	1.35
2	B	1113	HEC	C3B-CAB	8.77	1.53	1.35
2	D	1113	HEC	C3C-CAC	8.71	1.53	1.35
2	A	1109	HEC	FE-ND	5.97	2.18	1.92
2	D	1110	HEC	C3D-C2D	5.95	1.55	1.37
2	A	1108	HEC	C3D-C2D	5.88	1.55	1.37
2	B	1114	HEC	C3D-C2D	5.79	1.54	1.37
2	D	1105	HEC	C3D-C2D	5.79	1.54	1.37
2	D	1114	HEC	C3D-C2D	5.68	1.54	1.37
2	A	1114	HEC	C3D-C2D	5.68	1.54	1.37
2	B	1104	HEC	C1B-C2B	5.67	1.47	1.40
2	B	1105	HEC	C1D-C2D	5.63	1.47	1.40
2	D	1109	HEC	C3D-C2D	5.62	1.54	1.37
2	B	1111	HEC	C3D-C2D	5.60	1.54	1.37
2	B	1102	HEC	C3D-C2D	5.60	1.54	1.37
2	C	1114	HEC	C3D-C2D	5.58	1.54	1.37
2	C	1102	HEC	C3D-C2D	5.57	1.54	1.37
2	D	1110	HEC	C1C-C2C	5.55	1.47	1.40
2	A	1102	HEC	C3D-C2D	5.54	1.54	1.37
2	B	1105	HEC	C1B-C2B	5.52	1.47	1.40
2	D	1111	HEC	C3D-C2D	5.49	1.53	1.37
2	D	1107	HEC	C1C-C2C	5.49	1.47	1.40
2	D	1102	HEC	C3D-C2D	5.48	1.53	1.37
2	C	1116	HEC	C3D-C2D	5.47	1.53	1.37
2	C	1111	HEC	C3D-C2D	5.46	1.53	1.37
2	A	1111	HEC	C3D-C2D	5.45	1.53	1.37
2	D	1106	HEC	C3D-C2D	5.43	1.53	1.37
2	B	1113	HEC	C3D-C2D	5.42	1.53	1.37
2	D	1101	HEC	C3D-C2D	5.42	1.53	1.37
2	A	1110	HEC	C3D-C2D	5.40	1.53	1.37
2	C	1115	HEC	C3D-C2D	5.40	1.53	1.37
2	A	1103	HEC	C1C-C2C	5.39	1.46	1.40
2	A	1109	HEC	C3D-C2D	5.36	1.53	1.37
2	D	1103	HEC	C3D-C2D	5.36	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1104	HEC	C1C-C2C	5.35	1.46	1.40
2	C	1113	HEC	C1C-C2C	5.31	1.46	1.40
2	B	1115	HEC	C3D-C2D	5.30	1.53	1.37
2	D	1104	HEC	C3D-C2D	5.30	1.53	1.37
2	D	1113	HEC	C1C-C2C	5.29	1.46	1.40
2	C	1105	HEC	C3D-C2D	5.29	1.53	1.37
2	A	1113	HEC	C3D-C2D	5.29	1.53	1.37
2	A	1106	HEC	C3D-C2D	5.28	1.53	1.37
2	B	1108	HEC	C3D-C2D	5.28	1.53	1.37
2	A	1101	HEC	C3D-C2D	5.27	1.53	1.37
2	B	1101	HEC	C3D-C2D	5.26	1.53	1.37
2	D	1107	HEC	C3D-C2D	5.25	1.53	1.37
2	B	1105	HEC	C3D-C2D	5.25	1.53	1.37
2	A	1112	HEC	C3D-C2D	5.25	1.53	1.37
2	C	1111	HEC	C1B-C2B	5.24	1.46	1.40
2	B	1116	HEC	C3D-C2D	5.23	1.53	1.37
2	C	1108	HEC	C1B-C2B	5.23	1.46	1.40
2	B	1110	HEC	C3D-C2D	5.19	1.53	1.37
2	C	1101	HEC	C3D-C2D	5.17	1.53	1.37
2	C	1108	HEC	C3D-C2D	5.16	1.53	1.37
2	A	1107	HEC	C3D-C2D	5.16	1.53	1.37
2	A	1104	HEC	C3D-C2D	5.15	1.52	1.37
2	D	1115	HEC	FE-ND	5.15	2.14	1.92
2	A	1105	HEC	C3D-C2D	5.15	1.52	1.37
2	D	1109	HEC	C1B-C2B	5.13	1.46	1.40
2	C	1106	HEC	C3D-C2D	5.10	1.52	1.37
2	B	1107	HEC	C1C-C2C	5.09	1.46	1.40
2	A	1109	HEC	C1B-C2B	5.07	1.46	1.40
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	1109	HEC	C3D-C2D	5.06	1.52	1.37
2	D	1111	HEC	FE-ND	5.04	2.14	1.92
2	B	1109	HEC	C3D-C2D	5.03	1.52	1.37
2	D	1116	HEC	C3D-C2D	5.03	1.52	1.37
2	C	1103	HEC	C3D-C2D	5.03	1.52	1.37
2	D	1109	HEC	C1D-C2D	5.02	1.46	1.40
2	D	1101	HEC	C1B-C2B	5.02	1.46	1.40
2	D	1103	HEC	C1C-C2C	5.02	1.46	1.40
2	C	1110	HEC	C3D-C2D	5.01	1.52	1.37
2	A	1111	HEC	C1B-C2B	5.00	1.46	1.40
2	A	1111	HEC	FE-NA	5.00	2.14	1.92
2	B	1112	HEC	C3D-C2D	4.98	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1105	HEC	C1D-C2D	4.98	1.46	1.40
2	A	1116	HEC	C3D-C2D	4.98	1.52	1.37
2	A	1104	HEC	C1C-C2C	4.96	1.46	1.40
2	C	1115	HEC	C1C-C2C	4.96	1.46	1.40
2	C	1107	HEC	C3D-C2D	4.95	1.52	1.37
2	B	1106	HEC	C3D-C2D	4.94	1.52	1.37
2	B	1107	HEC	C3D-C2D	4.93	1.52	1.37
2	B	1109	HEC	C1B-C2B	4.93	1.46	1.40
2	A	1109	HEC	C1D-C2D	4.92	1.46	1.40
2	B	1114	HEC	C1D-C2D	4.91	1.46	1.40
2	C	1112	HEC	C3D-C2D	4.91	1.52	1.37
2	B	1103	HEC	C1C-C2C	4.89	1.46	1.40
2	C	1114	HEC	C1C-C2C	4.89	1.46	1.40
2	D	1115	HEC	C3D-C2D	4.88	1.52	1.37
2	D	1108	HEC	C1C-C2C	4.87	1.46	1.40
2	C	1113	HEC	FE-ND	4.87	2.13	1.92
2	C	1103	HEC	C1C-C2C	4.86	1.46	1.40
2	B	1103	HEC	C3D-C2D	4.85	1.52	1.37
2	D	1109	HEC	C1C-C2C	4.84	1.46	1.40
2	D	1115	HEC	C1C-C2C	4.84	1.46	1.40
2	C	1104	HEC	C3D-C2D	4.83	1.52	1.37
2	D	1108	HEC	C3D-C2D	4.81	1.51	1.37
2	A	1115	HEC	C1C-C2C	4.80	1.46	1.40
2	A	1112	HEC	C1C-C2C	4.78	1.46	1.40
2	B	1114	HEC	C1B-C2B	4.78	1.46	1.40
2	B	1113	HEC	C1C-C2C	4.78	1.46	1.40
2	A	1101	HEC	C1B-C2B	4.76	1.46	1.40
2	A	1114	HEC	FE-NA	4.76	2.12	1.92
2	D	1102	HEC	C1C-C2C	4.75	1.46	1.40
2	B	1104	HEC	C3D-C2D	4.75	1.51	1.37
2	B	1109	HEC	C3C-C4C	4.73	1.47	1.41
2	A	1115	HEC	C3D-C2D	4.72	1.51	1.37
2	C	1106	HEC	C1D-C2D	4.72	1.46	1.40
2	A	1103	HEC	C3D-C2D	4.72	1.51	1.37
2	B	1114	HEC	C1C-C2C	4.71	1.46	1.40
2	D	1105	HEC	C1B-C2B	4.70	1.46	1.40
2	D	1113	HEC	C3D-C2D	4.70	1.51	1.37
2	A	1108	HEC	C1B-C2B	4.69	1.46	1.40
2	B	1115	HEC	C1B-C2B	4.69	1.46	1.40
2	D	1114	HEC	C1C-C2C	4.68	1.46	1.40
2	D	1113	HEC	FE-NA	4.68	2.12	1.92
2	D	1108	HEC	C1B-C2B	4.64	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1116	HEC	C1D-C2D	4.64	1.46	1.40
2	A	1111	HEC	C1C-C2C	4.64	1.46	1.40
2	B	1115	HEC	C1C-C2C	4.64	1.46	1.40
2	D	1111	HEC	C1B-C2B	4.63	1.46	1.40
2	A	1114	HEC	C1D-C2D	4.62	1.45	1.40
2	C	1114	HEC	C1D-C2D	4.61	1.45	1.40
2	B	1112	HEC	C1D-C2D	4.59	1.45	1.40
2	B	1114	HEC	C3C-C4C	4.59	1.47	1.41
2	D	1101	HEC	C1C-C2C	4.57	1.45	1.40
2	D	1104	HEC	C1B-C2B	4.55	1.45	1.40
2	B	1111	HEC	C1B-C2B	4.55	1.45	1.40
2	B	1110	HEC	C1C-C2C	4.52	1.45	1.40
2	B	1108	HEC	C1C-C2C	4.52	1.45	1.40
2	B	1106	HEC	C1D-C2D	4.51	1.45	1.40
2	D	1112	HEC	C1D-C2D	4.48	1.45	1.40
2	C	1108	HEC	C1D-C2D	4.48	1.45	1.40
2	B	1101	HEC	C1C-C2C	4.45	1.45	1.40
2	C	1101	HEC	C1C-C2C	4.44	1.45	1.40
2	B	1113	HEC	C1B-C2B	4.43	1.45	1.40
2	A	1101	HEC	C1C-C2C	4.42	1.45	1.40
2	C	1102	HEC	C3C-C4C	4.42	1.47	1.41
2	C	1104	HEC	C1B-C2B	4.41	1.45	1.40
2	D	1115	HEC	C1B-C2B	4.39	1.45	1.40
2	B	1116	HEC	C1C-C2C	4.39	1.45	1.40
2	D	1106	HEC	C1B-C2B	4.39	1.45	1.40
2	A	1113	HEC	C1C-C2C	4.38	1.45	1.40
2	A	1102	HEC	C1B-C2B	4.38	1.45	1.40
2	B	1116	HEC	C1D-C2D	4.38	1.45	1.40
2	C	1107	HEC	C1C-C2C	4.37	1.45	1.40
2	C	1109	HEC	C1C-C2C	4.36	1.45	1.40
2	A	1101	HEC	FE-ND	4.36	2.11	1.92
2	C	1115	HEC	FE-ND	4.36	2.11	1.92
2	C	1109	HEC	FE-NC	4.35	2.11	1.92
2	A	1115	HEC	C3B-C4B	4.34	1.47	1.41
2	C	1111	HEC	C1C-C2C	4.33	1.45	1.40
2	C	1102	HEC	C1B-C2B	4.32	1.45	1.40
2	D	1102	HEC	C1B-C2B	4.32	1.45	1.40
2	C	1106	HEC	C1B-C2B	4.32	1.45	1.40
2	B	1109	HEC	C1C-C2C	4.30	1.45	1.40
2	A	1109	HEC	C1C-C2C	4.30	1.45	1.40
2	D	1102	HEC	C1D-C2D	4.29	1.45	1.40
2	A	1111	HEC	C1D-C2D	4.29	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	HEC	C3C-C4C	4.28	1.47	1.41
2	A	1102	HEC	FE-NA	4.27	2.10	1.92
2	D	1104	HEC	C1D-C2D	4.27	1.45	1.40
2	C	1112	HEC	C3B-C2B	-4.27	1.32	1.41
2	A	1106	HEC	C1B-C2B	4.27	1.45	1.40
2	D	1105	HEC	FE-NC	4.25	2.10	1.92
2	A	1114	HEC	C3C-C4C	4.25	1.46	1.41
2	B	1106	HEC	C1C-C2C	4.24	1.45	1.40
2	B	1115	HEC	FE-NA	4.24	2.10	1.92
2	A	1106	HEC	C1C-C2C	4.24	1.45	1.40
2	D	1113	HEC	C1B-C2B	4.23	1.45	1.40
2	C	1102	HEC	C1C-C2C	4.23	1.45	1.40
2	D	1114	HEC	C1B-C2B	4.23	1.45	1.40
2	A	1112	HEC	C1D-C2D	4.23	1.45	1.40
2	B	1115	HEC	FE-ND	4.22	2.10	1.92
2	D	1108	HEC	C3B-C2B	-4.22	1.32	1.41
2	A	1116	HEC	C1D-C2D	4.22	1.45	1.40
2	C	1105	HEC	C1C-C2C	4.21	1.45	1.40
2	C	1110	HEC	C1B-C2B	4.20	1.45	1.40
2	C	1105	HEC	C1D-C2D	4.20	1.45	1.40
2	C	1104	HEC	FE-ND	4.20	2.10	1.92
2	C	1114	HEC	FE-NC	4.20	2.10	1.92
2	A	1115	HEC	FE-NC	4.20	2.10	1.92
2	C	1115	HEC	FE-NC	4.20	2.10	1.92
2	C	1110	HEC	FE-NA	4.19	2.10	1.92
2	B	1103	HEC	FE-NB	4.19	2.10	1.92
2	A	1113	HEC	C1B-C2B	4.18	1.45	1.40
2	D	1113	HEC	C3C-C2C	-4.18	1.32	1.41
2	B	1115	HEC	C1D-C2D	4.16	1.45	1.40
2	C	1113	HEC	C3C-C2C	-4.15	1.32	1.41
2	B	1107	HEC	C1D-C2D	4.13	1.45	1.40
2	A	1115	HEC	C1D-C2D	4.13	1.45	1.40
2	D	1105	HEC	C1C-C2C	4.13	1.45	1.40
2	A	1110	HEC	C1D-C2D	4.12	1.45	1.40
2	D	1115	HEC	FE-NA	4.11	2.10	1.92
2	D	1107	HEC	C1D-C2D	4.10	1.45	1.40
2	B	1109	HEC	FE-ND	4.10	2.10	1.92
2	A	1113	HEC	C1D-C2D	4.09	1.45	1.40
2	B	1105	HEC	C3C-C4C	4.08	1.46	1.41
2	A	1107	HEC	C1C-C2C	4.07	1.45	1.40
2	A	1105	HEC	C1B-C2B	4.07	1.45	1.40
2	B	1109	HEC	C3C-C2C	-4.07	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1116	HEC	C3B-C2B	-4.06	1.32	1.41
2	D	1112	HEC	C1C-C2C	4.06	1.45	1.40
2	B	1101	HEC	C1D-C2D	4.05	1.45	1.40
2	D	1106	HEC	C1D-C2D	4.04	1.45	1.40
2	D	1114	HEC	C1D-C2D	4.04	1.45	1.40
2	B	1111	HEC	C1C-C2C	4.02	1.45	1.40
2	B	1111	HEC	C3B-C2B	-4.01	1.32	1.41
2	A	1104	HEC	C1B-C2B	4.01	1.45	1.40
2	D	1101	HEC	C3B-C4B	4.01	1.46	1.41
2	C	1113	HEC	FE-NC	4.00	2.09	1.92
