

Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 - 05:43 am BST

PDB ID	:	1H29
Title	:	Sulfate respiration in Desulfovibrio vulgaris Hildenborough: Structure of the
		16-heme Cytochrome c HmcA at 2.5 A resolution and a view of its role in
		transmembrane electron transfer
Authors	:	Matias, P.M.; Coelho, A.V.; Valente, F.M.A.; Placido, D.; Legall, J.; Xavier,
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Deposited on	:	2002-08-01
Resolution	:	2.51 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity Mogul Xtriage (Phenix) EDS buster-report Percentile statistics	······································	4.02b-467 1.8.5 (274361), CSD as541be (2020) NOT EXECUTED 1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019)
FDS		NOT EXECUTED
,	•	
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231(2.50-2.50)
Sidechain outliers	138945	5233(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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	А	514	74%	19%	••
1	В	514	75%	19%	••••
1	С	514	74%	21%	• •
1	D	514	69%	23%	• •



2 Entry composition (i)

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	501	Total	С	Ν	Ο	S	20	0	0
	A		3783	2323	717	699	44	30	0	0
1	в	400	Total	С	Ν	Ο	S	75	0	0
	D	499	3763	2312	712	695	44	10		0
1	C	501	Total	С	Ν	Ο	S	00	0	0
		106	3777	2320	714	699	44	90		0
1	1 D	D 400	Total	С	Ν	Ο	S	70	0	0
	492	3715	2284	699	688	44	10		0	

• Molecule 1 is a protein called HIGH-MOLECULAR-WEIGHT CYTOCHROME C.

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



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf
2	А	1	Total 43	С 34	Fe 1	N 4	0 4	0	0
2	А	1	Total 43	С 34	Fe 1	N 4	O 4	0	0



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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf		
0	٨	1	Total	С	Fe	Ν	Ο	0	0		
Z	A	1	43	34	1	4	4	0	0		
0	Δ	1	Total	С	Fe	Ν	Ο	0	0		
2	A	1	43	34	1	4	4	0	0		
0	٨	1	Total	С	Fe	Ν	Ο	0	0		
	A	1	43	34	1	4	4	0	0		
0	٨	1	Total	С	Fe	Ν	Ο	0	0		
	A	1	43	34	1	4	4	0	0		
0	٨	1	Total	С	Fe	Ν	Ο	0	0		
	A	1	43	34	1	4	4	0	0		
0	Λ	1	Total	С	Fe	Ν	Ο	0	0		
	A	1	43	34	1	4	4	0	0		
0	Λ	1	Total	С	Fe	Ν	Ο	0	0		
	A	1	43	34	1	4	4	0	0		
0	Δ	1	Total	С	Fe	Ν	Ο	0	0		
	А	L	43	34	1	4	4	0	0		
0	Δ	1	Total	С	Fe	Ν	Ο	0	0		
	А	L	43	34	1	4	4	0	U		
0	Δ	1	Total	С	Fe	Ν	Ο	0	0		
	А	L	43	34	1	4	4	0	0		
9	A	1	Total	С	Fe	Ν	Ο	0	0		
		I	43	34	1	4	4	0	0		
2	Δ	1	Total	С	Fe	Ν	Ο	0	0		
2	Л	L	43	34	1	4	4	0	0		
2	Δ	1	Total	С	Fe	Ν	Ο	0	0		
	11	L	43	34	1	4	4	0	0		
2	Δ	1	Total	С	Fe	Ν	Ο	0	0		
		L	43	34	1	4	4	0	0		
2	В	1	Total	С	Fe	Ν	Ο	0	0		
	D	1	43	34	1	4	4	0	0		
2	В	1	Total	С	Fe	Ν	Ο	0	0		
	D	1	43	34	1	4	4	0	0		
2	В	1	Total	С	Fe	Ν	Ο	0	0		
	D	1	43	34	1	4	4	0	0		
2	В	1	Total	\mathbf{C}	Fe	Ν	Ο	0	0		
		1	43	34	1	4	4	0	0		
2	В	1	Total	С	Fe	Ν	Ο	0	0		
		D	D	-	43	34	1	4	4		
2	B	1	Total	С	Fe	Ν	Ο	0	0		
		*	43	34	1	4	4				
2	В	1	Total	С	Fe	Ν	Ο	0	0		
			43	34	1	4	4				



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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	
0	р	1	Total	С	Fe	Ν	Ο	0	0	
	В	1	43	34	1	4	4	0	0	
0	р	1	Total	С	Fe	Ν	Ο	0	0	
	В	L	43	34	1	4	4	0	0	
0	D	1	Total	С	Fe	Ν	Ο	0	0	
	D	L	43	34	1	4	4	0	0	
0	D	1	Total	С	Fe	Ν	Ο	0	0	
	D	T	43	34	1	4	4	0	0	
0	В	1	Total	С	Fe	Ν	Ο	0	0	
	D	T	43	34	1	4	4	0	0	
9	В	1	Total	С	Fe	Ν	Ο	0	0	
	D	T	43	34	1	4	4	0	0	
2	В	1	Total	С	Fe	Ν	Ο	0	0	
	D	T	43	34	1	4	4	0	0	
2	В	1	Total	С	Fe	Ν	Ο	0	0	
	D	T	43	34	1	4	4	0	0	
2	В	1	Total	\mathbf{C}	Fe	Ν	Ο	0	0	
	D	*	43	34	1	4	4	0	0	
2	C	1	Total	С	Fe	Ν	Ο	0	0	
		1	43	34	1	4	4	0	0	
2	С	C	C 1	Total	С	Fe	Ν	Ο	0	0
		-	43	34	1	4	4		0	
2	С	1	Total	С	Fe	Ν	Ο	0	0	
		±	43	34	1	4	4	0	0	
2	С	1	Total	С	Fe	Ν	Ο	0	0	
		-	43	34	1	4	4	0		
2	С	1	Total	С	Fe	Ν	Ο	0	0	
		-	43	34	1	4	4	Ŭ		
2	С	1	Total	С	Fe	Ν	O	0	0	
			43	34	1	4	4		_	
2	С	1	Total	С	Fe	Ν	O	0	0	
	_		43	34	1	4	4		_	
2	С	1	Total	C	Fe	Ν	O	0	0	
			43	34		4	4			
2	С	1	Total	C	Fе	N	0	0	0	
			43	34		4	4			
2	C	1	lotal	C 1	Гe	N	U 4	0	0	
			43	<u>34</u>	1 E	4	4			
2	С	1	lotal	U 1	ге	IN 4	U 4	0	0	
			43	<u>34</u>	<u> </u>	4	4			
2	С	1	lotal	U a	ге	IN A	U 4	0	0	
			43	34	1	4	4			



Continued from previous page...

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	
0	C	1	Total	С	Fe	Ν	Ο	0	0	
2	C	1	43	34	1	4	4	0	0	
0	C	1	Total	С	Fe	Ν	Ο	0	0	
		T	43	34	1	4	4	0	0	
0	C	1	Total	С	Fe	Ν	Ο	0	0	
		L	43	34	1	4	4	0	0	
9	C	1	Total	С	Fe	Ν	Ο	0	0	
	U	T	43	34	1	4	4	0	0	
2	а	1	Total	С	Fe	Ν	Ο	0	Ο	
	D	T	43	34	1	4	4	0	0	
2	а	1	Total	С	Fe	Ν	Ο	0	0	
		T	43	34	1	4	4	0	0	
2	О	1	Total	С	Fe	Ν	Ο	0	Ο	
		1	43	34	1	4	4	0	0	
2	О	1	Total	С	Fe	Ν	Ο	0	0	
		1	43	34	1	4	4	U	U	
2	О	1	Total	С	Fe	Ν	Ο	0	0	
		*	43	34	1	4	4			
2	О	1	Total	С	Fe	Ν	Ο	0	0	
		1	43	34	1	4	4	0	0	
2	D	1	Total	С	Fe	Ν	Ο	0	0	
		-	43	34	1	4	4	0	0	
2	D	1	Total	С	Fe	Ν	Ο	0	0	
		-	43	34	1	4	4	Ŭ		
2	D	1	Total	С	Fe	Ν	Ο	0	0	
	_	_	43	34	1	4	4			
2	D	1	Total	С	Fe	Ν	O	0	0	
			43	34	1	4	4	_	_	
2	D	1	Total	C	Fe	Ν	O	0	0	
			43	34	1	4	4			
2	D	1	Total	C	Fе	N	0	0	0	
			43	34		4	4			
2	D	1	Total	C	Fе	N	U 1	0	0	
		-	43	34		4	4			
2	D	1	Total	\mathbf{C}	Гe	N	U 4	0	0	
			43	<u>54</u>	1 E	4	4			
2	2 D	1	Total	C	Fе	N	U 1	0	0	
		· · ·	43	<u>54</u>	1 E	4	4			
2	D	1	Total	C	Fе	IN	U 4	0	0	
				43	34	1	4	4	-	-

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	123	Total O 123 123	0	0
3	В	126	Total O 126 126	0	0
3	С	136	Total O 136 136	0	0
3	D	112	Total O 112 112	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are colorcoded 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.



• Molecule 1: HIGH-MOLECULAR-WEIGHT CYTOCHROME C









4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 62	Depositor	
Cell constants	220.39Å 220.39 Å 102.64 Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	30.00 - 2.51	Depositor	
% Data completeness	921 (30 00-2 51)	Depositor	
(in resolution range)	52.1 (50.00 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).

Mal	Chain	Bo	nd lengths	Bond angles			
Moi Chain		RMSZ	# Z > 5	RMSZ	# Z > 5		
1	А	0.59	0/3864	0.83	17/5201~(0.3%)		
1	В	0.59	1/3844~(0.0%)	0.83	21/5175~(0.4%)		
1	С	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	А	0	2
1	В	0	2
1	D	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	В	189	SER	CB-OG	7.80	1.52	1.42

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	С	218	ASP	CB-CG-OD2	10.44	127.69	118.30
1	А	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	С	97	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	С	428	ASP	CB-CG-OD2	7.37	124.93	118.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	79	ASP	CB-CG-OD2	7.15	124.73	118.30
1	В	132	ASP	CB-CG-OD2	7.08	124.68	118.30
1	В	79	ASP	CB-CG-OD2	6.94	124.55	118.30
1	С	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	А	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	В	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	А	425	ASP	CB-CG-OD2	6.56	124.20	118.30
1	А	186	ASP	CB-CG-OD2	6.50	124.15	118.30
1	А	58	ASP	CB-CG-OD2	6.48	124.13	118.30
1	А	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	С	330	ASP	CB-CG-OD2	6.33	123.99	118.30
1	С	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	В	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	С	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	В	212	ASP	CB-CG-OD2	5.83	123.55	118.30
1	С	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	В	100	ASP	CB-CG-OD2	5.75	123.48	118.30
1	В	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	В	99	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	173	ASP	CB-CG-OD2	5.50	123.25	118.30
	A	330	ASP	CB-CG-OD2	5.50	123.25	118.30
		344	ASP	CB-CG-OD2	5.47	123.22	118.30
	D	200	ASP	CB-CG-OD2	5.46	123.21	118.30
		396	GLY	N-CA-C	5.41	126.63	113.10
	A	389	ASP	CB-CG-OD2	5.39	123.15	118.30
		307	ASP	CB-CG-OD2	5.38	123.14	118.30
	В	218	ASP	CB-CG-OD2	5.36	123.13	118.30