2	D	1105	HEC	C1D-C2D	4.00	1.45	1.40
2	B	1107	HEC	C1B-C2B	3.99	1.45	1.40
2	A	1106	HEC	C1D-C2D	3.99	1.45	1.40
2	D	1107	HEC	C3C-C4C	3.98	1.46	1.41
2	A	1103	HEC	C3B-C2B	-3.98	1.33	1.41
2	C	1110	HEC	C1C-C2C	3.98	1.45	1.40
2	B	1113	HEC	C3B-C2B	-3.97	1.33	1.41
2	B	1104	HEC	FE-NC	3.97	2.09	1.92
2	B	1111	HEC	C1D-C2D	3.97	1.45	1.40
2	A	1110	HEC	C1C-C2C	3.95	1.45	1.40
2	D	1106	HEC	C1C-C2C	3.95	1.45	1.40
2	D	1110	HEC	C1D-C2D	3.95	1.45	1.40
2	D	1116	HEC	C1C-C2C	3.95	1.45	1.40
2	A	1102	HEC	C1D-C2D	3.95	1.45	1.40
2	C	1114	HEC	C1B-C2B	3.93	1.45	1.40
2	A	1110	HEC	C3B-C2B	-3.93	1.33	1.41
2	D	1112	HEC	FE-ND	3.93	2.09	1.92
2	B	1104	HEC	FE-ND	3.91	2.09	1.92
2	D	1110	HEC	C3C-C4C	3.90	1.46	1.41
2	D	1110	HEC	FE-NC	3.90	2.09	1.92
2	C	1107	HEC	C3B-C4B	3.88	1.46	1.41
2	A	1109	HEC	FE-NA	3.88	2.09	1.92
2	D	1116	HEC	C3C-C2C	-3.88	1.33	1.41
2	A	1106	HEC	C3C-C2C	-3.87	1.33	1.41
2	A	1104	HEC	C3B-C2B	-3.87	1.33	1.41
2	B	1104	HEC	C1C-C2C	3.86	1.45	1.40
2	B	1109	HEC	C1D-C2D	3.86	1.45	1.40
2	C	1115	HEC	FE-NB	3.85	2.09	1.92
2	C	1112	HEC	C1D-C2D	3.85	1.45	1.40
2	A	1107	HEC	C3C-C4C	3.84	1.46	1.41
2	D	1115	HEC	C1D-C2D	3.84	1.45	1.40
2	D	1108	HEC	FE-NC	3.84	2.08	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1105	HEC	C3C-C2C	-3.83	1.33	1.41
2	D	1110	HEC	C1B-C2B	3.83	1.45	1.40
2	B	1112	HEC	C1B-C2B	3.83	1.44	1.40
2	C	1103	HEC	C3B-C2B	-3.83	1.33	1.41
2	A	1101	HEC	C1D-C2D	3.82	1.44	1.40
2	B	1102	HEC	C1D-C2D	3.82	1.44	1.40
2	A	1110	HEC	C3C-C4C	3.82	1.46	1.41
2	A	1105	HEC	FE-ND	3.82	2.08	1.92
2	C	1115	HEC	C3B-C2B	-3.81	1.33	1.41
2	B	1103	HEC	C3B-C2B	-3.81	1.33	1.41
2	C	1106	HEC	FE-NA	3.81	2.08	1.92
2	C	1105	HEC	FE-NC	3.80	2.08	1.92
2	C	1109	HEC	C1D-C2D	3.80	1.44	1.40
2	C	1108	HEC	C1C-C2C	3.79	1.44	1.40
2	C	1105	HEC	C3B-C2B	-3.78	1.33	1.41
2	A	1106	HEC	CBC-CAC	-3.78	1.33	1.49
2	A	1105	HEC	C1C-C2C	3.78	1.44	1.40
2	C	1103	HEC	C1D-C2D	3.77	1.44	1.40
2	A	1105	HEC	CBC-CAC	-3.77	1.33	1.49
2	B	1111	HEC	C3C-C4C	3.77	1.46	1.41
2	D	1110	HEC	C3B-C4B	3.77	1.46	1.41
2	A	1114	HEC	C1B-C2B	3.77	1.44	1.40
2	A	1114	HEC	C1C-C2C	3.77	1.44	1.40
2	D	1113	HEC	FE-ND	3.76	2.08	1.92
2	B	1112	HEC	FE-ND	3.76	2.08	1.92
2	C	1105	HEC	C1B-C2B	3.76	1.44	1.40
2	C	1102	HEC	C3C-C2C	-3.76	1.33	1.41
2	B	1102	HEC	C1B-C2B	3.76	1.44	1.40
2	A	1116	HEC	FE-ND	3.76	2.08	1.92
2	A	1113	HEC	C3C-C4C	3.75	1.46	1.41
2	D	1104	HEC	FE-ND	3.76	2.08	1.92
2	D	1114	HEC	C3B-C4B	3.75	1.46	1.41
2	B	1112	HEC	CBC-CAC	-3.75	1.33	1.49
2	A	1114	HEC	C3B-C4B	3.74	1.46	1.41
2	C	1114	HEC	C3B-C2B	-3.74	1.33	1.41
2	B	1116	HEC	CBC-CAC	-3.74	1.33	1.49
2	A	1107	HEC	C1D-C2D	3.74	1.44	1.40
2	D	1111	HEC	C1D-C2D	3.73	1.44	1.40
2	A	1112	HEC	C3B-C2B	-3.73	1.33	1.41
2	D	1116	HEC	C1D-C2D	3.73	1.44	1.40
2	B	1105	HEC	C3B-C2B	-3.72	1.33	1.41
2	B	1101	HEC	FE-ND	3.72	2.08	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1112	HEC	C3B-C2B	-3.72	1.33	1.41
2	D	1107	HEC	CBB-CAB	-3.72	1.33	1.49
2	C	1116	HEC	CBC-CAC	-3.72	1.33	1.49
2	A	1104	HEC	C1D-C2D	3.72	1.44	1.40
2	B	1105	HEC	FE-NC	3.71	2.08	1.92
2	C	1110	HEC	CBB-CAB	-3.71	1.33	1.49
2	D	1101	HEC	C1D-C2D	3.71	1.44	1.40
2	B	1107	HEC	C3C-C2C	-3.71	1.33	1.41
2	C	1113	HEC	CBC-CAC	-3.70	1.33	1.49
2	B	1113	HEC	C3C-C2C	-3.70	1.33	1.41
2	C	1104	HEC	C1D-C2D	3.69	1.44	1.40
2	D	1105	HEC	FE-ND	3.69	2.08	1.92
2	B	1111	HEC	CBB-CAB	-3.69	1.33	1.49
2	C	1115	HEC	FE-NA	3.68	2.08	1.92
2	C	1112	HEC	C1B-C2B	3.68	1.44	1.40
2	A	1106	HEC	FE-NB	3.68	2.08	1.92
2	A	1109	HEC	C3C-C4C	3.68	1.46	1.41
2	C	1111	HEC	C3C-C2C	-3.68	1.33	1.41
2	B	1108	HEC	CBC-CAC	-3.67	1.33	1.49
2	B	1110	HEC	C1D-C2D	3.67	1.44	1.40
2	B	1104	HEC	C1D-C2D	3.67	1.44	1.40
2	C	1105	HEC	C3C-C2C	-3.67	1.33	1.41
2	A	1111	HEC	C3C-C2C	-3.67	1.33	1.41
2	D	1114	HEC	CBB-CAB	-3.67	1.33	1.49
2	B	1102	HEC	C3B-C2B	-3.66	1.33	1.41
2	B	1110	HEC	C1B-C2B	3.66	1.44	1.40
2	D	1116	HEC	C3B-C4B	3.65	1.46	1.41
2	B	1116	HEC	CBB-CAB	-3.65	1.33	1.49
2	A	1111	HEC	C3B-C2B	-3.65	1.33	1.41
2	A	1114	HEC	CBB-CAB	-3.65	1.33	1.49
2	B	1106	HEC	CBB-CAB	-3.64	1.33	1.49
2	C	1110	HEC	FE-NC	3.64	2.08	1.92
2	C	1109	HEC	CBC-CAC	-3.64	1.33	1.49
2	A	1115	HEC	FE-NB	3.63	2.08	1.92
2	A	1115	HEC	CBC-CAC	-3.63	1.33	1.49
2	D	1112	HEC	FE-NC	3.62	2.08	1.92
2	A	1105	HEC	C3C-C4C	3.62	1.46	1.41
2	C	1116	HEC	CBB-CAB	-3.62	1.33	1.49
2	D	1103	HEC	C3C-C4C	3.62	1.46	1.41
2	D	1108	HEC	FE-NB	3.61	2.08	1.92
2	A	1111	HEC	CBC-CAC	-3.61	1.33	1.49
2	B	1116	HEC	C3B-C2B	-3.61	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1112	HEC	C3C-C4C	3.61	1.46	1.41
2	A	1112	HEC	CBB-CAB	-3.61	1.33	1.49
2	D	1107	HEC	C1B-C2B	3.61	1.44	1.40
2	B	1110	HEC	CBB-CAB	-3.60	1.33	1.49
2	D	1112	HEC	C3B-C2B	-3.60	1.33	1.41
2	D	1111	HEC	C1C-C2C	3.60	1.44	1.40
2	A	1108	HEC	CBC-CAC	-3.60	1.33	1.49
2	D	1115	HEC	CBB-CAB	-3.60	1.33	1.49
2	A	1116	HEC	C1C-C2C	3.60	1.44	1.40
2	D	1101	HEC	FE-NA	3.60	2.07	1.92
2	A	1116	HEC	CBC-CAC	-3.59	1.33	1.49
2	C	1108	HEC	CBB-CAB	-3.59	1.34	1.49
2	B	1108	HEC	C3B-C2B	-3.58	1.33	1.41
2	D	1102	HEC	FE-NA	3.58	2.07	1.92
2	B	1115	HEC	CBB-CAB	-3.58	1.34	1.49
2	B	1106	HEC	C1B-C2B	3.58	1.44	1.40
2	B	1102	HEC	FE-NB	3.58	2.07	1.92
2	D	1113	HEC	C3B-C2B	-3.58	1.33	1.41
2	D	1116	HEC	CBC-CAC	-3.57	1.34	1.49
2	D	1108	HEC	C3C-C2C	-3.57	1.33	1.41
2	A	1109	HEC	CBC-CAC	-3.57	1.34	1.49
2	C	1114	HEC	CBB-CAB	-3.57	1.34	1.49
2	D	1115	HEC	C3B-C2B	-3.57	1.33	1.41
2	A	1115	HEC	C1B-C2B	3.57	1.44	1.40
2	C	1115	HEC	C3C-C2C	-3.57	1.33	1.41
2	D	1108	HEC	CBC-CAC	-3.56	1.34	1.49
2	C	1106	HEC	FE-NB	3.56	2.07	1.92
2	C	1104	HEC	CBC-CAC	-3.56	1.34	1.49
2	A	1107	HEC	C1B-C2B	3.56	1.44	1.40
2	B	1101	HEC	FE-NC	3.55	2.07	1.92
2	D	1111	HEC	CBB-CAB	-3.55	1.34	1.49
2	B	1113	HEC	CBB-CAB	-3.55	1.34	1.49
2	B	1111	HEC	CBC-CAC	-3.55	1.34	1.49
2	D	1104	HEC	CBB-CAB	-3.55	1.34	1.49
2	C	1111	HEC	CBB-CAB	-3.55	1.34	1.49
2	B	1111	HEC	C3C-C2C	-3.55	1.34	1.41
2	B	1105	HEC	CBB-CAB	-3.55	1.34	1.49
2	C	1115	HEC	C1B-C2B	3.55	1.44	1.40
2	C	1112	HEC	CBC-CAC	-3.54	1.34	1.49
2	D	1103	HEC	C3B-C2B	-3.54	1.34	1.41
2	D	1103	HEC	C3C-C2C	-3.54	1.34	1.41
2	B	1106	HEC	FE-NA	3.54	2.07	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1114	HEC	CBC-CAC	-3.53	1.34	1.49
2	B	1116	HEC	C3C-C2C	-3.53	1.34	1.41
2	B	1103	HEC	CBC-CAC	-3.53	1.34	1.49
2	D	1104	HEC	C1C-C2C	3.53	1.44	1.40
2	D	1102	HEC	C3C-C4C	3.53	1.46	1.41
2	A	1114	HEC	C3B-C2B	-3.52	1.34	1.41
2	B	1109	HEC	CBC-CAC	-3.52	1.34	1.49
2	D	1105	HEC	CBB-CAB	-3.51	1.34	1.49
2	A	1108	HEC	C1C-C2C	3.51	1.44	1.40
2	D	1101	HEC	CBC-CAC	-3.51	1.34	1.49
2	D	1103	HEC	FE-NC	3.51	2.07	1.92
2	C	1113	HEC	C3B-C2B	-3.51	1.34	1.41
2	B	1115	HEC	CBC-CAC	-3.51	1.34	1.49
2	B	1112	HEC	C1C-C2C	3.51	1.44	1.40
2	C	1106	HEC	C3C-C2C	-3.51	1.34	1.41
2	B	1114	HEC	CBB-CAB	-3.51	1.34	1.49
2	A	1113	HEC	CBC-CAC	-3.50	1.34	1.49
2	D	1103	HEC	CBB-CAB	-3.50	1.34	1.49
2	D	1109	HEC	C3C-C2C	-3.50	1.34	1.41
2	D	1115	HEC	CBC-CAC	-3.50	1.34	1.49
2	D	1101	HEC	C3B-C2B	-3.50	1.34	1.41
2	A	1113	HEC	C3B-C2B	-3.49	1.34	1.41
2	D	1114	HEC	CBC-CAC	-3.49	1.34	1.49
2	C	1114	HEC	C3C-C4C	3.49	1.46	1.41
2	B	1103	HEC	C1B-C2B	3.49	1.44	1.40
2	D	1108	HEC	CBB-CAB	-3.48	1.34	1.49
2	B	1112	HEC	CBB-CAB	-3.48	1.34	1.49
2	C	1103	HEC	C1B-C2B	3.48	1.44	1.40
2	A	1105	HEC	C3B-C2B	-3.48	1.34	1.41
2	B	1103	HEC	C1D-C2D	3.48	1.44	1.40
2	A	1116	HEC	C1B-C2B	3.48	1.44	1.40
2	C	1103	HEC	CBC-CAC	-3.48	1.34	1.49
2	A	1113	HEC	C3C-C2C	-3.47	1.34	1.41
2	C	1101	HEC	C3C-C4C	3.47	1.46	1.41
2	B	1105	HEC	CBC-CAC	-3.47	1.34	1.49
2	A	1106	HEC	C3B-C2B	-3.47	1.34	1.41
2	D	1103	HEC	C1D-C2D	3.47	1.44	1.40
2	C	1115	HEC	CBC-CAC	-3.46	1.34	1.49
2	C	1109	HEC	C3B-C2B	-3.46	1.34	1.41
2	C	1110	HEC	C3B-C2B	-3.46	1.34	1.41
2	B	1108	HEC	C3C-C2C	-3.46	1.34	1.41
2	C	1112	HEC	CBB-CAB	-3.46	1.34	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1103	HEC	C1B-C2B	3.46	1.44	1.40
2	D	1110	HEC	CBB-CAB	-3.46	1.34	1.49
2	C	1102	HEC	C3B-C2B	-3.45	1.34	1.41
2	B	1116	HEC	FE-NB	3.45	2.07	1.92
2	C	1116	HEC	C1C-C2C	3.45	1.44	1.40
2	D	1113	HEC	CBC-CAC	-3.45	1.34	1.49
2	A	1109	HEC	CBB-CAB	-3.45	1.34	1.49
2	D	1112	HEC	CBB-CAB	-3.44	1.34	1.49
2	A	1112	HEC	FE-ND	3.44	2.07	1.92
2	D	1107	HEC	FE-NC	3.44	2.07	1.92
2	D	1103	HEC	CBC-CAC	-3.44	1.34	1.49
2	D	1113	HEC	CBB-CAB	-3.44	1.34	1.49
2	D	1104	HEC	CBC-CAC	-3.44	1.34	1.49
2	C	1116	HEC	C3C-C2C	-3.43	1.34	1.41
2	B	1113	HEC	C3C-C4C	3.43	1.45	1.41
2	B	1108	HEC	C1B-C2B	3.43	1.44	1.40
2	C	1104	HEC	C3C-C2C	-3.43	1.34	1.41
2	D	1109	HEC	CBC-CAC	-3.42	1.34	1.49
2	B	1115	HEC	C3B-C2B	-3.42	1.34	1.41
2	C	1114	HEC	FE-NB	3.42	2.07	1.92
2	C	1114	HEC	C3C-C2C	-3.42	1.34	1.41
2	A	1102	HEC	CBC-CAC	-3.42	1.34	1.49
2	B	1103	HEC	FE-NA	3.42	2.07	1.92
2	A	1116	HEC	CBB-CAB	-3.42	1.34	1.49
2	B	1101	HEC	CBC-CAC	-3.42	1.34	1.49
2	C	1108	HEC	C3C-C2C	-3.42	1.34	1.41
2	B	1106	HEC	C3C-C4C	3.41	1.45	1.41
2	D	1106	HEC	CBC-CAC	-3.41	1.34	1.49
2	C	1105	HEC	CBC-CAC	-3.41	1.34	1.49
2	A	1115	HEC	C3B-C2B	-3.41	1.34	1.41
2	B	1109	HEC	CBB-CAB	-3.41	1.34	1.49
2	C	1112	HEC	C1C-C2C	3.41	1.44	1.40
2	C	1104	HEC	C3B-C4B	3.41	1.45	1.41
2	C	1115	HEC	CBB-CAB	-3.41	1.34	1.49
2	B	1116	HEC	C1B-C2B	3.41	1.44	1.40
2	B	1106	HEC	CBC-CAC	-3.41	1.34	1.49
2	A	1115	HEC	CBB-CAB	-3.41	1.34	1.49
2	D	1105	HEC	C3C-C4C	3.40	1.45	1.41
2	D	1107	HEC	CBC-CAC	-3.40	1.34	1.49
2	B	1109	HEC	C3B-C2B	-3.40	1.34	1.41
2	C	1101	HEC	C1B-C2B	3.40	1.44	1.40
2	C	1107	HEC	CBC-CAC	-3.40	1.34	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	HEC	FE-NA	3.40	2.07	1.92
2	A	1108	HEC	CBB-CAB	-3.40	1.34	1.49
2	C	1108	HEC	C3B-C2B	-3.40	1.34	1.41
2	C	1105	HEC	CBB-CAB	-3.40	1.34	1.49
2	A	1110	HEC	C1B-C2B	3.39	1.44	1.40
2	A	1106	HEC	C3C-C4C	3.39	1.45	1.41
2	D	1101	HEC	FE-NB	3.39	2.07	1.92
2	A	1109	HEC	C3C-C2C	-3.39	1.34	1.41
2	A	1106	HEC	CBB-CAB	-3.38	1.34	1.49
2	B	1116	HEC	C3B-C4B	3.39	1.45	1.41
2	B	1108	HEC	CBB-CAB	-3.38	1.34	1.49
2	A	1104	HEC	FE-NB	3.38	2.06	1.92
2	A	1115	HEC	FE-NA	3.38	2.06	1.92
2	B	1107	HEC	C3B-C2B	-3.37	1.34	1.41
2	D	1106	HEC	C3C-C2C	-3.37	1.34	1.41
2	B	1104	HEC	C3B-C4B	3.37	1.45	1.41
2	B	1103	HEC	CBB-CAB	-3.37	1.34	1.49
2	B	1116	HEC	FE-NA	3.37	2.06	1.92
2	A	1104	HEC	CBC-CAC	-3.36	1.34	1.49
2	D	1108	HEC	FE-NA	3.36	2.06	1.92
2	D	1110	HEC	FE-ND	3.36	2.06	1.92
2	B	1107	HEC	CBC-CAC	-3.36	1.35	1.49
2	D	1102	HEC	C3B-C2B	-3.36	1.34	1.41
2	A	1107	HEC	CBC-CAC	-3.36	1.35	1.49
2	D	1116	HEC	CBB-CAB	-3.35	1.35	1.49
2	A	1110	HEC	CBC-CAC	-3.36	1.35	1.49
2	A	1112	HEC	CBC-CAC	-3.35	1.35	1.49
2	C	1108	HEC	CBC-CAC	-3.35	1.35	1.49
2	C	1113	HEC	C1B-C2B	3.35	1.44	1.40
2	A	1110	HEC	CBB-CAB	-3.35	1.35	1.49
2	C	1116	HEC	FE-NC	3.35	2.06	1.92
2	C	1115	HEC	C3B-C4B	3.35	1.45	1.41
2	C	1104	HEC	CBB-CAB	-3.35	1.35	1.49
2	B	1108	HEC	C1D-C2D	3.35	1.44	1.40
2	D	1102	HEC	CBC-CAC	-3.35	1.35	1.49
2	D	1109	HEC	C3B-C2B	-3.35	1.34	1.41
2	A	1104	HEC	CBB-CAB	-3.34	1.35	1.49
2	A	1113	HEC	FE-NB	3.34	2.06	1.92
2	A	1108	HEC	C3C-C2C	-3.34	1.34	1.41
2	A	1111	HEC	CBB-CAB	-3.34	1.35	1.49
2	D	1107	HEC	C3C-C2C	-3.34	1.34	1.41
2	C	1102	HEC	CBB-CAB	-3.34	1.35	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1114	HEC	CBC-CAC	-3.34	1.35	1.49
2	B	1104	HEC	CBC-CAC	-3.33	1.35	1.49
2	A	1110	HEC	C3C-C2C	-3.33	1.34	1.41
2	D	1103	HEC	C3B-C4B	3.33	1.45	1.41
2	C	1112	HEC	C3C-C2C	-3.33	1.34	1.41
2	D	1109	HEC	FE-NA	3.33	2.06	1.92
2	C	1106	HEC	CBC-CAC	-3.32	1.35	1.49
2	A	1105	HEC	CBB-CAB	-3.32	1.35	1.49
2	A	1109	HEC	C3B-C2B	-3.32	1.34	1.41
2	C	1106	HEC	CBB-CAB	-3.32	1.35	1.49
2	B	1107	HEC	CBB-CAB	-3.32	1.35	1.49
2	D	1109	HEC	CBB-CAB	-3.32	1.35	1.49
2	A	1112	HEC	FE-NA	3.31	2.06	1.92
2	A	1110	HEC	FE-ND	3.31	2.06	1.92
2	C	1109	HEC	C3C-C2C	-3.31	1.34	1.41
2	D	1104	HEC	C3B-C2B	-3.31	1.34	1.41
2	C	1113	HEC	CBB-CAB	-3.30	1.35	1.49
2	C	1112	HEC	C3C-C4C	3.30	1.45	1.41
2	B	1101	HEC	C3B-C2B	-3.30	1.34	1.41
2	C	1107	HEC	C3B-C2B	-3.30	1.34	1.41
2	A	1111	HEC	C3B-C4B	3.29	1.45	1.41
2	C	1102	HEC	C3B-C4B	3.29	1.45	1.41
2	A	1108	HEC	FE-ND	3.29	2.06	1.92
2	D	1112	HEC	CBC-CAC	-3.29	1.35	1.49
2	A	1114	HEC	FE-NC	3.29	2.06	1.92
2	A	1101	HEC	CBB-CAB	-3.28	1.35	1.49
2	A	1115	HEC	C3C-C4C	3.28	1.45	1.41
2	D	1110	HEC	CBC-CAC	-3.28	1.35	1.49
2	C	1102	HEC	C1D-C2D	3.28	1.44	1.40
2	B	1113	HEC	CBC-CAC	-3.28	1.35	1.49
2	A	1107	HEC	C3C-C2C	-3.28	1.34	1.41
2	A	1112	HEC	C3C-C2C	-3.28	1.34	1.41
2	C	1107	HEC	FE-NB	3.27	2.06	1.92
2	A	1103	HEC	CBC-CAC	-3.27	1.35	1.49
2	D	1116	HEC	C1B-C2B	3.27	1.44	1.40
2	C	1110	HEC	CBC-CAC	-3.27	1.35	1.49
2	D	1105	HEC	C3B-C2B	-3.27	1.34	1.41
2	D	1107	HEC	C3B-C4B	3.27	1.45	1.41
2	A	1108	HEC	C1D-C2D	3.27	1.44	1.40
2	B	1102	HEC	CBC-CAC	-3.27	1.35	1.49
2	B	1101	HEC	CBB-CAB	-3.26	1.35	1.49
2	B	1105	HEC	C3B-C4B	3.26	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1114	HEC	C3B-C2B	-3.26	1.34	1.41
2	B	1108	HEC	FE-NA	3.25	2.06	1.92
2	D	1112	HEC	FE-NB	3.25	2.06	1.92
2	D	1106	HEC	CBB-CAB	-3.24	1.35	1.49
2	C	1107	HEC	C3C-C2C	-3.24	1.34	1.41
2	B	1102	HEC	C1C-C2C	3.24	1.44	1.40
2	A	1109	HEC	C3B-C4B	3.24	1.45	1.41
2	C	1105	HEC	C3B-C4B	3.24	1.45	1.41
2	C	1116	HEC	C3B-C2B	-3.24	1.34	1.41
2	A	1107	HEC	CBB-CAB	-3.24	1.35	1.49
2	C	1114	HEC	CBC-CAC	-3.23	1.35	1.49
2	D	1109	HEC	FE-NB	3.23	2.06	1.92
2	B	1115	HEC	C3B-C4B	3.23	1.45	1.41
2	D	1101	HEC	CBB-CAB	-3.23	1.35	1.49
2	A	1116	HEC	C3B-C2B	-3.23	1.34	1.41
2	A	1102	HEC	C3C-C2C	-3.23	1.34	1.41
2	D	1114	HEC	FE-ND	3.23	2.06	1.92
2	C	1111	HEC	C1D-C2D	3.23	1.44	1.40
2	D	1105	HEC	CBC-CAC	-3.22	1.35	1.49
2	B	1113	HEC	C1D-C2D	3.22	1.44	1.40
2	A	1104	HEC	C3C-C2C	-3.22	1.34	1.41
2	B	1105	HEC	C3C-C2C	-3.21	1.34	1.41
2	C	1102	HEC	CBC-CAC	-3.21	1.35	1.49
2	A	1113	HEC	CBB-CAB	-3.21	1.35	1.49
2	B	1106	HEC	C3B-C2B	-3.21	1.34	1.41
2	D	1109	HEC	C3C-C4C	3.21	1.45	1.41
2	D	1108	HEC	C3B-C4B	3.21	1.45	1.41
2	B	1101	HEC	FE-NB	3.21	2.06	1.92
2	D	1110	HEC	C3B-C2B	-3.21	1.34	1.41
2	C	1101	HEC	C3B-C2B	-3.21	1.34	1.41
2	D	1105	HEC	FE-NB	3.20	2.06	1.92
2	A	1116	HEC	C3C-C2C	-3.20	1.34	1.41
2	B	1112	HEC	C3C-C4C	3.20	1.45	1.41
2	C	1103	HEC	CBB-CAB	-3.20	1.35	1.49
2	D	1102	HEC	CBB-CAB	-3.19	1.35	1.49
2	B	1113	HEC	FE-NA	3.19	2.06	1.92
2	D	1107	HEC	C3B-C2B	-3.19	1.34	1.41
2	C	1109	HEC	CBB-CAB	-3.19	1.35	1.49
2	C	1103	HEC	C3B-C4B	3.19	1.45	1.41
2	C	1101	HEC	CBB-CAB	-3.19	1.35	1.49
2	A	1114	HEC	FE-NB	3.19	2.06	1.92
2	A	1102	HEC	FE-ND	3.19	2.06	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1112	HEC	FE-NA	3.19	2.06	1.92
2	A	1103	HEC	C3C-C2C	-3.19	1.34	1.41
2	A	1108	HEC	FE-NC	3.19	2.06	1.92
2	A	1103	HEC	C1B-C2B	3.18	1.44	1.40
2	B	1115	HEC	C3C-C2C	-3.18	1.34	1.41
2	D	1112	HEC	C1B-C2B	3.18	1.44	1.40
2	B	1114	HEC	FE-ND	3.18	2.06	1.92
2	A	1101	HEC	CBC-CAC	-3.18	1.35	1.49
2	B	1104	HEC	CBB-CAB	-3.18	1.35	1.49
2	D	1114	HEC	C3B-C2B	-3.18	1.34	1.41
2	B	1110	HEC	CBC-CAC	-3.18	1.35	1.49
2	C	1110	HEC	C3C-C4C	3.18	1.45	1.41
2	A	1104	HEC	FE-ND	3.18	2.06	1.92
2	C	1108	HEC	C3C-C4C	3.18	1.45	1.41
2	B	1108	HEC	C3C-C4C	3.17	1.45	1.41
2	D	1112	HEC	C3C-C2C	-3.17	1.34	1.41
2	B	1114	HEC	FE-NC	3.17	2.06	1.92
2	A	1108	HEC	C3B-C2B	-3.17	1.34	1.41
2	D	1114	HEC	FE-NC	3.17	2.06	1.92
2	D	1101	HEC	C3C-C4C	3.16	1.45	1.41
2	C	1109	HEC	C1B-C2B	3.16	1.44	1.40
2	C	1111	HEC	CBC-CAC	-3.16	1.35	1.49
2	B	1104	HEC	C3C-C2C	-3.16	1.34	1.41
2	D	1114	HEC	C3C-C4C	3.15	1.45	1.41
2	C	1111	HEC	C3B-C2B	-3.15	1.34	1.41
2	A	1102	HEC	CBB-CAB	-3.14	1.35	1.49
2	A	1103	HEC	CBB-CAB	-3.14	1.35	1.49
2	B	1102	HEC	CBB-CAB	-3.14	1.35	1.49
2	C	1110	HEC	C3B-C4B	3.14	1.45	1.41
2	C	1101	HEC	FE-ND	3.14	2.05	1.92
2	D	1107	HEC	FE-NB	3.14	2.05	1.92
2	C	1116	HEC	FE-ND	3.14	2.05	1.92
2	D	1102	HEC	C3B-C4B	3.14	1.45	1.41
2	C	1107	HEC	C1B-C2B	3.13	1.44	1.40
2	B	1108	HEC	FE-NC	3.13	2.05	1.92
2	C	1106	HEC	C3B-C4B	3.13	1.45	1.41
2	D	1104	HEC	C3B-C4B	3.13	1.45	1.41
2	D	1114	HEC	C3C-C2C	-3.12	1.34	1.41
2	D	1107	HEC	FE-NA	3.12	2.05	1.92
2	C	1101	HEC	CBC-CAC	-3.12	1.36	1.49
2	C	1103	HEC	C3C-C2C	-3.11	1.34	1.41
2	D	1111	HEC	CBC-CAC	-3.11	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1111	HEC	C3B-C2B	-3.10	1.35	1.41
2	B	1113	HEC	FE-NC	3.10	2.05	1.92
2	B	1110	HEC	C3C-C2C	-3.09	1.35	1.41
2	D	1101	HEC	FE-ND	3.09	2.05	1.92
2	A	1111	HEC	FE-ND	3.09	2.05	1.92
2	B	1106	HEC	C3C-C2C	-3.08	1.35	1.41