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	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	С	282	ASP	CB-CG-OD2	5.29	123.06	118.30
1	С	212	ASP	CB-CG-OD2	5.28	123.05	118.30
1	А	507	ASP	CB-CG-OD2	5.27	123.05	118.30
1	А	88	ASP	CB-CG-OD2	5.25	123.02	118.30
1	В	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	А	231	ASP	CB-CG-OD2	5.19	122.97	118.30
1	В	344	ASP	CB-CG-OD2	5.18	122.96	118.30
1	В	231	ASP	CB-CG-OD2	5.18	122.96	118.30
1	В	88	ASP	CB-CG-OD2	5.14	122.93	118.30
1	А	375	ASP	CB-CG-OD2	5.14	122.92	118.30
1	В	97	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	С	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	С	375	ASP	CB-CG-OD2	5.08	122.88	118.30
1	В	307	ASP	CB-CG-OD2	5.07	122.87	118.30
1	С	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	В	538	ASP	CB-CG-OD2	5.05	122.84	118.30
1	В	524	ASP	CB-CG-OD2	5.04	122.84	118.30
1	С	507	ASP	CB-CG-OD2	5.04	122.83	118.30
1	В	161	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	В	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	А	131	GLN	Peptide
1	А	217	LEU	Peptide
1	В	131	GLN	Peptide
1	В	154	PHE	Peptide
1	D	470	HIS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3783	0	3716	68	0
1	В	3763	0	3697	67	0
1	С	3777	0	3708	80	0
1	D	3715	0	3644	81	0
2	А	688	0	480	38	0
2	В	688	0	480	36	0
2	С	688	0	480	39	0
2	D	688	0	480	44	0
3	А	123	0	0	1	0
3	В	126	0	0	2	0
3	C	136	0	0	3	0
3	D	112	0	0	1	0
All	All	18287	0	16685	357	0

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (357) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:530:LYS:HB3	1:D:531:PRO:CD	1.85	1.07
1:B:530:LYS:HB2	1:B:531:PRO:HD3	1.34	1.06
1:D:530:LYS:HB3	1:D:531:PRO:HD3	1.29	1.06
1:C:522:CYS:SG	1:C:526:MET:HE2	1.97	1.03
1:B:530:LYS:CB	1:B:531:PRO:HD3	1.89	1.03
1:C:522:CYS:SG	1:C:526:MET:CE	2.54	0.96
1:C:409:VAL:HG12	1:C:413:MET:CE	1.97	0.95
1:C:409:VAL:HG12	1:C:413:MET:HE2	1.46	0.94
1:B:530:LYS:HB2	1:B:531:PRO:CD	1.99	0.92
1:C:161:ARG:HH11	1:C:161:ARG:HG2	1.40	0.87
1:D:528:ILE:CG2	1:D:530:LYS:HB2	2.06	0.85
1:D:410:ALA:HA	1:D:413:MET:HE2	1.57	0.84
1:D:530:LYS:CB	1:D:531:PRO:CD	2.55	0.83
1:A:530:LYS:HB3	1:A:531:PRO:HD3	1.60	0.82
1:A:186:ASP:HB3	1:A:189:SER:HB2	1.62	0.80
1:B:530:LYS:CB	1:B:531:PRO:CD	2.58	0.80
1:A:429:ILE:HD11	2:A:1113:HEC:HMB2	1.63	0.79
1:B:189:SER:HB2	1:B:191:LYS:HD3	1.67	0.76
1:B:526:MET:HE1	2:B:1115:HEC:HHD	1.67	0.76
1:A:429:ILE:CD1	2:A:1113:HEC:HMB2	2.15	0.76



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



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



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



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



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



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



Atom-1	Atom-2	Interatomic	Clash
	7100111 Z	distance (Å)	overlap (Å)
2:C:1111:HEC:CHA	2:C:1111:HEC:HBA2	2.48	0.43
1:C:349:CYS:HA	2:C:1110:HEC:CHC	2.48	0.43
1:A:121:LEU:CD1	2:A:1102:HEC:HMD3	2.48	0.43
2:D:1108:HEC:HBC1	2:D:1110:HEC:C2C	2.48	0.43
1:B:346:MET:HE1	1:B:355:THR:HB	2.00	0.43
1:C:342:GLN:HG2	1:C:345:SER:HB2	2.00	0.43
1:D: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
1:A:323:HIS:CE1	2:A:1109:HEC:ND	2.86	0.43
1:C:83:CYS:HB2	2:C:1101:HEC:C2C	2.48	0.43
1:C:161:ARG:CG	1:C:161:ARG:NH1	2.79	0.43
2:C:1111:HEC:HMC1	2:C:1111:HEC:HBC3	1.99	0.43
1:C:423:THR:CG2	1:C:424:PHE:H	2.29	0.43
1:C:528:ILE:CG2	1:C:530:LYS:HB2	2.48	0.43
1:A:72:ALA:HB1	2:A:1102:HEC:HMD2	2.00	0.43
2:B:1106:HEC:HBB3	2:B:1106:HEC:HMB1	2.01	0.43
1:D:308:CYS:SG	2:D:1104:HEC:HBA1	2.58	0.43
2:D:1108:HEC:HBC1	2:D:1110:HEC:HMC2	1.99	0.43
1:C:453:VAL:HG22	2:C:1113:HEC:HMC2	2.00	0.43
1:D:211:VAL:HG22	1:D:214:ARG:HB2	1.99	0.43
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.74	0.42
1:C:253:GLN:HA	1:C:256:PHE:CE2	2.54	0.42
1:B:214:ARG:HD3	2:B:1105:HEC:HMD3	2.01	0.42
1:B:475:THR:O	2:B:1111:HEC:HMD2	2.19	0.42
1:C:274:LEU:HD21	1:C:398:LEU:HD22	2.00	0.42
1:C:423:THR:CG2	1:C:424:PHE:N	2.81	0.42
1:D:88:ASP:C	1:D:90:LYS:H	2.22	0.42
2:B:1102:HEC:HMC1	2:B:1102:HEC:CBC	2.48	0.42
1:A:105:GLU:HG2	1:A:109:ILE:HD12	2.01	0.42
1:A:328:THR:HG22	1:A:330:ASP:N	2.34	0.42
1:B:387:GLY:O	1:B:388:PHE:C	2.57	0.42
1:C:334:VAL:HG13	1:C:338:LYS:HD3	2.01	0.42
1:D:122:ALA:HB2	1:D:128:THR:HG21	2.02	0.42
1:B:357:VAL:HG13	1:B:366:HIS:HB3	2.01	0.42
1:D:211:VAL:HG21	1:D:214:ARG:NH2	2.35	0.42
1:D:482:HIS:HE1	2:D:1114:HEC:CHA	2.33	0.42
1:A:483:ASN:HD22	2:A:1114:HEC:C1D	2.33	0.42
1:B:453:VAL:HG22	2:B:1113:HEC:HMC2	2.01	0.42
1:B:161:ARG:HG3	3:B:2113:HOH:O	2.19	0.42
1:C:42:ARG:HE	1:C:65:ARG:HG2	1.84	0.42
1:D:478:GLN:HA	1:D:481:HIS:O	2.20	0.42



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



1H29

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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	497/514~(97%)	463~(93%)	25~(5%)	9~(2%)	8	14
1	В	495/514~(96%)	460 (93%)	28~(6%)	7 (1%)	11	20
1	С	497/514~(97%)	468 (94%)	24~(5%)	5(1%)	15	28
1	D	484/514~(94%)	451 (93%)	26~(5%)	7 (1%)	11	20
All	All	1973/2056~(96%)	1842 (93%)	103 (5%)	28 (1%)	11	20

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	132	ASP
1	А	218	ASP
1	А	390	ALA
1	А	395	ALA
1	В	132	ASP
1	В	530	LYS



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

5.3.2 Protein sidechains (i)

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	Pe	erce	entiles
1	А	405/414~(98%)	363~(90%)	42 (10%)		7	13
1	В	403/414~(97%)	368~(91%)	35~(9%)		10	20
1	С	404/414~(98%)	374~(93%)	30~(7%)		13	27
1	D	400/414~(97%)	359~(90%)	41 (10%)		7	14
All	All	1612/1656~(97%)	1464 (91%)	148 (9%)		9	18

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



Mol	Chain	Res	Type
1	А	53	ARG
1	А	56	LYS
1	А	71	THR
1	А	90	LYS
1	А	97	ARG
1	А	123	LYS
1	А	127	LYS
1	А	132	ASP
1	А	150	LYS
1	А	151	GLU
1	А	155	ASP
1	А	158	LEU
1	А	169	LYS
1	A	184	VAL
1	А	255	LYS
1	А	257	LYS
1	А	267	ARG
1	А	269	GLN
1	А	288	LYS
1	А	299	LYS
1	А	306	ASN
1	А	356	ARG
1	А	361	THR
1	А	374	SER
1	А	388	PHE
1	А	391	LYS
1	А	419	GLN
1	A	421	LYS
1	А	426	LEU
1	А	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	$50\overline{5}$	ARG
1	A	508	ARG
1	A	511	LEU
1	A	534	THR
1	A	543	ARG
1	В	56	LYS