2	B	1102	HEC	C3C-C2C	-3.08	1.35	1.41
2	B	1116	HEC	C3C-C4C	3.08	1.45	1.41
2	C	1111	HEC	FE-ND	3.08	2.05	1.92
2	B	1110	HEC	FE-NC	3.07	2.05	1.92
2	B	1112	HEC	C3C-C2C	-3.07	1.35	1.41
2	A	1112	HEC	C3C-C4C	3.07	1.45	1.41
2	A	1102	HEC	C3B-C2B	-3.07	1.35	1.41
2	D	1113	HEC	C1D-C2D	3.07	1.44	1.40
2	B	1105	HEC	C1C-C2C	3.07	1.44	1.40
2	D	1111	HEC	C3C-C2C	-3.06	1.35	1.41
2	A	1103	HEC	FE-NC	3.05	2.05	1.92
2	C	1111	HEC	C3B-C4B	3.05	1.45	1.41
2	B	1114	HEC	C3C-C2C	-3.05	1.35	1.41
2	A	1102	HEC	C3C-C4C	3.05	1.45	1.41
2	A	1115	HEC	C3C-C2C	-3.04	1.35	1.41
2	D	1106	HEC	C3B-C4B	3.03	1.45	1.41
2	C	1107	HEC	CBB-CAB	-3.03	1.36	1.49
2	C	1105	HEC	FE-NA	3.03	2.05	1.92
2	B	1106	HEC	C3B-C4B	3.03	1.45	1.41
2	D	1106	HEC	FE-NB	3.01	2.05	1.92
2	D	1106	HEC	C3B-C2B	-3.01	1.35	1.41
2	D	1115	HEC	C3B-C4B	3.00	1.45	1.41
2	A	1107	HEC	FE-NA	2.99	2.05	1.92
2	D	1116	HEC	FE-ND	2.99	2.05	1.92
2	C	1106	HEC	C1C-C2C	2.99	1.43	1.40
2	C	1106	HEC	C3B-C2B	-2.99	1.35	1.41
2	D	1111	HEC	C3C-C4C	2.99	1.45	1.41
2	C	1107	HEC	FE-ND	2.99	2.05	1.92
2	B	1111	HEC	FE-NA	2.98	2.05	1.92
2	B	1105	HEC	FE-NB	2.98	2.05	1.92
2	C	1110	HEC	FE-ND	2.98	2.05	1.92
2	A	1103	HEC	C1D-C2D	2.97	1.43	1.40
2	A	1116	HEC	FE-NC	2.97	2.05	1.92
2	A	1103	HEC	FE-NB	2.97	2.05	1.92
2	C	1110	HEC	C3C-C2C	-2.97	1.35	1.41
2	A	1111	HEC	FE-NB	2.97	2.05	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1112	HEC	C1B-C2B	2.96	1.43	1.40
2	D	1108	HEC	FE-ND	2.95	2.05	1.92
2	D	1106	HEC	FE-NA	2.95	2.05	1.92
2	B	1110	HEC	C3C-C4C	2.94	1.45	1.41
2	D	1108	HEC	C1D-C2D	2.94	1.43	1.40
2	C	1101	HEC	C3C-C2C	-2.94	1.35	1.41
2	A	1101	HEC	FE-NB	2.93	2.05	1.92
2	D	1104	HEC	C3C-C2C	-2.93	1.35	1.41
2	A	1103	HEC	C3C-C4C	2.92	1.45	1.41
2	C	1105	HEC	C3C-C4C	2.91	1.45	1.41
2	B	1103	HEC	C3C-C4C	2.91	1.45	1.41
2	A	1101	HEC	C3C-C2C	-2.89	1.35	1.41
2	A	1107	HEC	FE-NC	2.89	2.04	1.92
2	B	1110	HEC	C3B-C2B	-2.89	1.35	1.41
2	C	1109	HEC	C3C-C4C	2.88	1.45	1.41
2	B	1111	HEC	FE-NB	2.88	2.04	1.92
2	D	1103	HEC	FE-NB	2.88	2.04	1.92
2	C	1113	HEC	C3C-C4C	2.88	1.45	1.41
2	A	1107	HEC	C3B-C2B	-2.87	1.35	1.41
2	D	1103	HEC	FE-NA	2.87	2.04	1.92
2	A	1111	HEC	C3C-C4C	2.86	1.45	1.41
2	A	1101	HEC	C3B-C2B	-2.86	1.35	1.41
2	A	1104	HEC	C3B-C4B	2.86	1.45	1.41
2	C	1113	HEC	C3B-C4B	2.86	1.45	1.41
2	D	1115	HEC	C3C-C2C	-2.86	1.35	1.41
2	A	1114	HEC	C3C-C2C	-2.86	1.35	1.41
2	C	1101	HEC	FE-NA	2.85	2.04	1.92
2	A	1103	HEC	C3B-C4B	2.85	1.45	1.41
2	B	1110	HEC	FE-NA	2.85	2.04	1.92
2	C	1103	HEC	FE-NC	2.85	2.04	1.92
2	D	1109	HEC	C3B-C4B	2.84	1.45	1.41
2	A	1113	HEC	FE-NC	2.84	2.04	1.92
2	D	1104	HEC	FE-NA	2.83	2.04	1.92
2	C	1113	HEC	C1D-C2D	2.83	1.43	1.40
2	B	1101	HEC	C1B-C2B	2.82	1.43	1.40
2	B	1111	HEC	C3B-C4B	2.82	1.45	1.41
2	B	1101	HEC	C3C-C4C	2.82	1.45	1.41
2	B	1107	HEC	FE-NB	2.81	2.04	1.92
2	C	1107	HEC	C1D-C2D	2.81	1.43	1.40
2	D	1111	HEC	FE-NC	2.80	2.04	1.92
2	B	1103	HEC	C3B-C4B	2.79	1.45	1.41
2	C	1104	HEC	C3C-C4C	2.79	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1108	HEC	C3C-C4C	2.78	1.45	1.41
2	D	1110	HEC	C3C-C2C	-2.77	1.35	1.41
2	B	1109	HEC	FE-NB	2.77	2.04	1.92
2	C	1105	HEC	FE-ND	2.77	2.04	1.92
2	C	1115	HEC	C1D-C2D	2.76	1.43	1.40
2	B	1101	HEC	C3C-C2C	-2.75	1.35	1.41
2	B	1104	HEC	C3B-C2B	-2.74	1.35	1.41
2	A	1115	HEC	FE-ND	2.74	2.04	1.92
2	C	1101	HEC	C1D-C2D	2.74	1.43	1.40
2	B	1113	HEC	FE-NB	2.74	2.04	1.92
2	B	1108	HEC	C3B-C4B	2.74	1.45	1.41
2	D	1102	HEC	C3C-C2C	-2.74	1.35	1.41
2	D	1114	HEC	FE-NB	2.72	2.04	1.92
2	A	1110	HEC	FE-NA	2.72	2.04	1.92
2	B	1102	HEC	C3B-C4B	2.72	1.45	1.41
2	D	1104	HEC	FE-NB	2.72	2.04	1.92
2	D	1105	HEC	C3C-C2C	-2.71	1.35	1.41
2	C	1108	HEC	FE-ND	2.70	2.04	1.92
2	B	1103	HEC	C3C-C2C	-2.70	1.35	1.41
2	D	1104	HEC	C3C-C4C	2.70	1.45	1.41
2	B	1115	HEC	FE-NC	2.70	2.04	1.92
2	C	1108	HEC	FE-NC	2.70	2.04	1.92
2	C	1116	HEC	C1B-C2B	2.70	1.43	1.40
2	C	1114	HEC	C3B-C4B	2.69	1.45	1.41
2	A	1108	HEC	C3B-C4B	2.68	1.45	1.41
2	C	1103	HEC	CAD-C3D	2.68	1.56	1.52
2	D	1101	HEC	C3C-C2C	-2.67	1.35	1.41
2	C	1111	HEC	FE-NB	2.67	2.03	1.92
2	A	1113	HEC	C3B-C4B	2.67	1.45	1.41
2	C	1112	HEC	FE-NC	2.67	2.03	1.92
2	A	1101	HEC	FE-NA	2.66	2.03	1.92
2	A	1116	HEC	FE-NA	2.66	2.03	1.92
2	B	1111	HEC	FE-ND	2.65	2.03	1.92
2	A	1110	HEC	FE-NB	2.65	2.03	1.92
2	B	1111	HEC	FE-NC	2.64	2.03	1.92
2	C	1109	HEC	FE-NB	2.63	2.03	1.92
2	B	1104	HEC	C3C-C4C	2.62	1.44	1.41
2	C	1104	HEC	C3B-C2B	-2.62	1.36	1.41
2	C	1110	HEC	C1D-C2D	2.62	1.43	1.40
2	A	1116	HEC	C3C-C4C	2.61	1.44	1.41
2	B	1107	HEC	FE-ND	2.61	2.03	1.92
2	A	1110	HEC	FE-NC	2.60	2.03	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1108	HEC	C3B-C4B	2.60	1.44	1.41
2	A	1103	HEC	FE-NA	2.60	2.03	1.92
2	D	1105	HEC	CAD-C3D	2.57	1.56	1.52
2	C	1102	HEC	FE-NA	2.56	2.03	1.92
2	B	1107	HEC	C3C-C4C	2.56	1.44	1.41
2	A	1108	HEC	C3C-C4C	2.56	1.44	1.41
2	C	1102	HEC	FE-ND	2.55	2.03	1.92
2	B	1112	HEC	FE-NB	2.55	2.03	1.92
2	B	1105	HEC	FE-NA	2.54	2.03	1.92
2	D	1110	HEC	CAD-C3D	2.54	1.56	1.52
2	B	1116	HEC	FE-ND	2.54	2.03	1.92
2	C	1103	HEC	FE-NB	2.53	2.03	1.92
2	A	1112	HEC	FE-NC	2.52	2.03	1.92
2	D	1116	HEC	C3C-C4C	2.51	1.44	1.41
2	A	1103	HEC	FE-ND	2.51	2.03	1.92
2	D	1106	HEC	C3C-C4C	2.51	1.44	1.41
2	A	1102	HEC	C3B-C4B	2.50	1.44	1.41
2	D	1115	HEC	FE-NC	2.50	2.03	1.92
2	C	1116	HEC	C3C-C4C	2.50	1.44	1.41
2	B	1109	HEC	C3B-C4B	2.47	1.44	1.41
2	D	1102	HEC	FE-NB	2.47	2.03	1.92
2	D	1110	HEC	FE-NA	2.47	2.03	1.92
2	D	1111	HEC	C3B-C4B	2.46	1.44	1.41
2	A	1110	HEC	C3B-C4B	2.46	1.44	1.41
2	A	1114	HEC	C4D-ND	2.46	1.41	1.36
2	A	1116	HEC	C3B-C4B	2.45	1.44	1.41
2	B	1104	HEC	FE-NB	2.44	2.02	1.92
2	A	1102	HEC	FE-NC	2.43	2.02	1.92
2	D	1114	HEC	FE-NA	2.42	2.02	1.92
2	B	1113	HEC	C3B-C4B	2.42	1.44	1.41
2	B	1102	HEC	C3C-C4C	2.42	1.44	1.41
2	A	1101	HEC	CAD-C3D	2.41	1.56	1.52
2	C	1103	HEC	C3C-C4C	2.40	1.44	1.41
2	B	1107	HEC	FE-NC	2.39	2.02	1.92
2	B	1102	HEC	FE-NC	2.39	2.02	1.92
2	C	1109	HEC	C3B-C4B	2.38	1.44	1.41
2	A	1112	HEC	C3B-C4B	2.37	1.44	1.41
2	B	1108	HEC	FE-NB	2.37	2.02	1.92
2	A	1103	HEC	CAD-C3D	2.37	1.56	1.52
2	B	1115	HEC	C3C-C4C	2.37	1.44	1.41
2	B	1109	HEC	CAD-C3D	2.37	1.56	1.52
2	A	1105	HEC	FE-NA	2.36	2.02	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1112	HEC	FE-NB	2.35	2.02	1.92
2	D	1115	HEC	FE-NB	2.35	2.02	1.92
2	B	1114	HEC	C3B-C4B	2.34	1.44	1.41
2	D	1109	HEC	FE-ND	2.34	2.02	1.92
2	A	1106	HEC	FE-NA	2.34	2.02	1.92
2	B	1110	HEC	C3B-C4B	2.33	1.44	1.41
2	A	1102	HEC	C1C-C2C	2.33	1.43	1.40
2	A	1106	HEC	FE-NC	2.33	2.02	1.92
2	B	1110	HEC	FE-ND	2.32	2.02	1.92
2	A	1101	HEC	C3B-C4B	2.32	1.44	1.41
2	C	1109	HEC	CAD-C3D	2.31	1.56	1.52
2	C	1111	HEC	C3C-C4C	2.30	1.44	1.41
2	A	1109	HEC	CAD-C3D	2.29	1.56	1.52
2	C	1104	HEC	C4A-NA	2.29	1.40	1.37
2	A	1108	HEC	C4D-ND	2.29	1.41	1.36
2	B	1114	HEC	CAD-C3D	2.29	1.56	1.52
2	B	1109	HEC	FE-NC	2.29	2.02	1.92
2	A	1112	HEC	FE-NB	2.28	2.02	1.92
2	A	1105	HEC	C3B-C4B	2.28	1.44	1.41
2	A	1111	HEC	CAA-C2A	2.27	1.57	1.52
2	C	1104	HEC	FE-NC	2.27	2.02	1.92
2	D	1106	HEC	FE-ND	2.25	2.02	1.92
2	B	1109	HEC	C4A-NA	2.25	1.40	1.37
2	D	1110	HEC	FE-NB	2.23	2.02	1.92
2	B	1105	HEC	CAD-C3D	2.23	1.55	1.52
2	B	1103	HEC	CAD-C3D	2.23	1.55	1.52
2	C	1109	HEC	FE-ND	2.22	2.01	1.92
2	D	1106	HEC	CAD-C3D	2.21	1.55	1.52
2	B	1114	HEC	FE-NB	2.21	2.01	1.92
2	A	1104	HEC	C3C-C4C	2.20	1.44	1.41
2	B	1108	HEC	FE-ND	2.18	2.01	1.92
2	C	1102	HEC	FE-NB	2.17	2.01	1.92
2	D	1102	HEC	FE-ND	2.16	2.01	1.92
2	B	1103	HEC	C4C-NC	2.16	1.40	1.37
2	C	1114	HEC	FE-ND	2.16	2.01	1.92
2	D	1105	HEC	C3B-C4B	2.14	1.44	1.41
2	B	1112	HEC	C3B-C4B	2.14	1.44	1.41
2	D	1102	HEC	C1D-ND	2.13	1.40	1.36
2	A	1106	HEC	CAD-C3D	2.12	1.55	1.52
2	B	1105	HEC	C4D-ND	2.12	1.40	1.36
2	C	1114	HEC	CMD-C2D	2.12	1.56	1.51
2	D	1111	HEC	FE-NB	2.12	2.01	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	HEC	FE-NC	2.12	2.01	1.92
2	A	1107	HEC	CAA-C2A	2.12	1.56	1.52
2	B	1113	HEC	CMD-C2D	2.11	1.56	1.51
2	C	1116	HEC	C3B-C4B	2.11	1.44	1.41
2	C	1106	HEC	C3C-C4C	2.11	1.44	1.41
2	A	1113	HEC	FE-ND	2.11	2.01	1.92
2	B	1106	HEC	FE-NB	2.10	2.01	1.92
2	C	1106	HEC	CAA-C2A	2.11	1.56	1.52
2	B	1115	HEC	FE-NB	2.10	2.01	1.92
2	B	1106	HEC	FE-ND	2.10	2.01	1.92
2	D	1116	HEC	FE-NC	2.09	2.01	1.92
2	C	1102	HEC	CAD-C3D	2.09	1.55	1.52
2	C	1108	HEC	FE-NB	2.09	2.01	1.92
2	C	1101	HEC	C3B-C4B	2.07	1.44	1.41
2	D	1109	HEC	CMD-C2D	2.07	1.56	1.51
2	B	1114	HEC	CMD-C2D	2.07	1.56	1.51
2	D	1113	HEC	C3C-C4C	2.06	1.44	1.41
2	C	1112	HEC	C3B-C4B	2.06	1.44	1.41
2	C	1103	HEC	FE-NA	2.05	2.01	1.92
2	A	1102	HEC	CMD-C2D	2.04	1.55	1.51
2	B	1108	HEC	CAA-C2A	2.04	1.56	1.52
2	B	1109	HEC	CAA-C2A	2.04	1.56	1.52
2	C	1106	HEC	CMD-C2D	2.04	1.55	1.51
2	D	1102	HEC	FE-NC	2.03	2.01	1.92
2	A	1106	HEC	C3B-C4B	2.02	1.44	1.41
2	C	1111	HEC	FE-NA	2.02	2.01	1.92
2	B	1105	HEC	FE-ND	2.02	2.01	1.92
2	D	1114	HEC	C4D-ND	2.01	1.40	1.36
2	B	1102	HEC	CAD-C3D	2.01	1.55	1.52
2	A	1107	HEC	C4B-NB	2.01	1.39	1.37

All (664) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1103	HEC	CBD-CAD-C3D	-7.45	99.57	112.69
2	C	1103	HEC	CBD-CAD-C3D	-6.70	100.89	112.69
2	B	1113	HEC	CBD-CAD-C3D	-6.03	102.07	112.69
2	A	1116	HEC	CBD-CAD-C3D	-6.03	102.07	112.69
2	C	1116	HEC	CBD-CAD-C3D	-5.84	102.40	112.69
2	B	1112	HEC	CBB-CAB-C3B	-5.29	113.56	128.44
2	A	1107	HEC	CBA-CAA-C2A	5.13	121.94	112.35
2	D	1116	HEC	CBD-CAD-C3D	-5.05	103.79	112.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1103	HEC	CBD-CAD-C3D	-4.98	103.92	112.69
2	D	1103	HEC	CBD-CAD-C3D	-4.83	104.18	112.69
2	C	1114	HEC	CBB-CAB-C3B	-4.76	115.03	128.44
2	A	1107	HEC	CMB-C2B-C1B	-4.69	121.41	128.62
2	B	1103	HEC	CBB-CAB-C3B	-4.65	115.34	128.44
2	D	1114	HEC	CBB-CAB-C3B	-4.60	115.49	128.44
2	B	1107	HEC	CBB-CAB-C3B	-4.44	115.93	128.44
2	D	1102	HEC	CBB-CAB-C3B	-4.44	115.94	128.44
2	C	1103	HEC	CBB-CAB-C3B	-4.43	115.96	128.44
2	B	1107	HEC	C4A-CHB-C1B	-4.38	121.71	127.47
2	D	1113	HEC	CBB-CAB-C3B	-4.38	116.11	128.44
2	A	1104	HEC	CBA-CAA-C2A	-4.37	104.18	112.35
2	B	1101	HEC	C4D-ND-C1D	4.36	112.50	106.76
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	A	1109	HEC	CBB-CAB-C3B	-4.24	116.51	128.44
2	D	1116	HEC	CBB-CAB-C3B	-4.23	116.53	128.44
2	D	1101	HEC	CBB-CAB-C3B	-4.22	116.56	128.44
2	A	1115	HEC	CBD-CAD-C3D	-4.22	105.26	112.69
2	C	1112	HEC	CBB-CAB-C3B	-4.19	116.65	128.44
2	A	1114	HEC	C4D-ND-C1D	4.12	112.19	106.76
2	C	1113	HEC	CBA-CAA-C2A	-4.09	104.71	112.35
2	D	1108	HEC	C4D-ND-C1D	4.08	112.14	106.76
2	D	1115	HEC	CBB-CAB-C3B	-4.08	116.95	128.44
2	B	1105	HEC	CMC-C2C-C1C	-4.06	122.38	128.62
2	C	1107	HEC	C4A-CHB-C1B	-4.06	122.13	127.47
2	B	1101	HEC	CMB-C2B-C1B	-4.05	122.40	128.62
2	A	1102	HEC	C4D-ND-C1D	4.00	112.03	106.76
2	B	1110	HEC	CMB-C2B-C3B	3.98	130.12	125.72
2	B	1110	HEC	CBD-CAD-C3D	-3.98	105.68	112.69
2	C	1101	HEC	CBB-CAB-C3B	-3.98	117.25	128.44
2	D	1104	HEC	CBA-CAA-C2A	-3.97	104.93	112.35
2	B	1110	HEC	CMC-C2C-C1C	-3.94	122.56	128.62
2	C	1104	HEC	CBA-CAA-C2A	-3.92	105.02	112.35
2	B	1116	HEC	CBD-CAD-C3D	-3.92	105.79	112.69
2	A	1108	HEC	CBD-CAD-C3D	-3.92	105.79	112.69
2	B	1105	HEC	CBB-CAB-C3B	-3.90	117.47	128.44
2	D	1113	HEC	CBC-CAC-C3C	-3.88	117.52	128.44
2	C	1109	HEC	CBA-CAA-C2A	-3.88	105.10	112.35
2	C	1107	HEC	CBB-CAB-C3B	-3.85	117.60	128.44
2	C	1115	HEC	C3C-C2C-C1C	3.85	109.63	107.07
2	C	1115	HEC	CBB-CAB-C3B	-3.85	117.61	128.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1103	HEC	CMB-C2B-C3B	3.83	129.95	125.72
2	D	1114	HEC	C4D-ND-C1D	3.82	111.80	106.76
2	D	1107	HEC	CBB-CAB-C3B	-3.79	117.76	128.44
2	C	1110	HEC	CBB-CAB-C3B	-3.77	117.81	128.44
2	D	1112	HEC	CBB-CAB-C3B	-3.78	117.81	128.44
2	C	1115	HEC	C4D-ND-C1D	3.77	111.73	106.76
2	A	1110	HEC	CBB-CAB-C3B	-3.75	117.89	128.44
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	C	1115	HEC	C2C-C1C-NC	-3.72	106.61	109.41
2	B	1111	HEC	C4D-ND-C1D	3.71	111.64	106.76
2	A	1113	HEC	CBB-CAB-C3B	-3.69	118.06	128.44
2	C	1105	HEC	CBB-CAB-C3B	-3.69	118.06	128.44
2	A	1115	HEC	CBB-CAB-C3B	-3.68	118.07	128.44
2	D	1115	HEC	C1D-C2D-C3D	-3.68	104.44	107.00
2	B	1116	HEC	CBB-CAB-C3B	-3.67	118.11	128.44
2	A	1108	HEC	CMC-C2C-C1C	-3.66	122.99	128.62
2	C	1109	HEC	CBB-CAB-C3B	-3.66	118.14	128.44
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	D	1106	HEC	CMC-C2C-C1C	-3.64	123.02	128.62
2	A	1112	HEC	CBB-CAB-C3B	-3.64	118.18	128.44
2	A	1105	HEC	C4B-CHC-C1C	-3.63	122.69	127.47
2	B	1114	HEC	CBB-CAB-C3B	-3.63	118.22	128.44
2	B	1110	HEC	CMB-C2B-C1B	-3.63	123.04	128.62
2	A	1104	HEC	CBC-CAC-C3C	-3.63	118.22	128.44
2	B	1106	HEC	CBD-CAD-C3D	-3.63	106.30	112.69
2	C	1102	HEC	CMC-C2C-C1C	-3.63	123.04	128.62
2	B	1113	HEC	C4D-ND-C1D	3.62	111.53	106.76
2	D	1110	HEC	CBB-CAB-C3B	-3.62	118.25	128.44
2	C	1106	HEC	CBD-CAD-C3D	-3.62	106.32	112.69
2	A	1101	HEC	C4D-ND-C1D	3.61	111.52	106.76
2	C	1102	HEC	CMC-C2C-C3C	3.61	129.71	125.72
2	C	1110	HEC	C4D-ND-C1D	3.61	111.52	106.76
2	D	1112	HEC	CMC-C2C-C1C	-3.61	123.07	128.62
2	D	1101	HEC	CMC-C2C-C3C	3.60	129.70	125.72
2	A	1102	HEC	CMC-C2C-C1C	-3.60	123.09	128.62
2	A	1113	HEC	C4D-ND-C1D	3.59	111.50	106.76
2	A	1111	HEC	CBB-CAB-C3B	-3.59	118.33	128.44
2	C	1106	HEC	CMB-C2B-C1B	-3.59	123.09	128.62
2	B	1112	HEC	C4A-CHB-C1B	-3.57	122.77	127.47
2	C	1107	HEC	C1D-C2D-C3D	-3.56	104.52	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1107	HEC	C4B-CHC-C1C	-3.55	122.80	127.47
2	B	1102	HEC	CBB-CAB-C3B	-3.54	118.47	128.44
2	D	1116	HEC	CBC-CAC-C3C	-3.53	118.50	128.44
2	C	1113	HEC	C2A-C1A-NA	-3.52	106.99	109.64
2	B	1102	HEC	CBA-CAA-C2A	-3.52	105.78	112.35
2	A	1109	HEC	CBC-CAC-C3C	-3.51	118.55	128.44
2	C	1106	HEC	CMC-C2C-C1C	-3.51	123.22	128.62
2	A	1109	HEC	C4B-CHC-C1C	-3.51	122.85	127.47
2	B	1108	HEC	C4D-ND-C1D	3.50	111.38	106.76
2	A	1101	HEC	CMC-C2C-C1C	-3.50	123.23	128.62
2	D	1116	HEC	C4A-CHB-C1B	-3.50	122.87	127.47
2	C	1110	HEC	CMC-C2C-C1C	-3.50	123.24	128.62
2	A	1105	HEC	CMB-C2B-C1B	-3.48	123.27	128.62
2	B	1112	HEC	CBC-CAC-C3C	-3.47	118.66	128.44
2	D	1111	HEC	CBC-CAC-C3C	-3.47	118.66	128.44
2	D	1102	HEC	C1D-C2D-C3D	-3.47	104.58	107.00
2	B	1104	HEC	CMB-C2B-C1B	-3.47	123.29	128.62
2	B	1102	HEC	C4D-ND-C1D	3.47	111.33	106.76
2	C	1102	HEC	C4D-ND-C1D	3.46	111.32	106.76
2	D	1102	HEC	CBA-CAA-C2A	-3.46	105.89	112.35
2	B	1112	HEC	C1D-C2D-C3D	-3.46	104.59	107.00
2	B	1113	HEC	CBB-CAB-C3B	-3.46	118.71	128.44
2	B	1115	HEC	C1D-C2D-C3D	-3.45	104.59	107.00
2	C	1108	HEC	CMC-C2C-C1C	-3.45	123.31	128.62
2	A	1116	HEC	C1D-C2D-C3D	-3.45	104.60	107.00
2	C	1115	HEC	CMB-C2B-C1B	-3.45	123.31	128.62
2	D	1107	HEC	C4D-ND-C1D	3.44	111.30	106.76
2	C	1106	HEC	CBC-CAC-C3C	-3.45	118.74	128.44
2	C	1101	HEC	C4D-C3D-C2D	-3.43	103.36	106.92
2	D	1112	HEC	CBC-CAC-C3C	-3.43	118.78	128.44
2	A	1107	HEC	CBB-CAB-C3B	-3.43	118.78	128.44
2	C	1111	HEC	CBC-CAC-C3C	-3.42	118.80	128.44
2	D	1108	HEC	CBD-CAD-C3D	-3.42	106.66	112.69
2	B	1113	HEC	CBC-CAC-C3C	-3.42	118.82	128.44
2	C	1115	HEC	C2A-C1A-NA	-3.41	107.08	109.64
2	A	1111	HEC	CBA-CAA-C2A	3.41	118.73	112.35
2	B	1110	HEC	C1D-C2D-C3D	-3.41	104.62	107.00
2	A	1103	HEC	C3C-C2C-C1C	3.40	109.33	107.07
2	B	1101	HEC	CMC-C2C-C1C	-3.40	123.39	128.62
2	A	1112	HEC	C4D-ND-C1D	3.39	111.22	106.76
2	A	1109	HEC	C4C-C3C-C2C	3.39	108.84	106.68
2	D	1114	HEC	CBC-CAC-C3C	-3.38	118.92	128.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1106	HEC	C4D-ND-C1D	3.38	111.22	106.76
2	A	1103	HEC	CMB-C2B-C1B	-3.37	123.43	128.62
2	D	1109	HEC	C1D-C2D-C3D	-3.37	104.65	107.00
2	A	1102	HEC	CBB-CAB-C3B	-3.37	118.96	128.44
2	C	1114	HEC	C4D-ND-C1D	3.36	111.19	106.76
2	A	1111	HEC	CBC-CAC-C3C	-3.36	118.97	128.44
2	A	1103	HEC	CBB-CAB-C3B	-3.36	118.99	128.44
2	A	1107	HEC	CMB-C2B-C3B	3.35	129.42	125.72
2	A	1116	HEC	CBC-CAC-C3C	-3.35	119.01	128.44
2	D	1103	HEC	C4B-C3B-C2B	3.35	108.81	106.68
2	A	1107	HEC	CAA-C2A-C1A	-3.34	118.64	124.67
2	A	1101	HEC	CMC-C2C-C3C	3.33	129.40	125.72
2	A	1102	HEC	CMC-C2C-C3C	3.32	129.39	125.72
2	D	1101	HEC	C4D-ND-C1D	3.31	111.12	106.76
2	A	1109	HEC	C1D-C2D-C3D	-3.31	104.70	107.00
2	A	1112	HEC	CBD-CAD-C3D	-3.31	106.87	112.69
2	B	1107	HEC	CBC-CAC-C3C	-3.30	119.15	128.44
2	C	1113	HEC	CBB-CAB-C3B	-3.30	119.15	128.44
2	B	1101	HEC	CBB-CAB-C3B	-3.30	119.15	128.44
2	D	1112	HEC	C4D-ND-C1D	3.30	111.11	106.76