Mol	Chain	Res	Type
1	В	71	THR
1	В	127	LYS
1	В	132	ASP
1	В	142	LYS
1	В	144	SER
1	В	151	GLU
1	В	155	ASP
1	В	156	LYS
1	В	161	ARG
1	В	187	GLU
1	В	191	LYS
1	В	193	VAL
1	В	209	LYS
1	В	261	GLU
1	В	267	ARG
1	В	269	GLN
1	В	325	VAL
1	В	326	ASN
1	В	345	SER
1	В	369	ILE
1	В	370	LYS
1	В	389	ASP
1	В	391	LYS
1	В	392	GLN
1	В	421	LYS
1	В	437	SER
1	В	445	SER
1	В	451	LYS
1	В	482	HIS
1	В	499	LYS
1	В	505	ARG
1	В	507	ASP
1	В	508	ARG
1	В	512	LYS
1	С	88	ASP
1	С	126	LYS
1	С	132	ASP
1	C	147	SER
1	С	151	GLU
1	C	161	ARG
1	С	171	VAL
1	С	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 1 C 373 LYS 1 C 373 LYS 1 C 389 ASP 1 C 407 SER 1 C 408 GLN 1 C 407 SER 1 C 421 LYS 1 C 441 GLU 1 C 512 LYS 1 C 529 GLU 1 C 543 ARG 1 D 41 LYS	ł	Mol	Chain		Res	Type
1 C 190 LYS 1 C 198 LYS 1 C 213 LYS 1 C 257 LYS 1 C 267 ARG 1 C 269 GLN 1 C 281 LYS 1 C 285 ARG 1 C 342 GLN 1 C 342 GLN 1 C 373 LYS 1 C 389 ASP 1 C 389 ASP 1 C 407 SER 1 C 407 SER 1 C 407 SER 1 C 421 LYS 1 C 441 GLU 1 C 512 LYS 1 C 529 GLU 1 C 543 ARG 1 D 41 LYS <tbr> <t< td=""><td></td><td>1</td><td>С</td><td></td><td>189</td><td>SER</td></t<></tbr>		1	С		189	SER
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		190	LYS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		198	LYS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		213	LYS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		257	LYS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		267	ARG
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		269	GLN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		281	LYS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		285	ARG
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		342	GLN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		373	LYS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		389	ASP
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		407	SER
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		408	GLN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		421	LYS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С	l	437	SER
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		441	GLU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		482	HIS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	С		512	LYS
$ \begin{array}{c ccccc} 1 & C & 540 & HIS \\ \hline 1 & C & 543 & ARG \\ \hline 1 & D & 41 & LYS \\ \hline 1 & D & 42 & ABC \\ \end{array} $		1	С		529	GLU
1 C 543 ARG 1 D 41 LYS 1 D 42 ARG		1	С		540	HIS
$\begin{array}{c cccc} 1 & D & 41 & LYS \\ \hline 1 & D & 42 & ABC \end{array}$		1	С		543	ARG
1 D 42 ARC		1	D		41	LYS
$1 \mid D \mid 42 \mid And \mid$		1	D		42	ARG
1 D 53 ARG		1	D		53	ARG
1 D 56 LYS		1	D		56	LYS
1 D 71 THR		1	D		71	THR
1 D 80 CYS		1	D		80	CYS
1 D 90 LYS		1	D		90	LYS
1 D 127 LYS		1	D		127	LYS
1 D 132 ASP		1	D		132	ASP
1 D 151 GLU		1	D		151	GLU
1 D 158 LEU		1	D		158	LEU
1 D 166 LYS		1	D		166	LYS
1 D 198 LYS		1	D		198	LYS
1 D 236 LYS		1	D		236	LYS
1 D 257 LYS		1	D		257	LYS
1 D 262 VAL		1	D	T	262	VAL
1 D 269 GLN		1	D		269	GLN
1 D 281 LYS		1	D		281	LYS
1 D 287 MET		1	D	T	287	MET
1 D 288 LYS		1	D		288	LYS



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

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

Mol	Chain	Res	Type
1	А	68	GLN
1	А	359	GLN
1	А	408	GLN
1	А	483	ASN
1	В	197	ASN
1	В	326	ASN
1	В	335	GLN
1	В	342	GLN
1	В	358	GLN
1	В	377	GLN
1	В	392	GLN
1	В	483	ASN
1	С	68	GLN
1	С	358	GLN
1	С	377	GLN
1	С	419	GLN
1	С	483	ASN



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

 $Continued \ from \ previous \ page...$

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

64 ligands are modelled in this entry.

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

Mal	Turne	Chain	n Res L		В	ond leng	gths	Bond angles		
	туре	Chain	nes	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	В	1107	1	26,50,50	2.55	<mark>5 (19%)</mark>	18,82,82	1.76	3(16%)
2	HEC	С	1107	1	26,50,50	2.41	<mark>5 (19%)</mark>	18,82,82	1.86	<mark>5 (27%)</mark>
2	HEC	В	1105	1	26,50,50	2.69	9 (34%)	18,82,82	1.46	3(16%)
2	HEC	D	1105	1	26,50,50	2.51	<mark>6 (23%)</mark>	18,82,82	1.77	4 (22%)
2	HEC	С	1114	1	26,50,50	2.67	<mark>6 (23%)</mark>	18,82,82	1.49	3 (16%)



Mol	Type	Chain	Bos	Link	В	ond leng	Bond lengths		Bond angles		
	туре	Cham	Ites		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
2	HEC	В	1108	1	26,50,50	<mark>2.61</mark>	7 (26%)	18,82,82	1.48	4 (22%)	
2	HEC	А	1113	1	26,50,50	<mark>2.58</mark>	<mark>5 (19%)</mark>	18,82,82	1.55	3 (16%)	
2	HEC	В	1106	1	26,50,50	2.50	6 (23%)	18,82,82	1.91	<mark>6 (33%)</mark>	
2	HEC	А	1111	1	26,50,50	2.72	<mark>6 (23%)</mark>	18,82,82	1.39	2 (11%)	
2	HEC	D	1102	1	26,50,50	2.52	6 (23%)	18,82,82	1.82	5 (27%)	
2	HEC	А	1102	1	26,50,50	2.47	7 (26%)	18,82,82	1.75	<mark>5 (27%)</mark>	
2	HEC	D	1106	1	26,50,50	2.50	<u>6 (23%)</u>	18,82,82	1.71	<mark>6 (33%)</mark>	
2	HEC	А	1105	1	26,50,50	2.67	6 (23%)	18,82,82	1.67	4 (22%)	
2	HEC	С	1105	1	26,50,50	2.72	7 (26%)	18,82,82	1.56	5 (27%)	
2	HEC	В	1103	1	26,50,50	2.55	7 (26%)	18,82,82	1.91	5 (27%)	
2	HEC	А	1101	1	26,50,50	2.43	10 (38%)	18,82,82	1.69	5 (27%)	
2	HEC	D	1107	1	26,50,50	2.52	<mark>5 (19%)</mark>	18,82,82	1.65	<mark>6 (33%)</mark>	
2	HEC	С	1116	1	26,50,50	<mark>2.61</mark>	<mark>6 (23%)</mark>	18,82,82	2.25	7 (38%)	
2	HEC	В	1104	1	26,50,50	<mark>2.35</mark>	<mark>6 (23%)</mark>	18,82,82	1.87	4 (22%)	
2	HEC	D	1104	1	26, 50, 50	2.50	<mark>6 (23%)</mark>	18,82,82	1.95	<mark>6 (33%)</mark>	
2	HEC	D	1108	1	26, 50, 50	2.72	5(19%)	18,82,82	1.69	<mark>3 (16%)</mark>	
2	HEC	А	1107	1	26, 50, 50	2.39	<mark>6 (23%)</mark>	18,82,82	<mark>2.33</mark>	8 (44%)	
2	HEC	В	1101	1	26,50,50	2.42	6 (23%)	18,82,82	1.72	5 (27%)	
2	HEC	А	1103	1	26,50,50	2.55	6 (23%)	18,82,82	<mark>2.23</mark>	5 (27%)	
2	HEC	С	1102	1	26,50,50	<mark>2.69</mark>	7 (26%)	18,82,82	1.89	<mark>6 (33%)</mark>	
2	HEC	В	1102	1	26, 50, 50	2.58	7 (26%)	18,82,82	1.71	<mark>6 (33%)</mark>	
2	HEC	D	1116	1	26, 50, 50	2.82	<mark>6 (23%)</mark>	18,82,82	1.88	<mark>3 (16%)</mark>	
2	HEC	D	1114	1	26, 50, 50	2.57	<mark>6 (23%)</mark>	18,82,82	1.56	<mark>3 (16%)</mark>	
2	HEC	А	1108	1	26, 50, 50	2.58	<mark>6 (23%)</mark>	18,82,82	1.98	<mark>9 (50%)</mark>	
2	HEC	С	1106	1	26, 50, 50	2.53	7 (26%)	18,82,82	2.06	7 (38%)	
2	HEC	С	1104	1	26,50,50	2.41	5(19%)	18,82,82	1.76	5 (27%)	
2	HEC	В	1110	1	26,50,50	2.43	7 (26%)	18,82,82	2.25	7 (38%)	
2	HEC	С	1110	1	26,50,50	2.45	5(19%)	18,82,82	1.85	<mark>6 (33%)</mark>	
2	HEC	В	1112	1	26,50,50	<mark>2.57</mark>	6 (23%)	18,82,82	1.86	7 (38%)	
2	HEC	D	1112	1	26,50,50	<mark>2.55</mark>	5 (19%)	18,82,82	1.59	4 (22%)	
2	HEC	С	1103	1	26,50,50	2.57	6 (23%)	18,82,82	2.08	5 (27%)	
2	HEC	А	1104	1	26,50,50	<mark>2.58</mark>	5 (19%)	18,82,82	1.50	1(5%)	
2	HEC	В	1111	1	26,50,50	<mark>2.79</mark>	5 (19%)	18,82,82	1.51	4 (22%)	
2	HEC	А	1106	1	26,50,50	2.71	6 (23%)	18,82,82	1.66	5 (27%)	
2	HEC	D	1115	1	26,50,50	2.48	6 (23%)	18,82,82	1.57	4 (22%)	



1H29

Mal	Tuno	Chain	Pos	Link	B	ond leng	\mathbf{gths}	В	ond ang	les
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	А	1109	1	26,50,50	2.62	6 (23%)	18,82,82	1.62	3 (16%)
2	HEC	А	1115	1	26,50,50	2.48	7 (26%)	$18,\!82,\!82$	2.03	6 (33%)
2	HEC	D	1111	1	26,50,50	2.45	5 (19%)	$18,\!82,\!82$	1.68	5 (27%)
2	HEC	А	1112	1	26,50,50	2.61	5 (19%)	18,82,82	1.45	<mark>4 (22%)</mark>
2	HEC	С	1112	1	26,50,50	2.72	6 (23%)	18,82,82	1.31	3(16%)
2	HEC	В	1114	1	26,50,50	2.59	8 (30%)	18,82,82	1.48	<mark>4 (22%)</mark>
2	HEC	А	1116	1	26,50,50	2.48	5 (19%)	18,82,82	2.05	4 (22%)
2	HEC	D	1110	1	26,50,50	2.56	7 (26%)	18,82,82	1.64	<mark>5 (27%)</mark>
2	HEC	С	1101	1	26,50,50	2.41	6 (23%)	18,82,82	1.59	4 (22%)
2	HEC	D	1109	1	26,50,50	2.62	6 (23%)	18,82,82	1.38	3 (16%)
2	HEC	В	1113	1	26,50,50	2.77	8 (30%)	18,82,82	1.95	3 (16%)
2	HEC	D	1113	1	26,50,50	2.68	6 (23%)	18,82,82	1.52	4 (22%)
2	HEC	А	1110	1	26,50,50	2.69	6 (23%)	18,82,82	1.66	3(16%)
2	HEC	В	1116	1	26,50,50	2.67	<mark>5 (19%)</mark>	18,82,82	1.89	<mark>4 (22%)</mark>
2	HEC	А	1114	1	26,50,50	2.60	8 (30%)	18,82,82	1.30	1 (5%)
2	HEC	С	1115	1	26,50,50	2.70	7 (26%)	18,82,82	2.01	7 (38%)
2	HEC	В	1115	1	26,50,50	2.52	5 (19%)	18,82,82	1.57	4 (22%)
2	HEC	В	1109	1	26,50,50	2.79	8 (30%)	18,82,82	1.29	2 (11%)
2	HEC	С	1109	1	26,50,50	2.57	7 (26%)	18,82,82	1.77	4 (22%)
2	HEC	D	1101	1	26,50,50	2.54	7 (26%)	18,82,82	1.53	<mark>3 (16%)</mark>
2	HEC	D	1103	1	26,50,50	2.67	8 (30%)	18,82,82	2.05	<mark>6 (33%)</mark>
2	HEC	С	1108	1	26,50,50	2.53	5 (19%)	18,82,82	1.70	<mark>6 (33%)</mark>
2	HEC	С	1111	1	26,50,50	2.59	6 (23%)	18,82,82	1.47	3(16%)
2	HEC	С	1113	1	26,50,50	2.73	5(19%)	18,82,82	1.97	7(38%)