2	B	1114	HEC	C4D-ND-C1D	3.29	111.10	106.76
2	C	1109	HEC	CMB-C2B-C1B	-3.29	123.56	128.62
2	A	1114	HEC	CBB-CAB-C3B	-3.29	119.19	128.44
2	B	1116	HEC	CMB-C2B-C1B	-3.28	123.57	128.62
2	A	1111	HEC	C4D-ND-C1D	3.27	111.07	106.76
2	D	1105	HEC	C4D-ND-C1D	3.26	111.06	106.76
2	D	1103	HEC	CBB-CAB-C3B	-3.26	119.27	128.44
2	B	1102	HEC	C4A-CHB-C1B	-3.25	123.19	127.47
2	B	1101	HEC	C2D-C1D-ND	-3.24	106.97	109.41
2	B	1104	HEC	C4D-ND-C1D	3.23	111.02	106.76
2	C	1116	HEC	CMB-C2B-C1B	-3.23	123.65	128.62
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	B	1107	HEC	C4B-C3B-C2B	3.22	108.73	106.68
2	C	1113	HEC	CBC-CAC-C3C	-3.21	119.41	128.44
2	A	1114	HEC	C2A-C1A-NA	-3.21	107.23	109.64
2	B	1115	HEC	CBB-CAB-C3B	-3.21	119.41	128.44
2	B	1108	HEC	CMB-C2B-C1B	-3.21	123.69	128.62
2	D	1106	HEC	C4D-ND-C1D	3.20	110.98	106.76
2	A	1115	HEC	C4D-ND-C1D	3.20	110.98	106.76
2	B	1114	HEC	C4B-CHC-C1C	-3.20	123.26	127.47
2	D	1110	HEC	C4D-ND-C1D	3.20	110.98	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1110	HEC	CBB-CAB-C3B	-3.20	119.44	128.44
2	A	1102	HEC	CBD-CAD-C3D	-3.19	107.08	112.69
2	A	1104	HEC	CBB-CAB-C3B	-3.17	119.50	128.44
2	B	1106	HEC	C4D-ND-C1D	3.17	110.94	106.76
2	C	1102	HEC	CBA-CAA-C2A	-3.17	106.42	112.35
2	B	1108	HEC	CBC-CAC-C3C	-3.17	119.52	128.44
2	A	1107	HEC	C3B-C2B-C1B	3.16	109.17	107.07
2	B	1101	HEC	CMB-C2B-C3B	3.16	129.21	125.72
2	C	1116	HEC	CBB-CAB-C3B	-3.15	119.56	128.44
2	C	1101	HEC	CMB-C2B-C1B	-3.14	123.79	128.62
2	D	1109	HEC	CBB-CAB-C3B	-3.14	119.61	128.44
2	A	1110	HEC	C4D-ND-C1D	3.14	110.90	106.76
2	B	1103	HEC	CMB-C2B-C1B	-3.13	123.80	128.62
2	D	1115	HEC	C4B-C3B-C2B	3.12	108.67	106.68
2	D	1101	HEC	CMC-C2C-C1C	-3.12	123.82	128.62
2	A	1113	HEC	CBA-CAA-C2A	-3.12	106.53	112.35
2	D	1112	HEC	CMC-C2C-C3C	3.12	129.16	125.72
2	B	1109	HEC	CMB-C2B-C1B	-3.11	123.83	128.62
2	C	1115	HEC	C4A-CHB-C1B	-3.11	123.38	127.47
2	D	1111	HEC	C4D-ND-C1D	3.11	110.86	106.76
2	B	1109	HEC	CBB-CAB-C3B	-3.09	119.73	128.44
2	A	1101	HEC	CMB-C2B-C1B	-3.09	123.87	128.62
2	C	1111	HEC	CBB-CAB-C3B	-3.09	119.75	128.44
2	C	1103	HEC	CMB-C2B-C1B	-3.08	123.89	128.62
2	D	1103	HEC	C3C-C2C-C1C	3.08	109.11	107.07
2	D	1111	HEC	C1D-C2D-C3D	-3.07	104.86	107.00
2	A	1115	HEC	CMC-C2C-C1C	-3.07	123.89	128.62
2	D	1107	HEC	CBD-CAD-C3D	-3.07	107.28	112.69
2	A	1108	HEC	C4D-ND-C1D	3.06	110.79	106.76
2	D	1103	HEC	CMB-C2B-C1B	-3.05	123.92	128.62
2	C	1101	HEC	CMC-C2C-C1C	-3.05	123.93	128.62
2	C	1115	HEC	CMC-C2C-C1C	-3.04	123.94	128.62
2	B	1103	HEC	CMB-C2B-C3B	3.04	129.07	125.72
2	C	1107	HEC	C4D-ND-C1D	3.03	110.75	106.76
2	A	1101	HEC	C4D-C3D-C2D	-3.03	103.78	106.92
2	B	1106	HEC	CMB-C2B-C1B	-3.03	123.96	128.62
2	C	1107	HEC	CMB-C2B-C1B	-3.03	123.97	128.62
2	C	1114	HEC	CBA-CAA-C2A	-3.02	106.70	112.35
2	C	1115	HEC	CMB-C2B-C3B	3.02	129.05	125.72
2	C	1116	HEC	CMB-C2B-C3B	3.02	129.05	125.72
2	A	1115	HEC	C1D-C2D-C3D	-3.02	104.90	107.00
2	C	1101	HEC	CBC-CAC-C3C	-3.02	119.95	128.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1105	HEC	CMB-C2B-C1B	-3.01	123.99	128.62
2	C	1116	HEC	C1D-C2D-C3D	-3.01	104.90	107.00
2	C	1105	HEC	C4D-ND-C1D	3.00	110.71	106.76
2	B	1116	HEC	CMC-C2C-C1C	-3.00	124.01	128.62
2	D	1110	HEC	C4D-C3D-C2D	-3.00	103.82	106.92
2	A	1104	HEC	C4D-C3D-C2D	-2.99	103.82	106.92
2	C	1106	HEC	C4D-ND-C1D	2.99	110.70	106.76
2	A	1110	HEC	CBC-CAC-C3C	-2.99	120.03	128.44
2	B	1110	HEC	C4D-ND-C1D	2.98	110.69	106.76
2	A	1105	HEC	C1D-C2D-C3D	-2.98	104.92	107.00
2	C	1104	HEC	CMB-C2B-C1B	-2.98	124.04	128.62
2	D	1114	HEC	CBA-CAA-C2A	-2.98	106.78	112.35
2	B	1105	HEC	C4D-ND-C1D	2.98	110.68	106.76
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	D	1112	HEC	CMB-C2B-C1B	-2.97	124.05	128.62
2	C	1108	HEC	C4D-ND-C1D	2.97	110.67	106.76
2	B	1112	HEC	CMC-C2C-C1C	-2.97	124.06	128.62
2	C	1107	HEC	CBD-CAD-C3D	-2.96	107.47	112.69
2	A	1101	HEC	CBB-CAB-C3B	-2.95	120.13	128.44
2	A	1115	HEC	CMB-C2B-C1B	-2.95	124.08	128.62
2	D	1103	HEC	C4D-ND-C1D	2.95	110.65	106.76
2	D	1105	HEC	CBA-CAA-C2A	2.95	117.86	112.35
2	C	1113	HEC	CMB-C2B-C1B	-2.95	124.09	128.62
2	D	1102	HEC	CBD-CAD-C3D	-2.94	107.50	112.69
2	C	1102	HEC	CBB-CAB-C3B	-2.93	120.18	128.44
2	D	1113	HEC	C4C-CHD-C1D	-2.93	123.61	127.47
2	B	1114	HEC	C1D-C2D-C3D	-2.93	104.96	107.00
2	D	1115	HEC	CBD-CAD-C3D	-2.93	107.53	112.69
2	C	1101	HEC	C4A-CHB-C1B	-2.93	123.62	127.47
2	B	1116	HEC	C4A-CHB-C1B	-2.93	123.62	127.47
2	A	1102	HEC	CMB-C2B-C1B	-2.93	124.12	128.62
2	C	1110	HEC	CMC-C2C-C3C	2.92	128.95	125.72
2	A	1106	HEC	CBD-CAD-C3D	-2.92	107.54	112.69
2	B	1104	HEC	CMC-C2C-C1C	-2.92	124.13	128.62
2	A	1115	HEC	CBA-CAA-C2A	-2.92	106.89	112.35
2	C	1108	HEC	C4B-CHC-C1C	-2.90	123.66	127.47
2	D	1104	HEC	CMC-C2C-C1C	-2.90	124.17	128.62
2	C	1102	HEC	CBD-CAD-C3D	-2.90	107.59	112.69
2	C	1113	HEC	C4D-ND-C1D	2.90	110.58	106.76
2	B	1110	HEC	CMC-C2C-C3C	2.89	128.91	125.72
2	C	1112	HEC	CMB-C2B-C1B	-2.89	124.18	128.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1110	HEC	CBD-CAD-C3D	-2.88	107.61	112.69
2	C	1115	HEC	C1D-C2D-C3D	-2.88	104.99	107.00
2	D	1106	HEC	CMB-C2B-C1B	-2.88	124.19	128.62
2	B	1106	HEC	C1D-C2D-C3D	-2.87	105.00	107.00
2	D	1102	HEC	C4D-ND-C1D	2.88	110.55	106.76
2	B	1106	HEC	C4B-CHC-C1C	-2.87	123.69	127.47
2	D	1108	HEC	C2B-C1B-NB	-2.87	107.24	109.41
2	B	1105	HEC	CMC-C2C-C3C	2.87	128.89	125.72
2	C	1115	HEC	C1A-C2A-C3A	2.87	108.95	106.69
2	C	1114	HEC	CBC-CAC-C3C	-2.86	120.38	128.44
2	B	1111	HEC	CBB-CAB-C3B	-2.86	120.38	128.44
2	C	1113	HEC	C1A-C2A-C3A	2.86	108.94	106.69
2	B	1113	HEC	C4A-C3A-C2A	2.86	108.71	106.89
2	B	1103	HEC	CMC-C2C-C1C	-2.85	124.23	128.62
2	C	1116	HEC	CMC-C2C-C1C	-2.84	124.25	128.62
2	D	1102	HEC	CMB-C2B-C1B	-2.84	124.26	128.62
2	B	1111	HEC	CMB-C2B-C1B	-2.83	124.26	128.62
2	D	1111	HEC	CMC-C2C-C1C	-2.83	124.27	128.62
2	A	1102	HEC	CBC-CAC-C3C	-2.83	120.47	128.44
2	B	1104	HEC	CAD-CBD-CGD	-2.83	104.37	113.47
2	C	1103	HEC	C4D-C3D-C2D	-2.83	103.99	106.92
2	D	1103	HEC	CBC-CAC-C3C	-2.82	120.51	128.44
2	C	1112	HEC	CBD-CAD-C3D	-2.81	107.74	112.69
2	A	1106	HEC	CBB-CAB-C3B	-2.80	120.55	128.44
2	B	1111	HEC	CMC-C2C-C1C	-2.80	124.31	128.62
2	D	1105	HEC	CMC-C2C-C1C	-2.80	124.32	128.62
2	D	1107	HEC	CMB-C2B-C1B	-2.80	124.32	128.62
2	A	1114	HEC	CMC-C2C-C1C	-2.80	124.32	128.62
2	D	1107	HEC	C4A-CHB-C1B	-2.80	123.79	127.47
2	A	1106	HEC	CMB-C2B-C1B	-2.80	124.32	128.62
2	C	1105	HEC	CBD-CAD-C3D	-2.79	107.78	112.69
2	B	1109	HEC	C4D-ND-C1D	2.78	110.43	106.76
2	C	1106	HEC	C4B-CHC-C1C	-2.78	123.81	127.47
2	C	1108	HEC	C1D-C2D-C3D	-2.78	105.06	107.00
2	C	1113	HEC	CBD-CAD-C3D	-2.78	107.80	112.69
2	D	1105	HEC	C4D-C3D-C2D	-2.77	104.05	106.92
2	C	1106	HEC	CMB-C2B-C3B	2.76	128.77	125.72
2	B	1104	HEC	C4A-CHB-C1B	-2.76	123.84	127.47
2	A	1108	HEC	C1D-C2D-C3D	-2.76	105.08	107.00
2	D	1111	HEC	C4C-C3C-C2C	2.75	108.43	106.68
2	D	1113	HEC	CBD-CAD-C3D	-2.75	107.84	112.69
2	B	1108	HEC	CBD-CAD-C3D	-2.75	107.85	112.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1108	HEC	C3A-C4A-NA	-2.74	107.34	109.41
2	D	1108	HEC	C4B-C3B-C2B	2.75	108.43	106.68
2	C	1115	HEC	C3B-C4B-NB	-2.74	107.56	111.52
2	A	1110	HEC	CMB-C2B-C1B	-2.74	124.41	128.62
2	C	1110	HEC	C4B-C3B-C2B	2.74	108.42	106.68
2	B	1112	HEC	CMA-C3A-C2A	2.73	130.09	124.94
2	D	1109	HEC	C4B-CHC-C1C	-2.73	123.87	127.47
2	D	1114	HEC	C4A-CHB-C1B	-2.73	123.88	127.47
2	D	1101	HEC	C1D-C2D-C3D	-2.73	105.10	107.00
2	C	1106	HEC	CBB-CAB-C3B	-2.72	120.78	128.44
2	C	1107	HEC	CBC-CAC-C3C	-2.71	120.80	128.44
2	C	1107	HEC	CMC-C2C-C1C	-2.71	124.45	128.62
2	D	1104	HEC	C4D-ND-C1D	2.71	110.33	106.76
2	C	1101	HEC	CBA-CAA-C2A	-2.71	107.29	112.35
2	A	1106	HEC	CBC-CAC-C3C	-2.70	120.83	128.44
2	D	1111	HEC	CBB-CAB-C3B	-2.70	120.84	128.44
2	A	1115	HEC	CMB-C2B-C3B	2.70	128.70	125.72
2	D	1111	HEC	C3C-C4C-NC	-2.69	107.63	111.52
2	D	1109	HEC	C4D-ND-C1D	2.69	110.31	106.76
2	C	1111	HEC	C4D-ND-C1D	2.69	110.31	106.76
2	C	1109	HEC	CBC-CAC-C3C	-2.68	120.89	128.44
2	C	1113	HEC	C1D-C2D-C3D	-2.68	105.13	107.00
2	D	1108	HEC	C2A-C1A-NA	-2.68	107.63	109.64
2	C	1112	HEC	C4D-ND-C1D	2.67	110.28	106.76