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	В	1107	1	-	4/6/54/54	-
2	HEC	С	1107	1	-	1/6/54/54	-
2	HEC	В	1105	1	-	0/6/54/54	-
2	HEC	D	1105	1	-	2/6/54/54	-
2	HEC	С	1114	1	-	0/6/54/54	-
2	HEC	В	1108	1	-	0/6/54/54	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	А	1113	1	-	0/6/54/54	-
2	HEC	В	1106	1	-	0/6/54/54	-
2	HEC	А	1111	1	_	1/6/54/54	-
2	HEC	D	1102	1	-	0/6/54/54	-
2	HEC	А	1102	1	-	0/6/54/54	-
2	HEC	D	1106	1	-	0/6/54/54	-
2	HEC	А	1105	1	-	2/6/54/54	-
2	HEC	С	1105	1	-	3/6/54/54	-
2	HEC	В	1103	1	-	0/6/54/54	-
2	HEC	А	1101	1	-	1/6/54/54	-
2	HEC	D	1107	1	_	0/6/54/54	-
2	HEC	С	1116	1	_	0/6/54/54	_
2	HEC	В	1104	1	-	0/6/54/54	-
2	HEC	D	1104	1	-	0/6/54/54	-
2	HEC	D	1108	1	-	0/6/54/54	-
2	HEC	А	1107	1	-	2/6/54/54	-
2	HEC	В	1101	1	_	1/6/54/54	-
2	HEC	А	1103	1	-	0/6/54/54	-
2	HEC	С	1102	1	-	0/6/54/54	-
2	HEC	В	1102	1	-	0/6/54/54	-
2	HEC	D	1116	1	-	0/6/54/54	-
2	HEC	D	1114	1	-	0/6/54/54	-
2	HEC	А	1108	1	-	0/6/54/54	-
2	HEC	С	1106	1	-	0/6/54/54	-
2	HEC	С	1104	1	-	0/6/54/54	-
2	HEC	В	1110	1	-	0/6/54/54	-
2	HEC	С	1110	1	-	1/6/54/54	-
2	HEC	В	1112	1	-	0/6/54/54	-
2	HEC	D	1112	1	-	0/6/54/54	-
2	HEC	С	1103	1	_	0/6/54/54	_
2	HEC	A	1104	1	-	1/6/54/54	-
2	HEC	В	1111	1	-	0/6/54/54	-
2	HEC	A	1106	1	-	0/6/54/54	-
2	HEC	D	1115	1	-	0/6/54/54	-
2	HEC	А	1109	1	-	5/6/54/54	_
2	HEC	А	1115	1	-	0/6/54/54	-
2	HEC	D	11111		-	$0/6/\overline{54/54}$	_
2	HEC	A	1112	1	-	0/6/54/54	-
2	HEC	C	1112	1	-	0/6/54/54	-
2	HEC	В	11114	1	-	0/6/54/54	-
2	HEC	A	1116	1	_	0/6/54/54	_



Mol	Type	Chain	\mathbf{Res}	Link	Chirals	Torsions	Rings
2	HEC	D	1110	1	-	2/6/54/54	-
2	HEC	С	1101	1	-	1/6/54/54	-
2	HEC	D	1109	1	-	5/6/54/54	-
2	HEC	В	1113	1	-	0/6/54/54	-
2	HEC	D	1113	1	-	0/6/54/54	-
2	HEC	А	1110	1	-	0/6/54/54	-
2	HEC	В	1116	1	-	0/6/54/54	-
2	HEC	А	1114	1	-	0/6/54/54	-
2	HEC	С	1115	1	-	0/6/54/54	-
2	HEC	В	1115	1	-	0/6/54/54	-
2	HEC	В	1109	1	_	0/6/54/54	_
2	HEC	С	1109	1	-	0/6/54/54	-
2	HEC	D	1101	1	-	$1\overline{/6/54/54}$	-
2	HEC	D	1103	1	-	0/6/54/54	_
2	HEC	С	1108	1	-	$0\overline{/6/54/54}$	-
2	HEC	С	1111	1	-	2/6/54/54	-
2	HEC	С	1113	1	-	0/6/54/54	_

All (397) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	С	1112	HEC	C3B-C2B	-8.05	1.32	1.40
2	D	1108	HEC	C3B-C2B	-7.94	1.32	1.40
2	D	1113	HEC	C3C-C2C	-7.85	1.32	1.40
2	С	1113	HEC	C3C-C2C	-7.79	1.32	1.40
2	В	1109	HEC	C3C-C2C	-7.62	1.32	1.40
2	D	1116	HEC	C3B-C2B	-7.59	1.32	1.40
2	В	1111	HEC	C3B-C2B	-7.50	1.32	1.40
2	А	1103	HEC	C3B-C2B	-7.43	1.33	1.40
2	В	1113	HEC	C3B-C2B	-7.41	1.33	1.40
2	А	1110	HEC	C3B-C2B	-7.33	1.33	1.40
2	D	1116	HEC	C3C-C2C	-7.22	1.33	1.40
2	А	1106	HEC	C3C-C2C	-7.19	1.33	1.40
2	А	1104	HEC	C3B-C2B	-7.18	1.33	1.40
2	А	1105	HEC	C3C-C2C	-7.12	1.33	1.40
2	С	1103	HEC	C3B-C2B	-7.10	1.33	1.40
2	С	1115	HEC	C3B-C2B	-7.07	1.33	1.40
2	В	1103	HEC	C3B-C2B	-7.07	1.33	1.40
2	С	1105	HEC	C3B-C2B	-7.00	1.33	1.40
2	С	1102	HEC	C3C-C2C	-6.95	1.33	1.40
2	С	1114	HEC	C3B-C2B	-6.92	1.33	1.40
2	А	1112	HEC	C3B-C2B	-6.89	1.33	1.40



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	1105	HEC	C3B-C2B	-6.88	1.33	1.40
2	В	1112	HEC	C3B-C2B	-6.87	1.33	1.40
2	В	1107	HEC	C3C-C2C	-6.84	1.33	1.40
2	В	1113	HEC	C3C-C2C	-6.82	1.33	1.40
2	С	1111	HEC	C3C-C2C	-6.78	1.33	1.40
2	С	1105	HEC	C3C-C2C	-6.76	1.33	1.40
2	А	1111	HEC	C3C-C2C	-6.75	1.33	1.40
2	В	1102	HEC	C3B-C2B	-6.74	1.33	1.40
2	А	1111	HEC	C3B-C2B	-6.72	1.33	1.40
2	В	1116	HEC	C3B-C2B	-6.64	1.33	1.40
2	D	1112	HEC	C3B-C2B	-6.61	1.33	1.40
2	В	1108	HEC	C3B-C2B	-6.57	1.33	1.40
2	D	1113	HEC	C3B-C2B	-6.56	1.33	1.40
2	D	1108	HEC	C3C-C2C	-6.56	1.33	1.40
2	D	1115	HEC	C3B-C2B	-6.55	1.33	1.40
2	С	1115	HEC	C3C-C2C	-6.54	1.33	1.40
2	В	1111	HEC	C3C-C2C	-6.51	1.34	1.40
2	D	1103	HEC	C3B-C2B	-6.49	1.34	1.40
2	D	1103	HEC	C3C-C2C	-6.48	1.34	1.40
2	В	1116	HEC	C3C-C2C	-6.46	1.34	1.40
2	А	1114	HEC	C3B-C2B	-6.45	1.34	1.40
2	С	1113	HEC	C3B-C2B	-6.42	1.34	1.40
2	С	1106	HEC	C3C-C2C	-6.41	1.34	1.40
2	D	1109	HEC	C3C-C2C	-6.40	1.34	1.40
2	D	1101	HEC	C3B-C2B	-6.40	1.34	1.40
2	А	1113	HEC	C3B-C2B	-6.39	1.34	1.40
2	А	1105	HEC	C3B-C2B	-6.36	1.34	1.40
2	А	1113	HEC	C3C-C2C	-6.34	1.34	1.40
2	А	1106	HEC	C3B-C2B	-6.34	1.34	1.40
2	С	1109	HEC	C3B-C2B	-6.33	1.34	1.40
2	С	1110	HEC	C3B-C2B	-6.32	1.34	1.40
2	В	1108	HEC	C3C-C2C	-6.31	1.34	1.40
2	С	1102	HEC	C3B-C2B	-6.30	1.34	1.40
2	С	1116	HEC	C3C-C2C	-6.26	1.34	1.40
2	С	1104	HEC	C3C-C2C	-6.24	1.34	1.40
2	В	1115	HEC	C3B-C2B	-6.24	1.34	1.40
2	C _	1114	HEC	C3C-C2C	-6.22	1.34	1.40
2	С	1108	HEC	C3C-C2C	-6.22	1.34	1.40
2	A	1115	HEC	C3B-C2B	-6.22	1.34	1.40
2	В	1109	HEC	C3B-C2B	-6.19	1.34	1.40
2	C	1108	HEC	C3B-C2B	-6.18	1.34	1.40
2	A	1109	HEC	C3C-C2C	-6.16	1.34	1.40



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	1107	HEC	C3B-C2B	-6.13	1.34	1.40
2	D	1106	HEC	C3C-C2C	-6.13	1.34	1.40
2	D	1102	HEC	C3B-C2B	-6.09	1.34	1.40
2	D	1109	HEC	C3B-C2B	-6.07	1.34	1.40
2	A	1108	HEC	C3C-C2C	-6.06	1.34	1.40
2	D	1107	HEC	C3C-C2C	-6.06	1.34	1.40
2	А	1110	HEC	C3C-C2C	-6.04	1.34	1.40
2	С	1112	HEC	C3C-C2C	-6.03	1.34	1.40
2	А	1109	HEC	C3B-C2B	-6.02	1.34	1.40
2	С	1109	HEC	C3C-C2C	-6.00	1.34	1.40
2	D	1104	HEC	C3B-C2B	-5.99	1.34	1.40
2	В	1101	HEC	C3B-C2B	-5.97	1.34	1.40
2	С	1107	HEC	C3B-C2B	-5.97	1.34	1.40
2	D	1110	HEC	C3D-C2D	5.95	1.55	1.37
2	А	1107	HEC	C3C-C2C	-5.92	1.34	1.40
2	А	1112	HEC	C3C-C2C	-5.92	1.34	1.40
2	D	1105	HEC	C3B-C2B	-5.91	1.34	1.40
2	В	1114	HEC	C3B-C2B	-5.88	1.34	1.40
2	A	1108	HEC	C3D-C2D	5.88	1.55	1.37
2	C	1107	HEC	C3C-C2C	-5.85	1.34	1.40
2	C	1116	HEC	C3B-C2B	-5.84	1.34	1.40
2	A	1116	HEC	C3B-C2B	-5.83	1.34	1.40
2	A	1102	HEC	C3C-C2C	-5.81	1.34	1.40
2	A	1104	HEC	C3C-C2C	-5.80	1.34	1.40
2	В	1114	HEC	C3D-C2D	5.79	1.54	1.37
2	В	1105	HEC	C3C-C2C	-5.79	1.34	1.40
2	D	1105	HEC	C3D-C2D	5.79	1.54	1.37
2	В	1106	HEC	C3B-C2B	-5.78	1.34	1.40
2	C	1101	HEC	C3B-C2B	-5.77	1.34	1.40
2	D	1110	HEC	C3B-C2B	-5.77	1.34	1.40
2	A	1116	HEC	C3C-C2C	-5.76	1.34	1.40
2	D	1107	HEC	C3B-C2B	-5.74	1.34	1.40
2	A	1103	HEC	C3C-C2C	-5.73	1.34	1.40
2	B		HEC	C3C-C2C	-5.72	1.34	1.40
2	D	1114	HEC	C3B-C2B	-5.71	1.34	1.40
$\boxed{2}$	D A	1112	HEC	C3C-C2C	-5.70	1.34	1.40
	A	1108	HEC	C3B-C2B	-5.69	1.34	1.40
2	D A	1114	HEC	C3D-C2D	5.68	1.54	1.37
2	A	1114	HEC	C3D-C2D	5.68	1.54	1.37
$\boxed{2}$	B	1104	HEC	$\begin{array}{c} C3C-C2C \\ \hline C3D \\ \hline C3D \\ \hline \end{array}$	-5.67	1.34	1.40
2			HEC	C3B-C2B	-5.64	1.34	1.40
2		1109	HEC	C3D-C2D	5.62	1.54	1.37



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	1111	HEC	C3D-C2D	5.60	1.54	1.37
2	В	1102	HEC	C3D-C2D	5.60	1.54	1.37
2	D	1114	HEC	C3C-C2C	-5.59	1.34	1.40
2	С	1114	HEC	C3D-C2D	5.58	1.54	1.37
2	С	1102	HEC	C3D-C2D	5.57	1.54	1.37
2	С	1103	HEC	C3C-C2C	-5.56	1.34	1.40
2	D	1111	HEC	C3B-C2B	-5.54	1.35	1.40
2	А	1102	HEC	C3D-C2D	5.54	1.54	1.37
2	В	1110	HEC	C3C-C2C	-5.52	1.35	1.40
2	В	1106	HEC	C3C-C2C	-5.51	1.35	1.40
2	В	1102	HEC	C3C-C2C	-5.50	1.35	1.40
2	D	1111	HEC	C3D-C2D	5.49	1.53	1.37
2	В	1112	HEC	C3C-C2C	-5.49	1.35	1.40
2	А	1102	HEC	C3B-C2B	-5.48	1.35	1.40
2	D	1102	HEC	C3D-C2D	5.48	1.53	1.37
2	С	1116	HEC	C3D-C2D	5.47	1.53	1.37
2	С	1111	HEC	C3D-C2D	5.46	1.53	1.37
2	D	1111	HEC	C3C-C2C	-5.45	1.35	1.40
2	А	1111	HEC	C3D-C2D	5.45	1.53	1.37
2	В	1114	HEC	C3C-C2C	-5.43	1.35	1.40
2	D	1106	HEC	C3D-C2D	5.43	1.53	1.37
2	А	1115	HEC	C3C-C2C	-5.43	1.35	1.40
2	В	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	С	1115	HEC	C3D-C2D	5.40	1.53	1.37
2	A	1109	HEC	C3D-C2D	5.36	1.53	1.37
2	D	1103	HEC	C3D-C2D	5.36	1.53	1.37
2	D	1106	HEC	C3B-C2B	-5.35	1.35	1.40
2	С	1106	HEC	C3B-C2B	-5.30	1.35	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	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	В	1108	HEC	C3D-C2D	5.28	1.53	1.37
2	A		HEC	C3D-C2D	5.27	1.53	1.37
2			HEC	C3C-C2C	-5.26	1.35	1.40
$\frac{2}{2}$	R B	1101	HEC	C3D-C2D	5.26	1.53	1.37
$ \frac{2}{2}$		1107	HEC	C3D-C2D	5.25	1.53	1.37
$\frac{2}{2}$	В	1105	HEC	C3D-C2D	5.25	1.53	1.37
2	A	1112	HEC	U3D-02D	5.25	1.53	1.37


Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	1116	HEC	C3D-C2D	5.23	1.53	1.37
2	С	1101	HEC	C3C-C2C	-5.20	1.35	1.40
2	В	1110	HEC	C3D-C2D	5.19	1.53	1.37
2	D	1104	HEC	C3C-C2C	-5.18	1.35	1.40
2	С	1101	HEC	C3D-C2D	5.17	1.53	1.37
2	С	1108	HEC	C3D-C2D	5.16	1.53	1.37
2	А	1107	HEC	C3D-C2D	5.16	1.53	1.37
2	А	1104	HEC	C3D-C2D	5.15	1.52	1.37
2	А	1105	HEC	C3D-C2D	5.15	1.52	1.37
2	А	1101	HEC	C3C-C2C	-5.10	1.35	1.40
2	С	1106	HEC	C3D-C2D	5.10	1.52	1.37
2	В	1110	HEC	C3B-C2B	-5.09	1.35	1.40
2	С	1113	HEC	C3D-C2D	5.07	1.52	1.37
2	D	1112	HEC	C3D-C2D	5.07	1.52	1.37
2	С	1109	HEC	C3D-C2D	5.06	1.52	1.37
2	А	1107	HEC	C3B-C2B	-5.05	1.35	1.40
2	А	1101	HEC	C3B-C2B	-5.04	1.35	1.40
2	В	1109	HEC	C3D-C2D	5.03	1.52	1.37
2	D	1116	HEC	C3D-C2D	5.03	1.52	1.37
2	С	1103	HEC	C3D-C2D	5.03	1.52	1.37
2	A	1114	HEC	C3C-C2C	-5.02	1.35	1.40
2	D	1115	HEC	C3C-C2C	-5.02	1.35	1.40
2	С	1110	HEC	C3D-C2D	5.01	1.52	1.37
2	В	1112	HEC	C3D-C2D	4.98	1.52	1.37
2	A	1116	HEC	C3D-C2D	4.98	1.52	1.37
2	С	1107	HEC	C3D-C2D	4.95	1.52	1.37
2	В	1106	HEC	C3D-C2D	4.94	1.52	1.37
2	В	1107	HEC	C3D-C2D	4.93	1.52	1.37
2	C	1112	HEC	C3D-C2D	4.91	1.52	1.37
2	D	1115	HEC	C3D-C2D	4.88	1.52	1.37
2	B	1103	HEC	C3D-C2D	4.85	1.52	1.37
2	D	1110	HEC	C3C-C2C	-4.84	1.35	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	B	1101	HEC	C3C-C2C	-4.79	1.35	1.40
2	B	1104	HEC	C3B-C2B	-4.78	1.35	1.40
2		1102	HEC	C3C-C2C	-4.77	1.35	1.40
2	В	1104	HEC	C3D-C2D	4.75	1.51	1.37
$\boxed{2}$	A	1115	HEC	C3D-C2D	4.72	1.51	1.37
$\boxed{2}$	A	1103	HEC	C3D-C2D	4.72	1.51	1.37
2		1105	HEC	C3C-C2C	-4.70	1.35	1.40
2		1113	HEC	C3D-C2D	4.70	1.51	1.37



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	1103	HEC	C3C-C2C	-4.69	1.35	1.40
2	D	1101	HEC	C3C-C2C	-4 63	1.35	1 40
$\frac{-}{2}$	C	1104	HEC	C3B-C2B	-4.52	1.36	1.40
2	A	1106	HEC	CBC-CAC	-4.36	1.33	1.49
$\frac{-}{2}$	A	1105	HEC	CBC-CAC	-4.34	1.33	1.49
2	В	1112	HEC	CBC-CAC	-4.32	1.33	1.49
2	В	1116	HEC	CBC-CAC	-4.31	1.33	1.49
2	D	1107	HEC	CBB-CAB	-4.29	1.33	1.49
2	С	1116	HEC	CBC-CAC	-4.29	1.33	1.49
2	С	1110	HEC	CBB-CAB	-4.28	1.33	1.49
2	С	1113	HEC	CBC-CAC	-4.26	1.33	1.49
2	В	1111	HEC	CBB-CAB	-4.26	1.33	1.49
2	В	1108	HEC	CBC-CAC	-4.23	1.33	1.49
2	D	1114	HEC	CBB-CAB	-4.23	1.33	1.49
2	В	1116	HEC	CBB-CAB	-4.21	1.33	1.49
2	А	1114	HEC	CBB-CAB	-4.21	1.33	1.49
2	В	1106	HEC	CBB-CAB	-4.20	1.33	1.49
2	С	1109	HEC	CBC-CAC	-4.20	1.33	1.49
2	А	1115	HEC	CBC-CAC	-4.19	1.33	1.49
2	С	1116	HEC	CBB-CAB	-4.18	1.33	1.49
2	А	1111	HEC	CBC-CAC	-4.17	1.33	1.49
2	А	1112	HEC	CBB-CAB	-4.16	1.33	1.49
2	В	1110	HEC	CBB-CAB	-4.16	1.33	1.49
2	А	1108	HEC	CBC-CAC	-4.15	1.33	1.49
2	D	1115	HEC	CBB-CAB	-4.15	1.33	1.49
2	А	1116	HEC	CBC-CAC	-4.14	1.33	1.49
2	С	1108	HEC	CBB-CAB	-4.14	1.34	1.49
2	В	1115	HEC	CBB-CAB	-4.13	1.34	1.49
2	D	1116	HEC	CBC-CAC	-4.12	1.34	1.49
2	А	1109	HEC	CBC-CAC	-4.12	1.34	1.49
2	С	1114	HEC	CBB-CAB	-4.11	1.34	1.49
2	D	1108	HEC	CBC-CAC	-4.11	1.34	1.49
2	С	1104	HEC	CBC-CAC	-4.10	1.34	1.49
2	D	1111	HEC	CBB-CAB	-4.10	1.34	1.49
2	В	1113	HEC	CBB-CAB	-4.10	1.34	1.49
2	В	1111	HEC	CBC-CAC	-4.10	1.34	1.49
2	D	1104	HEC	CBB-CAB	-4.10	1.34	1.49
2	С	1111	HEC	CBB-CAB	-4.09	1.34	1.49
2	В	1105	HEC	CBB-CAB	-4.09	1.34	1.49
2	С	1112	HEC	CBC-CAC	-4.08	1.34	1.49
2	A	1114	HEC	CBC-CAC	-4.07	1.34	1.49
2	B	1103	HEC	CBC-CAC	-4.07	1.34	1.49