2	B	1115	HEC	C4D-ND-C1D	2.67	110.28	106.76
2	A	1103	HEC	CMB-C2B-C3B	2.67	128.66	125.72
2	C	1106	HEC	C3C-C4C-NC	-2.67	107.67	111.52
2	B	1108	HEC	C3B-C2B-C1B	2.66	108.84	107.07
2	A	1105	HEC	CBB-CAB-C3B	-2.66	120.94	128.44
2	A	1103	HEC	C2C-C1C-NC	-2.66	107.40	109.41
2	B	1112	HEC	CMB-C2B-C1B	-2.66	124.52	128.62
2	D	1109	HEC	C1A-CHA-C4D	-2.66	123.97	127.47
2	A	1114	HEC	C3C-C4C-NC	-2.65	107.69	111.52
2	D	1104	HEC	CBB-CAB-C3B	-2.65	120.99	128.44
2	B	1107	HEC	CAD-CBD-CGD	-2.64	104.97	113.47
2	C	1111	HEC	C1D-C2D-C3D	-2.64	105.16	107.00
2	D	1113	HEC	CBA-CAA-C2A	-2.64	107.42	112.35
2	C	1115	HEC	CBD-CAD-C3D	-2.64	108.05	112.69
2	C	1107	HEC	C3B-C4B-NB	-2.63	107.72	111.52
2	C	1116	HEC	CMC-C2C-C3C	2.63	128.62	125.72
2	D	1108	HEC	CBB-CAB-C3B	-2.63	121.04	128.44
2	B	1102	HEC	CMC-C2C-C1C	-2.63	124.58	128.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1110	HEC	CMB-C2B-C1B	-2.63	124.58	128.62
2	C	1101	HEC	C4D-ND-C1D	2.63	110.23	106.76
2	B	1106	HEC	CMB-C2B-C3B	2.63	128.62	125.72
2	C	1108	HEC	CBB-CAB-C3B	-2.62	121.05	128.44
2	D	1110	HEC	C2A-C1A-NA	-2.62	107.67	109.64
2	B	1116	HEC	CBC-CAC-C3C	-2.62	121.06	128.44
2	A	1113	HEC	CBD-CAD-C3D	-2.62	108.08	112.69
2	D	1108	HEC	C3B-C4B-NB	-2.62	107.74	111.52
2	C	1103	HEC	C4D-ND-C1D	2.62	110.21	106.76
2	A	1113	HEC	C4D-C3D-C2D	-2.61	104.21	106.92
2	B	1111	HEC	CBC-CAC-C3C	-2.61	121.10	128.44
2	D	1115	HEC	CMC-C2C-C1C	-2.61	124.61	128.62
2	A	1106	HEC	C4B-CHC-C1C	-2.60	124.06	127.47
2	B	1109	HEC	C4D-C3D-C2D	-2.60	104.23	106.92
2	C	1116	HEC	CBC-CAC-C3C	-2.59	121.14	128.44
2	A	1108	HEC	C2A-C1A-NA	-2.59	107.69	109.64
2	A	1108	HEC	C4C-CHD-C1D	-2.59	124.06	127.47
2	A	1107	HEC	C4D-ND-C1D	2.58	110.17	106.76
2	A	1116	HEC	CMC-C2C-C1C	-2.58	124.65	128.62
2	D	1104	HEC	C4C-CHD-C1D	-2.58	124.08	127.47
2	D	1110	HEC	C1A-C2A-C3A	2.56	108.71	106.69
2	A	1108	HEC	C4A-CHB-C1B	-2.56	124.10	127.47
2	A	1116	HEC	CBB-CAB-C3B	-2.56	121.23	128.44
2	D	1105	HEC	C2B-C1B-NB	-2.56	107.48	109.41
2	A	1113	HEC	CBC-CAC-C3C	-2.56	121.23	128.44
2	D	1115	HEC	C3B-C4B-NB	-2.56	107.83	111.52
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	A	1115	HEC	C4A-CHB-C1B	-2.56	124.11	127.47
2	A	1116	HEC	CMB-C2B-C1B	-2.55	124.70	128.62
2	A	1103	HEC	C4D-C3D-C2D	-2.55	104.28	106.92
2	A	1106	HEC	CMB-C2B-C3B	2.54	128.53	125.72
2	D	1107	HEC	C3B-C4B-NB	-2.53	107.86	111.52
2	A	1108	HEC	CBC-CAC-C3C	-2.54	121.30	128.44
2	D	1110	HEC	CBA-CAA-C2A	-2.54	107.61	112.35
2	A	1109	HEC	C4D-ND-C1D	2.53	110.10	106.76
2	B	1112	HEC	C4D-ND-C1D	2.52	110.09	106.76
2	C	1104	HEC	CMB-C2B-C3B	2.52	128.50	125.72
2	D	1113	HEC	C4D-ND-C1D	2.52	110.08	106.76
2	A	1104	HEC	C1A-CHA-C4D	-2.52	124.16	127.47
2	A	1114	HEC	C4A-CHB-C1B	-2.52	124.16	127.47
2	D	1114	HEC	C4C-C3C-C2C	2.51	108.28	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1114	HEC	C4B-C3B-C2B	2.51	108.28	106.68
2	C	1109	HEC	CMB-C2B-C3B	2.51	128.49	125.72
2	C	1104	HEC	CBC-CAC-C3C	-2.51	121.38	128.44
2	A	1110	HEC	C4C-C3C-C2C	2.51	108.28	106.68
2	B	1105	HEC	C4B-CHC-C1C	-2.50	124.18	127.47
2	C	1106	HEC	CMC-C2C-C3C	2.50	128.48	125.72
2	B	1105	HEC	C3C-C2C-C1C	2.49	108.73	107.07
2	A	1113	HEC	CMC-C2C-C1C	-2.49	124.78	128.62
2	D	1106	HEC	C4B-CHC-C1C	-2.49	124.19	127.47
2	C	1108	HEC	CBD-CAD-C3D	-2.50	108.30	112.69
2	A	1105	HEC	CMB-C2B-C3B	2.49	128.47	125.72
2	C	1102	HEC	CBC-CAC-C3C	-2.49	121.42	128.44
2	C	1101	HEC	CMC-C2C-C3C	2.49	128.47	125.72
2	B	1112	HEC	CMC-C2C-C3C	2.48	128.46	125.72
2	C	1112	HEC	C4A-CHB-C1B	-2.48	124.20	127.47
2	D	1103	HEC	C4A-CHB-C1B	-2.48	124.20	127.47
2	B	1115	HEC	CMC-C2C-C1C	-2.48	124.81	128.62
2	C	1105	HEC	CMA-C3A-C2A	2.48	129.61	124.94
2	B	1116	HEC	C4C-CHD-C1D	-2.48	124.21	127.47
2	A	1102	HEC	C1D-C2D-C3D	-2.47	105.28	107.00
2	A	1107	HEC	C4A-CHB-C1B	-2.47	124.22	127.47
2	C	1102	HEC	C4D-C3D-C2D	-2.47	104.36	106.92
2	D	1113	HEC	C4B-C3B-C2B	2.47	108.25	106.68
2	A	1112	HEC	CBC-CAC-C3C	-2.47	121.49	128.44
2	A	1108	HEC	CMC-C2C-C3C	2.47	128.44	125.72
2	B	1102	HEC	CMC-C2C-C3C	2.47	128.44	125.72
2	D	1114	HEC	C2A-C1A-NA	-2.46	107.79	109.64
2	A	1106	HEC	C4C-C3C-C2C	2.46	108.25	106.68
2	C	1104	HEC	C4D-C3D-C2D	-2.46	104.37	106.92
2	B	1102	HEC	CBD-CAD-C3D	-2.46	108.36	112.69
2	D	1112	HEC	C1D-C2D-C3D	-2.45	105.29	107.00
2	A	1104	HEC	C4D-ND-C1D	2.45	109.99	106.76
2	B	1115	HEC	C4B-C3B-C2B	2.45	108.24	106.68
2	B	1101	HEC	CMC-C2C-C3C	2.44	128.42	125.72
2	B	1115	HEC	C3B-C4B-NB	-2.44	107.99	111.52
2	C	1114	HEC	C4D-C3D-C2D	-2.44	104.39	106.92
2	A	1107	HEC	C2B-C1B-NB	-2.44	107.57	109.41
2	A	1101	HEC	CBA-CAA-C2A	-2.44	107.80	112.35
2	A	1103	HEC	C4D-ND-C1D	2.44	109.97	106.76
2	B	1111	HEC	CBA-CAA-C2A	-2.43	107.80	112.35
2	B	1106	HEC	CMC-C2C-C1C	-2.43	124.89	128.62
2	B	1112	HEC	CMB-C2B-C3B	2.43	128.40	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1109	HEC	C3C-C4C-NC	-2.43	108.01	111.52
2	D	1106	HEC	C3C-C2C-C1C	2.43	108.68	107.07
2	C	1105	HEC	C4B-C3B-C2B	2.43	108.22	106.68
2	C	1115	HEC	C4B-C3B-C2B	2.43	108.22	106.68
2	C	1109	HEC	C1D-C2D-C3D	-2.43	105.31	107.00
2	B	1107	HEC	C3B-C4B-NB	-2.42	108.02	111.52
2	C	1103	HEC	C3C-C2C-C1C	2.43	108.68	107.07
2	C	1116	HEC	C4D-ND-C1D	2.42	109.94	106.76
2	B	1102	HEC	CMB-C2B-C1B	-2.41	124.91	128.62
2	B	1116	HEC	C4D-ND-C1D	2.41	109.94	106.76
2	D	1103	HEC	CMA-C3A-C2A	2.41	129.48	124.94
2	B	1112	HEC	C4B-C3B-C2B	2.41	108.21	106.68
2	D	1116	HEC	C4C-C3C-C2C	2.40	108.21	106.68
2	C	1112	HEC	CBC-CAC-C3C	-2.40	121.68	128.44
2	C	1108	HEC	CMC-C2C-C3C	2.40	128.37	125.72
2	D	1113	HEC	CMB-C2B-C1B	-2.39	124.94	128.62
2	D	1107	HEC	C1D-C2D-C3D	-2.39	105.33	107.00
2	B	1103	HEC	C4D-ND-C1D	2.39	109.91	106.76
2	D	1107	HEC	CMB-C2B-C3B	2.39	128.35	125.72
2	D	1114	HEC	C3C-C4C-NC	-2.38	108.08	111.52
2	B	1107	HEC	C4B-CHC-C1C	-2.38	124.34	127.47
2	D	1114	HEC	CBD-CAD-C3D	-2.38	108.50	112.69
2	A	1106	HEC	CMA-C3A-C2A	2.38	129.43	124.94
2	C	1103	HEC	CMC-C2C-C1C	-2.37	124.97	128.62
2	A	1112	HEC	CMB-C2B-C1B	-2.37	124.97	128.62
2	D	1113	HEC	C4A-CHB-C1B	-2.37	124.35	127.47
2	B	1104	HEC	CMB-C2B-C3B	2.37	128.34	125.72
2	D	1113	HEC	C1D-C2D-C3D	-2.37	105.35	107.00
2	C	1109	HEC	C4D-C3D-C2D	-2.37	104.47	106.92
2	C	1111	HEC	C4D-C3D-C2D	-2.37	104.47	106.92
2	B	1114	HEC	CBC-CAC-C3C	-2.37	121.78	128.44
2	A	1110	HEC	C3C-C4C-NC	-2.37	108.10	111.52
2	C	1102	HEC	CMB-C2B-C1B	-2.36	124.99	128.62
2	C	1114	HEC	CMB-C2B-C1B	-2.36	125.00	128.62
2	D	1103	HEC	C3B-C4B-NB	-2.35	108.13	111.52
2	C	1103	HEC	CMB-C2B-C3B	2.35	128.31	125.72
2	D	1113	HEC	C3B-C4B-NB	-2.35	108.13	111.52
2	D	1105	HEC	CAA-CBA-CGA	-2.34	105.94	113.47
2	A	1116	HEC	C4B-C3B-C2B	2.34	108.17	106.68
2	D	1106	HEC	CMC-C2C-C3C	2.34	128.30	125.72
2	D	1108	HEC	C4A-NA-C1A	2.33	109.08	105.58
2	A	1108	HEC	C1A-C2A-C3A	2.34	108.53	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1116	HEC	C4D-ND-C1D	2.33	109.84	106.76
2	C	1105	HEC	CMB-C2B-C3B	2.33	128.30	125.72
2	C	1115	HEC	C4C-CHD-C1D	-2.33	124.40	127.47
2	D	1109	HEC	CBC-CAC-C3C	-2.33	121.88	128.44
2	B	1106	HEC	C3B-C4B-NB	-2.33	108.16	111.52
2	B	1109	HEC	CMB-C2B-C3B	2.33	128.29	125.72
2	B	1101	HEC	C3B-C4B-NB	-2.33	108.16	111.52
2	B	1103	HEC	C4B-C3B-C2B	2.32	108.16	106.68
2	D	1114	HEC	CMB-C2B-C1B	-2.32	125.05	128.62
2	C	1106	HEC	C4A-CHB-C1B	-2.32	124.42	127.47
2	D	1110	HEC	CMD-C2D-C1D	-2.32	125.05	128.62
2	A	1114	HEC	C3B-C4B-NB	-2.32	108.17	111.52
2	A	1116	HEC	C4A-CHB-C1B	-2.31	124.43	127.47
2	B	1109	HEC	CBC-CAC-C3C	-2.31	121.93	128.44
2	A	1114	HEC	C4A-C3A-C2A	2.31	108.36	106.89
2	D	1102	HEC	CMC-C2C-C1C	-2.31	125.08	128.62
2	D	1110	HEC	C3B-C4B-NB	-2.31	108.19	111.52
2	A	1103	HEC	C1A-C2A-C3A	2.31	108.50	106.69
2	B	1113	HEC	CMD-C2D-C3D	2.31	129.29	124.94
2	C	1110	HEC	C3A-C4A-NA	-2.30	107.67	109.41
2	D	1112	HEC	C4B-CHC-C1C	-2.30	124.44	127.47
2	C	1108	HEC	CBC-CAC-C3C	-2.30	121.96	128.44
2	B	1102	HEC	CBC-CAC-C3C	-2.30	121.96	128.44
2	D	1106	HEC	C4D-C3D-C2D	-2.30	104.54	106.92
2	A	1108	HEC	CMB-C2B-C1B	-2.30	125.09	128.62
2	C	1104	HEC	O1A-CGA-CBA	-2.30	115.12	123.03
2	C	1113	HEC	CMB-C2B-C3B	2.30	128.26	125.72