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	1109	HEC	CBC-CAC	-4.05	1.34	1.49
2	D	1101	HEC	CBC-CAC	-4.05	1.34	1.49
2	D	1105	HEC	CBB-CAB	-4.05	1.34	1.49
2	В	1115	HEC	CBC-CAC	-4.05	1.34	1.49
2	В	1114	HEC	CBB-CAB	-4.04	1.34	1.49
2	D	1103	HEC	CBB-CAB	-4.04	1.34	1.49
2	A	1113	HEC	CBC-CAC	-4.04	1.34	1.49
2	D	1115	HEC	CBC-CAC	-4.03	1.34	1.49
2	D	1114	HEC	CBC-CAC	-4.03	1.34	1.49
2	D	1108	HEC	CBB-CAB	-4.02	1.34	1.49
2	В	1112	HEC	CBB-CAB	-4.02	1.34	1.49
2	С	1103	HEC	CBC-CAC	-4.01	1.34	1.49
2	В	1105	HEC	CBC-CAC	-4.00	1.34	1.49
2	С	1115	HEC	CBC-CAC	-4.00	1.34	1.49
2	С	1112	HEC	CBB-CAB	-3.99	1.34	1.49
2	D	1110	HEC	CBB-CAB	-3.99	1.34	1.49
2	D	1113	HEC	CBC-CAC	-3.98	1.34	1.49
2	А	1109	HEC	CBB-CAB	-3.97	1.34	1.49
2	D	1112	HEC	CBB-CAB	-3.97	1.34	1.49
2	D	1103	HEC	CBC-CAC	-3.97	1.34	1.49
2	D	1113	HEC	CBB-CAB	-3.96	1.34	1.49
2	D	1104	HEC	CBC-CAC	-3.96	1.34	1.49
2	D	1109	HEC	CBC-CAC	-3.95	1.34	1.49
2	А	1116	HEC	CBB-CAB	-3.94	1.34	1.49
2	A	1102	HEC	CBC-CAC	-3.94	1.34	1.49
2	В	1101	HEC	CBC-CAC	-3.94	1.34	1.49
2	В	1109	HEC	CBB-CAB	-3.94	1.34	1.49
2	D	1106	HEC	CBC-CAC	-3.94	1.34	1.49
2	С	1105	HEC	CBC-CAC	-3.94	1.34	1.49
2	C	1115	HEC	CBB-CAB	-3.93	1.34	1.49
2	B	1106	HEC	CBC-CAC	-3.93	1.34	1.49
2	A	1115	HEC	CBB-CAB	-3.93	1.34	1.49
2	D	1107	HEC	CBC-CAC	-3.93	1.34	1.49
2	C	1107	HEC	CBC-CAC	-3.92	1.34	1.49
2	A	1108	HEC	CBB-CAB	-3.92	1.34	1.49
2		1105	HEC	CBB-CAB	-3.92	1.34	1.49
2	A	1106	HEC	CBB-CAB	-3.90	1.34	1.49
$\boxed{2}$	В	1108	HEC	CBB-CAB	-3.90	1.34	1.49
2	В	1103	HEC	CBB-CAB	-3.88	1.34	1.49
$\boxed{2}$	A	1104	HEC	CBC-CAC	-3.88	1.34	1.49
2	В	1107	HEC	CBC-CAC	-3.87	1.35	1.49
2	A	1107	HEC	CBC-CAC	-3.87	1.35	1.49



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1110	HEC	CBC-CAC	-3.87	1.35	1.49
2	D	1116	HEC	CBB-CAB	-3.87	1.35	1.49
2	C	1108	HEC	CBC-CAC	-3.87	1.35	1.49
2	A	1112	HEC	CBC-CAC	-3.87	1.35	1.49
2	A	1110	HEC	CBB-CAB	-3.87	1.35	1.49
2	С	1104	HEC	CBB-CAB	-3.86	1.35	1.49
2	D	1102	HEC	CBC-CAC	-3.86	1.35	1.49
2	A	1104	HEC	CBB-CAB	-3.86	1.35	1.49
2	A	1111	HEC	CBB-CAB	-3.85	1.35	1.49
2	В	1114	HEC	CBC-CAC	-3.85	1.35	1.49
2	С	1102	HEC	CBB-CAB	-3.85	1.35	1.49
2	В	1104	HEC	CBC-CAC	-3.84	1.35	1.49
2	С	1106	HEC	CBC-CAC	-3.83	1.35	1.49
2	А	1105	HEC	CBB-CAB	-3.83	1.35	1.49
2	С	1106	HEC	CBB-CAB	-3.83	1.35	1.49
2	В	1107	HEC	CBB-CAB	-3.83	1.35	1.49
2	D	1109	HEC	CBB-CAB	-3.83	1.35	1.49
2	С	1113	HEC	CBB-CAB	-3.81	1.35	1.49
2	D	1112	HEC	CBC-CAC	-3.79	1.35	1.49
2	А	1101	HEC	CBB-CAB	-3.79	1.35	1.49
2	D	1110	HEC	CBC-CAC	-3.79	1.35	1.49
2	В	1113	HEC	CBC-CAC	-3.78	1.35	1.49
2	C	1110	HEC	CBC-CAC	-3.78	1.35	1.49
2	A	1103	HEC	CBC-CAC	-3.78	1.35	1.49
2	В	1102	HEC	CBC-CAC	-3.77	1.35	1.49
2	В	1101	HEC	CBB-CAB	-3.76	1.35	1.49
2	D	1106	HEC	CBB-CAB	-3.74	1.35	1.49
2	A	1107	HEC	CBB-CAB	-3.74	1.35	1.49
2	C	1114	HEC	CBC-CAC	-3.73	1.35	1.49
2	D	1101	HEC	CBB-CAB	-3.73	1.35	1.49
2	D	1105	HEC	CBC-CAC	-3.72	1.35	1.49
2	C	1102	HEC	CBC-CAC	-3.71	1.35	1.49
2	A	1113	HEC	CBB-CAB	-3.70	1.35	1.49
2	C	1103	HEC	CBB-CAB	-3.69	1.35	1.49
2	D	1102	HEC	CBB-CAB	-3.68	1.35	1.49
$\frac{2}{2}$		1109	HEC	CBB-CAB	-3.68	1.35	1.49
2		1101	HEC	CBB-CAB	-3.68	1.35	1.49
2	A		HEC	CBC-CAC	-3.67	1.35	1.49
$\boxed{2}$	В	1104	HEC	CBB-CAB	-3.66	1.35	1.49
	B		HEC	UBC-CAC	-3.66	1.35	1.49
$\boxed{2}$			HEC	CBC-CAC	-3.65	1.35	1.49
2	A	1102	HEC	CBB-CAB	-3.63	1.35	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	1103	HEC	CBB-CAB	-3.62	1.35	1.49
2	В	1102	HEC	CBB-CAB	-3.62	1.35	1.49
2	С	1101	HEC	CBC-CAC	-3.60	1.36	1.49
2	D	1111	HEC	CBC-CAC	-3.58	1.36	1.49
2	С	1107	HEC	CBB-CAB	-3.50	1.36	1.49
2	С	1103	HEC	CAD-C3D	3.19	1.56	1.52
2	D	1105	HEC	CAD-C3D	3.07	1.56	1.52
2	D	1110	HEC	CAD-C3D	3.03	1.56	1.52
2	А	1101	HEC	CAD-C3D	2.87	1.56	1.52
2	А	1103	HEC	CAD-C3D	2.82	1.56	1.52
2	В	1109	HEC	CAD-C3D	2.82	1.56	1.52
2	С	1109	HEC	CAD-C3D	2.75	1.56	1.52
2	А	1109	HEC	CAD-C3D	2.74	1.56	1.52
2	В	1114	HEC	CAD-C3D	2.73	1.56	1.52
2	А	1111	HEC	CAA-C2A	2.72	1.57	1.52
2	В	1105	HEC	CAD-C3D	2.66	1.55	1.52
2	В	1103	HEC	CAD-C3D	2.66	1.55	1.52
2	D	1106	HEC	CAD-C3D	2.64	1.55	1.52
2	А	1106	HEC	CAD-C3D	2.53	1.55	1.52
2	А	1114	HEC	C4D-ND	2.53	1.41	1.36
2	А	1107	HEC	CAA-C2A	2.53	1.56	1.52
2	С	1106	HEC	CAA-C2A	2.52	1.56	1.52
2	С	1102	HEC	CAD-C3D	2.49	1.55	1.52
2	В	1109	HEC	C3C-C4C	2.47	1.47	1.43
2	В	1109	HEC	CAA-C2A	2.44	1.56	1.52
2	В	1108	HEC	CAA-C2A	2.44	1.56	1.52
2	В	1102	HEC	CAD-C3D	2.40	1.55	1.52
2	A	1108	HEC	C4D-ND	2.38	1.41	1.36
2	В	1114	HEC	C3C-C4C	2.37	1.47	1.43
2	С	1111	HEC	CAD-C3D	2.36	1.55	1.52
2	A	1101	HEC	C4A-C3A	2.36	1.47	1.42
2	С	1109	HEC	CMA-C3A	2.33	1.57	1.51
2	С	1105	HEC	CAD-C3D	2.31	1.55	1.52
2	D	1103	HEC	CAD-C3D	2.30	1.55	1.52
2	D	1115	HEC	CAA-C2A	2.29	1.56	1.52
2	A	1114	HEC	CAD-C3D	2.27	1.55	1.52
2	C	1112	HEC	CAA-C2A	2.26	1.56	1.52
2	C	1102	HEC	C3C-C4C	2.26	1.47	1.43
2	D	1113	HEC	CAA-C2A	2.23	1.56	1.52
2	B	1103	HEC	CMB-C2B	2.23	1.56	1.51
2	D	1102	HEC	C1D-ND	2.22	1.40	1.36
2	В	1104	HEC	CAA-C2A	2.22	1.56	1.52



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	А	1101	HEC	CAA-C2A	2.22	1.56	1.52
2	В	1105	HEC	C4D-ND	2.22	1.40	1.36
2	D	1103	HEC	CAA-C2A	2.21	1.56	1.52
2	А	1115	HEC	C3B-C4B	2.20	1.47	1.43
2	С	1116	HEC	CAD-C3D	2.17	1.55	1.52
2	А	1105	HEC	CAD-C3D	2.17	1.55	1.52
2	D	1101	HEC	CMC-C2C	2.17	1.56	1.51
2	С	1101	HEC	CAD-C3D	2.16	1.55	1.52
2	А	1101	HEC	C3C-C4C	2.16	1.47	1.43
2	С	1114	HEC	CMD-C2D	2.15	1.56	1.51
2	В	1106	HEC	CAA-C2A	2.14	1.56	1.52
2	В	1113	HEC	CAA-C2A	2.14	1.56	1.52
2	А	1114	HEC	C3C-C4C	2.14	1.46	1.43
2	С	1105	HEC	CAA-C2A	2.14	1.56	1.52
2	В	1113	HEC	CMD-C2D	2.14	1.56	1.51
2	D	1114	HEC	C4D-ND	2.12	1.40	1.36
2	В	1102	HEC	CAA-C2A	2.10	1.55	1.52
2	D	1101	HEC	CAD-C3D	2.10	1.55	1.52
2	D	1109	HEC	CMD-C2D	2.09	1.56	1.51
2	D	1116	HEC	CMA-C3A	2.09	1.56	1.51
2	В	1108	HEC	C4D-ND	2.09	1.40	1.36
2	В	1114	HEC	CMD-C2D	2.09	1.56	1.51
2	D	1110	HEC	CMC-C2C	2.09	1.56	1.51
2	В	1112	HEC	CMA-C3A	2.08	1.56	1.51
2	С	1115	HEC	CAA-C2A	2.07	1.55	1.52
2	А	1102	HEC	CMD-C2D	2.07	1.55	1.51
2	С	1106	HEC	CMD-C2D	2.06	1.55	1.51
2	В	1101	HEC	CAD-C3D	2.05	1.55	1.52
2	A	1115	HEC	C1D-ND	2.05	1.40	1.36
2	A	1102	HEC	CAD-C3D	2.05	1.55	1.52
2	D	1103	HEC	CMB-C2B	2.05	1.56	1.51
2	A	1101	HEC	CMC-C2C	2.03	1.56	1.51
2	В	1110	HEC	C4D-ND	2.03	1.40	1.36
2	В	1105	HEC	C3C-C4C	2.02	1.46	1.43
2	В	1110	HEC	C1A-C2A	2.02	1.47	1.42
2	A	1110	HEC	CAA-C2A	2.02	1.55	1.52
2	В	1105	HEC	C1D-ND	2.01	1.40	1.36
2	C	1115	HEC	C1D-ND	2.01	1.40	1.36
2	D	1104	HEC	CAA-C2A	2.01	1.55	1.52
2	В	1113	HEC	C1D-ND	2.00	1.40	1.36

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All (292) bond angle outliers are listed below:



1U	20
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	1103	HEC	CBD-CAD-C3D	-7.00	99.57	112.49
2	С	1103	HEC	CBD-CAD-C3D	-6.29	100.89	112.49
2	В	1113	HEC	CBD-CAD-C3D	-5.65	102.07	112.49
2	А	1116	HEC	CBD-CAD-C3D	-5.65	102.07	112.49
2	С	1116	HEC	CBD-CAD-C3D	-5.47	102.40	112.49
2	А	1107	HEC	CBA-CAA-C2A	5.14	121.94	112.48
2	В	1104	HEC	CAD-CBD-CGD	-4.95	104.37	112.67
2	D	1116	HEC	CBD-CAD-C3D	-4.71	103.79	112.49
2	В	1103	HEC	CBD-CAD-C3D	-4.64	103.92	112.49
2	В	1107	HEC	CAD-CBD-CGD	-4.59	104.97	112.67
2	А	1107	HEC	CMB-C2B-C1B	-4.59	121.41	128.46
2	А	1104	HEC	CBA-CAA-C2A	-4.50	104.18	112.48
2	D	1103	HEC	CBD-CAD-C3D	-4.50	104.18	112.49
2	D	1116	HEC	C1D-C2D-C3D	-4.30	104.00	107.00
2	В	1116	HEC	C1D-C2D-C3D	-4.27	104.02	107.00
2	С	1113	HEC	CBA-CAA-C2A	-4.21	104.71	112.48
2	D	1104	HEC	CBA-CAA-C2A	-4.10	104.93	112.48
2	С	1104	HEC	CBA-CAA-C2A	-4.05	105.02	112.48
2	D	1105	HEC	CAA-CBA-CGA	-4.01	105.94	112.67
2	С	1109	HEC	CBA-CAA-C2A	-4.00	105.10	112.48
2	В	1105	HEC	CMC-C2C-C1C	-3.96	122.38	128.46
2	В	1101	HEC	CMB-C2B-C1B	-3.95	122.40	128.46
2	А	1115	HEC	CBD-CAD-C3D	-3.92	105.26	112.49
2	В	1110	HEC	CMC-C2C-C1C	-3.84	122.56	128.46
2	В	1106	HEC	CAD-CBD-CGD	-3.81	106.28	112.67
2	D	1108	HEC	C1D-C2D-C3D	-3.75	104.39	107.00
2	В	1113	HEC	C1D-C2D-C3D	-3.74	104.39	107.00
2	С	1104	HEC	CAD-CBD-CGD	-3.73	106.41	112.67
2	В	1110	HEC	CBD-CAD-C3D	-3.69	105.68	112.49
2	D	1115	HEC	C1D-C2D-C3D	-3.68	104.44	107.00
2	В	1110	HEC	CMB-C2B-C3B	3.65	130.12	125.82
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	B	1102	HEC	CBA-CAA-C2A	-3.64	105.78	112.48
2	B	1116	HEC	CBD-CAD-C3D	-3.63	105.79	112.49
2	A	1108	HEC	CBD-CAD-C3D	-3.63	105.79	112.49
2	D	1102	HEC	CBA-CAA-C2A	-3.58	105.89	112.48
2	A	1108	HEC	CMC-C2C-C1C	-3.56	122.99	128.46
2	C	1107	HEC	C1D-C2D-C3D	-3.56	$1\overline{04.52}$	107.00
2	D	1106	HEC	CMC-C2C-C1C	-3.54	$1\overline{23.02}$	128.46
2	B	1110	HEC	CMB-C2B-C1B	-3.53	123.04	128.46
2	C	1102	HEC	CMC-C2C-C1C	-3.53	$123.0\overline{4}$	128.46
2	D	1103	HEC	CMB-C2B-C3B	3.51	129.95	125.82



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Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$ $ Ideal(o)	
2	D	1112	HEC	CMC-C2C-C1C	-3.51	123.07	128.46	
2	А	1102	HEC	CMC-C2C-C1C	-3.50	123.09	128.46	
2	С	1106	HEC	CMB-C2B-C1B	-3.49	123.09	128.46	
2	D	1102	HEC	C1D-C2D-C3D	-3.47	104.58	107.00	
2	В	1112	HEC	C1D-C2D-C3D	-3.46	104.59	107.00	
2	В	1115	HEC	C1D-C2D-C3D	-3.45	104.59	107.00	
2	А	1116	HEC	C1D-C2D-C3D	-3.45	104.60	107.00	
2	В	1110	HEC	C1D-C2D-C3D	-3.41	104.62	107.00	
2	С	1106	HEC	CMC-C2C-C1C	-3.41	123.22	128.46	
2	А	1101	HEC	CMC-C2C-C1C	-3.40	123.23	128.46	
2	С	1110	HEC	CMC-C2C-C1C	-3.40	123.24	128.46	
2	А	1111	HEC	CBA-CAA-C2A	3.39	118.73	112.48	
2	А	1105	HEC	CMB-C2B-C1B	-3.38	123.27	128.46	
2	D	1109	HEC	C1D-C2D-C3D	-3.37	104.65	107.00	
2	В	1104	HEC	CMB-C2B-C1B	-3.37	123.29	128.46	
2	С	1108	HEC	CMC-C2C-C1C	-3.35	123.31	128.46	
2	В	1106	HEC	CBD-CAD-C3D	-3.35	106.30	112.49	
2	С	1115	HEC	CMB-C2B-C1B	-3.35	123.31	128.46	
2	С	1106	HEC	CBD-CAD-C3D	-3.34	106.32	112.49	
2	С	1115	HEC	CAA-CBA-CGA	-3.33	107.08	112.67	
2	С	1102	HEC	CMC-C2C-C3C	3.31	129.71	125.82	
2	A	1109	HEC	C1D-C2D-C3D	-3.31	104.70	107.00	
2	В	1101	HEC	CMC-C2C-C1C	-3.30	123.39	128.46	
2	D	1101	HEC	CMC-C2C-C3C	3.30	129.70	125.82	
2	С	1102	HEC	CBA-CAA-C2A	-3.29	106.42	112.48	
2	A	1103	HEC	CMB-C2B-C1B	-3.28	123.43	128.46	
2	A	1113	HEC	CBA-CAA-C2A	-3.23	106.53	112.48	
2	В	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	С	1109	HEC	CMB-C2B-C1B	-3.19	123.56	128.46	
2	В	1116	HEC	CMB-C2B-C1B	-3.18	123.57	128.46	
2	D	1108	HEC	CBD-CAD-C3D	-3.16	106.66	112.49	
2	D	1108	HEC	CAD-CBD-CGD	-3.15	107.38	112.67	
2	С	1114	HEC	CBA-CAA-C2A	-3.14	106.70	112.48	
2	C	1116	HEC	CMB-C2B-C1B	-3.13	123.65	128.46	
2	B	1108	HEC	CMB-C2B-C1B	-3.11	123.69	128.46	
2	D	1114	HEC	CBA-CAA-C2A	-3.09	106.78	112.48	
$\frac{1}{2}$	D	1111	HEC	C1D-C2D-C3D	-3.07	104.86	107.00	
2	A	1107	HEC	CMB-C2B-C3B	3.06	129.42	125.82	
$\frac{-}{2}$	A	1112	HEC	CBD-CAD-C3D	-3.05	106.87	112.49	
$\frac{-}{2}$	C	1111	HEC	CAA-CBA-CGA	-3.04	107.56	112.67	
$\frac{-}{2}$	A	1101	HEC	CMC-C2C-C3C	3.04	129.40	125.82	
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1H29

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	1101	HEC	CMB-C2B-C1B	-3.04	123.79	128.46
2	А	1102	HEC	CMC-C2C-C3C	3.03	129.39	125.82
2	В	1103	HEC	CMB-C2B-C1B	-3.03	123.80	128.46
2	А	1115	HEC	CBA-CAA-C2A	-3.03	106.89	112.48
2	D	1101	HEC	CMC-C2C-C1C	-3.02	123.82	128.46
2	А	1115	HEC	C1D-C2D-C3D	-3.02	104.90	107.00
2	В	1109	HEC	CMB-C2B-C1B	-3.01	123.83	128.46
2	С	1116	HEC	C1D-C2D-C3D	-3.01	104.90	107.00
2	А	1101	HEC	CMB-C2B-C1B	-2.99	123.87	128.46
2	А	1109	HEC	CAA-CBA-CGA	-2.98	107.67	112.67
2	А	1105	HEC	C1D-C2D-C3D	-2.98	104.92	107.00
2	С	1103	HEC	CMB-C2B-C1B	-2.98	123.89	128.46
2	В	1103	HEC	C1D-C2D-C3D	-2.98	104.92	107.00
2	В	1107	HEC	C1D-C2D-C3D	-2.98	104.93	107.00
2	А	1115	HEC	CMC-C2C-C1C	-2.97	123.89	128.46
2	D	1103	HEC	CMB-C2B-C1B	-2.95	123.92	128.46
2	С	1101	HEC	CMC-C2C-C1C	-2.95	123.93	128.46
2	С	1115	HEC	CMC-C2C-C1C	-2.94	123.94	128.46
2	В	1114	HEC	C1D-C2D-C3D	-2.93	104.96	107.00
2	А	1102	HEC	CBD-CAD-C3D	-2.93	107.08	112.49
2	В	1106	HEC	CMB-C2B-C1B	-2.93	123.96	128.46
2	С	1107	HEC	CMB-C2B-C1B	-2.93	123.97	128.46
2	В	1115	HEC	CAA-CBA-CGA	-2.93	107.76	112.67
2	D	1105	HEC	CBA-CAA-C2A	2.92	117.86	112.48
2	С	1102	HEC	CAA-CBA-CGA	-2.91	107.78	112.67
2	С	1110	HEC	CAD-CBD-CGD	-2.91	107.79	112.67
2	С	1105	HEC	CMB-C2B-C1B	-2.91	123.99	128.46
2	В	1116	HEC	CMC-C2C-C1C	-2.90	124.01	128.46
2	С	1108	HEC	CAA-CBA-CGA	-2.89	107.83	112.67
2	С	1115	HEC	C1D-C2D-C3D	-2.88	104.99	107.00
2	В	1101	HEC	CMB-C2B-C3B	2.88	129.21	125.82
2	С	1104	HEC	CMB-C2B-C1B	-2.88	124.04	128.46
2	В	1106	HEC	C1D-C2D-C3D	-2.87	105.00	107.00
2	D	1112	HEC	CMB-C2B-C1B	-2.87	124.05	128.46
2	В	1112	HEC	CMC-C2C-C1C	-2.87	124.06	128.46
2	A	$1\overline{115}$	HEC	CMB-C2B-C1B	-2.85	124.08	128.46
2	С	1113	HEC	CMB-C2B-C1B	-2.85	124.09	128.46
2	D	1112	HEC	CMC-C2C-C3C	2.84	129.16	125.82
2	A	1102	HEC	CMB-C2B-C1B	-2.83	124.12	128.46
2	B	1104	HEC	CMC-C2C-C1C	-2.82	124.13	128.46
2	D	1107	HEC	CBD-CAD-C3D	-2.82	107.28	112.49
2	С	1101	HEC	CBA-CAA-C2A	-2.81	107.29	112.48