2	B	1106	HEC	CBC-CAC-C3C	-2.30	121.97	128.44
2	A	1101	HEC	CMB-C2B-C3B	2.29	128.25	125.72
2	A	1107	HEC	CBD-CAD-C3D	-2.29	108.65	112.69
2	B	1101	HEC	CBD-CAD-C3D	-2.29	108.65	112.69
2	C	1104	HEC	C4D-ND-C1D	2.29	109.78	106.76
2	D	1102	HEC	CBC-CAC-C3C	-2.29	122.00	128.44
2	C	1108	HEC	CMB-C2B-C1B	-2.29	125.10	128.62
2	C	1107	HEC	C2C-C1C-NC	-2.28	107.69	109.41
2	D	1107	HEC	C4B-C3B-C2B	2.28	108.13	106.68
2	D	1109	HEC	CMB-C2B-C1B	-2.28	125.11	128.62
2	D	1116	HEC	CMA-C3A-C2A	2.28	129.24	124.94
2	B	1108	HEC	CMC-C2C-C1C	-2.28	125.12	128.62
2	D	1114	HEC	C3B-C4B-NB	-2.28	108.23	111.52
2	D	1109	HEC	CMC-C2C-C1C	-2.28	125.12	128.62
2	B	1104	HEC	C3C-C2C-C1C	2.27	108.58	107.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1114	HEC	CMB-C2B-C1B	-2.27	125.12	128.62
2	A	1111	HEC	C4C-C3C-C2C	2.27	108.13	106.68
2	B	1103	HEC	C4A-CHB-C1B	-2.27	124.48	127.47
2	C	1114	HEC	C3B-C4B-NB	-2.27	108.24	111.52
2	B	1112	HEC	C4C-CHD-C1D	-2.27	124.49	127.47
2	A	1116	HEC	C4C-CHD-C1D	-2.26	124.49	127.47
2	D	1106	HEC	CMB-C2B-C3B	2.26	128.22	125.72
2	B	1116	HEC	C3C-C2C-C1C	2.26	108.57	107.07
2	C	1106	HEC	C2C-C1C-NC	-2.26	107.70	109.41
2	D	1102	HEC	C4A-CHB-C1B	-2.26	124.50	127.47
2	A	1103	HEC	CMA-C3A-C2A	2.25	129.19	124.94
2	A	1108	HEC	C3C-C2C-C1C	2.25	108.57	107.07
2	A	1116	HEC	O1D-CGD-CBD	-2.25	115.28	123.03
2	C	1103	HEC	C4B-CHC-C1C	-2.25	124.51	127.47
2	B	1107	HEC	C4C-CHD-C1D	-2.24	124.52	127.47
2	A	1112	HEC	CMC-C2C-C1C	-2.24	125.17	128.62
2	C	1113	HEC	C4C-C3C-C2C	2.24	108.11	106.68
2	D	1104	HEC	CMB-C2B-C1B	-2.24	125.18	128.62
2	B	1106	HEC	CAD-CBD-CGD	-2.24	106.28	113.47
2	C	1113	HEC	C3B-C4B-NB	-2.24	108.29	111.52
2	A	1109	HEC	C1A-CHA-C4D	-2.23	124.53	127.47
2	C	1105	HEC	C3B-C4B-NB	-2.23	108.30	111.52
2	C	1111	HEC	CMB-C2B-C1B	-2.23	125.19	128.62
2	D	1115	HEC	C4D-ND-C1D	2.23	109.70	106.76
2	B	1107	HEC	C4D-ND-C1D	2.22	109.68	106.76
2	B	1110	HEC	C4B-C3B-C2B	2.22	108.09	106.68
2	A	1108	HEC	O1D-CGD-CBD	-2.21	115.41	123.03
2	A	1105	HEC	CMA-C3A-C2A	2.21	129.11	124.94
2	C	1107	HEC	C2A-C1A-NA	-2.21	107.98	109.64
2	A	1116	HEC	C4D-ND-C1D	2.21	109.67	106.76
2	D	1104	HEC	C4B-C3B-C2B	2.20	108.08	106.68
2	C	1101	HEC	CMB-C2B-C3B	2.20	128.15	125.72
2	C	1109	HEC	C4D-ND-C1D	2.20	109.66	106.76
2	A	1108	HEC	CBB-CAB-C3B	-2.20	122.25	128.44
2	C	1110	HEC	C3B-C4B-NB	-2.20	108.34	111.52
2	D	1111	HEC	CMC-C2C-C3C	2.20	128.15	125.72
2	C	1101	HEC	C4B-CHC-C1C	-2.20	124.58	127.47
2	C	1104	HEC	CAD-CBD-CGD	-2.20	106.41	113.47
2	A	1105	HEC	C4D-C3D-C2D	-2.19	104.65	106.92
2	C	1107	HEC	C1A-C2A-C3A	2.19	108.41	106.69
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1114	HEC	C3C-C4C-NC	-2.19	108.36	111.52
2	A	1115	HEC	C3B-C4B-NB	-2.19	108.36	111.52
2	D	1103	HEC	C2C-C1C-NC	-2.19	107.76	109.41
2	A	1105	HEC	CBC-CAC-C3C	-2.19	122.29	128.44
2	A	1101	HEC	C4B-CHC-C1C	-2.18	124.60	127.47
2	A	1102	HEC	CHA-C4D-ND	2.18	128.22	124.58
2	D	1113	HEC	C2B-C1B-NB	-2.17	107.77	109.41
2	B	1116	HEC	C3B-C2B-C1B	2.18	108.52	107.07
2	B	1115	HEC	CMB-C2B-C1B	-2.18	125.27	128.62
2	C	1104	HEC	C1A-C2A-C3A	2.17	108.40	106.69
2	A	1112	HEC	CBA-CAA-C2A	-2.17	108.30	112.35
2	A	1112	HEC	C4D-C3D-C2D	-2.17	104.68	106.92
2	C	1110	HEC	CHD-C1D-ND	2.16	128.19	124.58
2	D	1103	HEC	O1A-CGA-CBA	-2.17	115.58	123.03
2	A	1109	HEC	O1A-CGA-CBA	-2.16	115.59	123.03
2	C	1110	HEC	CMB-C2B-C1B	-2.16	125.30	128.62
2	A	1111	HEC	C4D-C3D-C2D	-2.16	104.69	106.92
2	B	1115	HEC	C3C-C2C-C1C	2.15	108.50	107.07
2	B	1110	HEC	C3C-C2C-C1C	2.15	108.50	107.07
2	C	1106	HEC	C4A-C3A-C2A	2.15	108.26	106.89
2	C	1107	HEC	CMB-C2B-C3B	2.15	128.09	125.72
2	A	1112	HEC	C4B-C3B-C2B	2.14	108.04	106.68
2	B	1103	HEC	C3C-C2C-C1C	2.14	108.49	107.07
2	C	1116	HEC	C4C-C3C-C2C	2.14	108.04	106.68
2	C	1102	HEC	C4B-CHC-C1C	-2.14	124.66	127.47
2	B	1110	HEC	C4B-CHC-C1C	-2.14	124.66	127.47
2	B	1111	HEC	C3C-C4C-NC	-2.14	108.43	111.52
2	C	1108	HEC	C4D-C3D-C2D	-2.14	104.70	106.92
2	C	1112	HEC	CMC-C2C-C1C	-2.14	125.33	128.62
2	D	1107	HEC	CBC-CAC-C3C	-2.14	122.43	128.44
2	A	1103	HEC	C3B-C4B-NB	-2.13	108.44	111.52
2	A	1115	HEC	CMC-C2C-C3C	2.13	128.07	125.72
2	D	1109	HEC	C3B-C2B-C1B	2.13	108.48	107.07
2	D	1105	HEC	CMB-C2B-C1B	-2.13	125.35	128.62
2	A	1107	HEC	CMC-C2C-C1C	-2.13	125.35	128.62
2	B	1106	HEC	C4B-C3B-C2B	2.13	108.03	106.68
2	B	1103	HEC	CBC-CAC-C3C	-2.13	122.46	128.44
2	D	1111	HEC	CMB-C2B-C1B	-2.13	125.35	128.62
2	D	1110	HEC	CMB-C2B-C3B	2.13	128.07	125.72
2	D	1110	HEC	C4B-C3B-C2B	2.13	108.03	106.68
2	B	1105	HEC	C3C-C4C-NC	-2.12	108.45	111.52
2	D	1115	HEC	C4A-CHB-C1B	-2.12	124.68	127.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1108	HEC	C4A-C3A-C2A	2.12	108.24	106.89
2	C	1116	HEC	C4A-CHB-C1B	-2.12	124.69	127.47
2	B	1101	HEC	C3C-C4C-NC	-2.12	108.46	111.52
2	A	1105	HEC	C4D-ND-C1D	2.11	109.55	106.76
2	A	1107	HEC	CHB-C1B-NB	2.11	128.11	124.58
2	A	1103	HEC	O1A-CGA-CBA	-2.11	115.75	123.03
2	A	1106	HEC	C1D-C2D-C3D	-2.11	105.53	107.00
2	B	1105	HEC	C4D-C3D-C2D	-2.11	104.73	106.92
2	D	1106	HEC	CBB-CAB-C3B	-2.11	122.50	128.44
2	C	1105	HEC	C4B-CHC-C1C	-2.11	124.69	127.47
2	B	1104	HEC	CBC-CAC-C3C	-2.11	122.50	128.44
2	C	1113	HEC	CMD-C2D-C3D	2.11	128.92	124.94
2	D	1110	HEC	CMD-C2D-C3D	2.11	128.92	124.94
2	B	1107	HEC	CBD-CAD-C3D	-2.10	108.98	112.69
2	C	1111	HEC	C4B-CHC-C1C	-2.11	124.70	127.47
2	C	1104	HEC	C3B-C4B-NB	-2.10	108.49	111.52
2	A	1113	HEC	CMB-C2B-C1B	-2.09	125.40	128.62
2	B	1101	HEC	C4D-C3D-C2D	-2.09	104.75	106.92
2	A	1109	HEC	C4D-C3D-C2D	-2.09	104.75	106.92
2	A	1111	HEC	C1D-C2D-C3D	-2.09	105.54	107.00
2	C	1113	HEC	C4C-CHD-C1D	-2.09	124.73	127.47
2	C	1108	HEC	C1A-CHA-C4D	-2.08	124.73	127.47
2	A	1105	HEC	CMC-C2C-C1C	-2.08	125.42	128.62
2	C	1104	HEC	C1D-C2D-C3D	-2.08	105.55	107.00
2	B	1106	HEC	C3C-C4C-NC	-2.08	108.52	111.52
2	D	1109	HEC	O1D-CGD-CBD	-2.07	115.91	123.03
2	A	1103	HEC	CBC-CAC-C3C	-2.07	122.61	128.44
2	B	1112	HEC	C4D-C3D-C2D	-2.07	104.78	106.92
2	B	1113	HEC	C3B-C4B-NB	-2.07	108.53	111.52
2	B	1115	HEC	C2C-C1C-NC	-2.07	107.85	109.41
2	C	1109	HEC	C4B-CHC-C1C	-2.07	124.75	127.47
2	B	1107	HEC	C4D-C3D-C2D	-2.06	104.79	106.92
2	B	1111	HEC	C4D-C3D-C2D	-2.06	104.79	106.92
2	D	1101	HEC	C4A-C3A-C2A	2.06	108.20	106.89
2	C	1109	HEC	CMC-C2C-C1C	-2.06	125.46	128.62
2	D	1111	HEC	C3A-C4A-NA	-2.05	107.86	109.41
2	C	1116	HEC	O1D-CGD-CBD	-2.05	115.97	123.03
2	A	1110	HEC	C4B-C3B-C2B	2.05	107.99	106.68
2	A	1106	HEC	C4A-C3A-C2A	2.05	108.20	106.89
2	A	1110	HEC	CMB-C2B-C3B	2.05	127.98	125.72
2	D	1104	HEC	CMA-C3A-C2A	2.05	128.80	124.94
2	C	1116	HEC	C4D-C3D-C2D	-2.04	104.80	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1110	HEC	CBA-CAA-C2A	-2.04	108.53	112.35
2	D	1101	HEC	C3B-C4B-NB	-2.04	108.57	111.52
2	C	1106	HEC	C4C-C3C-C2C	2.04	107.98	106.68
2	A	1114	HEC	C4B-C3B-C2B	2.04	107.98	106.68
2	C	1110	HEC	CMA-C3A-C2A	2.04	128.78	124.94
2	A	1112	HEC	C3B-C4B-NB	-2.04	108.58	111.52
2	D	1103	HEC	CMC-C2C-C1C	-2.03	125.49	128.62
2	B	1108	HEC	C4A-CHB-C1B	-2.03	124.80	127.47
2	B	1114	HEC	CMC-C2C-C1C	-2.03	125.50	128.62
2	B	1103	HEC	C3B-C4B-NB	-2.03	108.59	111.52
2	A	1106	HEC	CMC-C2C-C1C	-2.02	125.51	128.62
2	B	1113	HEC	CHD-C1D-ND	2.02	127.96	124.58
2	C	1110	HEC	O1D-CGD-CBD	-2.02	116.08	123.03
2	D	1109	HEC	O2D-CGD-CBD	2.02	121.36	114.22
2	B	1101	HEC	C2B-C1B-NB	-2.02	107.89	109.41
2	C	1115	HEC	CMD-C2D-C3D	2.02	128.75	124.94
2	B	1109	HEC	CBD-CAD-C3D	-2.02	109.14	112.69
2	A	1105	HEC	C3C-C2C-C1C	2.01	108.41	107.07
2	A	1101	HEC	O2D-CGD-O1D	-2.01	118.18	123.30
2	D	1105	HEC	CBB-CAB-C3B	-2.01	122.79	128.44
2	A	1116	HEC	CMC-C2C-C3C	2.01	127.94	125.72
2	D	1106	HEC	C3C-C4C-NC	-2.01	108.62	111.52
2	B	1110	HEC	C1A-C2A-C3A	2.01	108.27	106.69
2	B	1112	HEC	C3C-C4C-NC	-2.01	108.62	111.52
2	C	1105	HEC	C3C-C4C-NC	-2.00	108.63	111.52
2	A	1110	HEC	C3B-C4B-NB	-2.00	108.63	111.52

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.

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 ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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