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	1114	HEC	CAD-CBD-CGD	2.80	117.36	112.67
2	D	1104	HEC	CMC-C2C-C1C	-2.80	124.17	128.46
2	С	1112	HEC	CMB-C2B-C1B	-2.79	124.18	128.46
2	D	1106	HEC	CMB-C2B-C1B	-2.78	124.19	128.46
2	С	1108	HEC	C1D-C2D-C3D	-2.78	105.06	107.00
2	С	1107	HEC	CAA-CBA-CGA	-2.77	108.03	112.67
2	В	1103	HEC	CMB-C2B-C3B	2.76	129.07	125.82
2	А	1108	HEC	C1D-C2D-C3D	-2.76	105.08	107.00
2	В	1103	HEC	CMC-C2C-C1C	-2.75	124.23	128.46
2	С	1115	HEC	CMB-C2B-C3B	2.75	129.05	125.82
2	С	1116	HEC	CMB-C2B-C3B	2.75	129.05	125.82
2	D	1113	HEC	CBA-CAA-C2A	-2.75	107.42	112.48
2	С	1116	HEC	CMC-C2C-C1C	-2.74	124.25	128.46
2	В	1111	HEC	CAD-CBD-CGD	-2.74	108.08	112.67
2	D	1102	HEC	CMB-C2B-C1B	-2.74	124.26	128.46
2	В	1111	HEC	CMB-C2B-C1B	-2.73	124.26	128.46
2	В	1112	HEC	CMA-C3A-C2A	2.73	130.09	124.94
2	D	1111	HEC	CMC-C2C-C1C	-2.73	124.27	128.46
2	D	1101	HEC	C1D-C2D-C3D	-2.73	105.10	107.00
2	С	1107	HEC	CBD-CAD-C3D	-2.72	107.47	112.49
2	D	1102	HEC	CBD-CAD-C3D	-2.70	107.50	112.49
2	В	1111	HEC	CMC-C2C-C1C	-2.70	124.31	128.46
2	D	1107	HEC	CMB-C2B-C1B	-2.70	124.32	128.46
2	А	1114	HEC	CMC-C2C-C1C	-2.70	124.32	128.46
2	D	1105	HEC	CMC-C2C-C1C	-2.70	124.32	128.46
2	А	1106	HEC	CMB-C2B-C1B	-2.70	124.32	128.46
2	D	1115	HEC	CBD-CAD-C3D	-2.69	107.53	112.49
2	С	1113	HEC	C1D-C2D-C3D	-2.68	105.13	107.00
2	А	1106	HEC	CBD-CAD-C3D	-2.68	107.54	112.49
2	С	1110	HEC	CMC-C2C-C3C	2.66	128.95	125.82
2	С	1102	HEC	CBD-CAD-C3D	-2.65	107.59	112.49
2	С	1116	HEC	CAD-CBD-CGD	2.65	117.12	112.67
2	С	1111	HEC	C1D-C2D-C3D	-2.64	105.16	107.00
2	С	1110	HEC	CBD-CAD-C3D	-2.64	107.61	112.49
2	D	1110	HEC	CBA-CAA-C2A	-2.64	107.61	112.48
2	A	1110	HEC	CMB-C2B-C1B	-2.64	124.41	128.46
2	В	1110	HEC	CMC-C2C-C3C	2.63	128.91	125.82
2	С	1107	HEC	CMC-C2C-C1C	-2.61	124.45	128.46
2	В	1105	HEC	CMC-C2C-C3C	2.61	128.89	125.82
2	С	1113	HEC	CAA-CBA-CGA	-2.57	108.35	112.67
2	C	1112	HEC	CBD-CAD-C3D	-2.57	107.74	112.49
2	В	1112	HEC	CMB-C2B-C1B	-2.56	124.52	128.46



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	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	С	1105	HEC	CBD-CAD-C3D	-2.55	107.78	112.49
2	А	1107	HEC	CAA-C2A-C3A	2.55	134.57	127.25
2	А	1101	HEC	CBA-CAA-C2A	-2.54	107.80	112.48
2	С	1113	HEC	CBD-CAD-C3D	-2.54	107.80	112.49
2	В	1111	HEC	CBA-CAA-C2A	-2.54	107.80	112.48
2	В	1102	HEC	CMC-C2C-C1C	-2.53	124.58	128.46
2	D	1110	HEC	CMB-C2B-C1B	-2.53	124.58	128.46
2	D	1113	HEC	CBD-CAD-C3D	-2.52	107.84	112.49
2	В	1108	HEC	CBD-CAD-C3D	-2.52	107.85	112.49
2	С	1106	HEC	CMB-C2B-C3B	2.51	128.77	125.82
2	D	1115	HEC	CMC-C2C-C1C	-2.51	124.61	128.46
2	D	1111	HEC	CAA-CBA-CGA	-2.50	108.47	112.67
2	D	1104	HEC	CAD-CBD-CGD	-2.50	108.48	112.67
2	А	1116	HEC	CMC-C2C-C1C	-2.48	124.65	128.46
2	С	1106	HEC	CAD-CBD-CGD	-2.48	108.51	112.67
2	С	1105	HEC	CMA-C3A-C2A	2.48	129.61	124.94
2	А	1102	HEC	C1D-C2D-C3D	-2.47	105.28	107.00
2	D	1112	HEC	C1D-C2D-C3D	-2.45	105.29	107.00
2	А	1116	HEC	CMB-C2B-C1B	-2.45	124.70	128.46
2	А	1115	HEC	CMB-C2B-C3B	2.45	128.70	125.82
2	С	1109	HEC	C1D-C2D-C3D	-2.43	105.31	107.00
2	А	1103	HEC	CMB-C2B-C3B	2.42	128.66	125.82
2	D	1106	HEC	CAD-CBD-CGD	-2.41	108.62	112.67
2	D	1103	HEC	CMA-C3A-C2A	2.41	129.48	124.94
2	С	1115	HEC	CBD-CAD-C3D	-2.41	108.05	112.49
2	А	1113	HEC	CMC-C2C-C1C	-2.39	124.78	128.46
2	D	1107	HEC	C1D-C2D-C3D	-2.39	105.33	107.00
2	A	1113	HEC	CBD-CAD-C3D	-2.39	108.08	112.49
2	С	1116	HEC	CMC-C2C-C3C	2.38	128.62	125.82
2	В	1106	HEC	CMB-C2B-C3B	2.38	128.62	125.82
2	В	1112	HEC	CAD-CBD-CGD	-2.38	108.68	112.67
2	В	1115	HEC	CMC-C2C-C1C	-2.38	124.81	128.46
2	A	1106	HEC	CMA-C3A-C2A	2.38	129.43	124.94
2	D	1113	HEC	C1D-C2D-C3D	-2.37	105.35	107.00
2	D	1107	HEC	CAD-CBD-CGD	-2.36	108.70	112.67
2	A	1103	HEC	CAD-CBD-CGD	2.36	116.64	112.67
2	В	1106	HEC	CMC-C2C-C1C	-2.33	124.89	128.46
2	B	1102	HEC	CMB-C2B-C1B	-2.31	124.91	128.46
2	В	1113	HEC	CMD-C2D-C3D	2.31	129.29	124.94
2	A	1106	HEC	CMB-C2B-C3B	2.30	128.53	125.82



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	1109	HEC	C4C-C3C-C2C	2.30	108.84	106.35
2	D	1107	HEC	CAA-CBA-CGA	-2.30	108.82	112.67
2	С	1103	HEC	CAD-CBD-CGD	2.30	116.52	112.67
2	D	1113	HEC	CMB-C2B-C1B	-2.29	124.94	128.46
2	С	1104	HEC	CMB-C2B-C3B	2.28	128.50	125.82
2	D	1103	HEC	C4B-C3B-C2B	2.28	108.81	106.35
2	D	1116	HEC	CMA-C3A-C2A	2.28	129.24	124.94
2	С	1103	HEC	CMC-C2C-C1C	-2.27	124.97	128.46
2	А	1112	HEC	CMB-C2B-C1B	-2.27	124.97	128.46
2	С	1109	HEC	CMB-C2B-C3B	2.27	128.49	125.82
2	С	1108	HEC	CBD-CAD-C3D	-2.27	108.30	112.49
2	А	1112	HEC	CBA-CAA-C2A	-2.27	108.30	112.48
2	С	1106	HEC	CMC-C2C-C3C	2.26	128.48	125.82
2	С	1102	HEC	CMB-C2B-C1B	-2.26	124.99	128.46
2	А	1105	HEC	CMB-C2B-C3B	2.26	128.47	125.82
2	С	1114	HEC	CMB-C2B-C1B	-2.26	125.00	128.46
2	А	1103	HEC	CMA-C3A-C2A	2.25	129.19	124.94
2	С	1101	HEC	CMC-C2C-C3C	2.25	128.47	125.82
2	В	1112	HEC	CMC-C2C-C3C	2.25	128.46	125.82
2	А	1108	HEC	CAA-CBA-CGA	-2.25	108.90	112.67
2	В	1102	HEC	CBD-CAD-C3D	-2.24	108.36	112.49
2	А	1108	HEC	CMC-C2C-C3C	2.23	128.44	125.82
2	В	1102	HEC	CMC-C2C-C3C	2.23	128.44	125.82
2	D	1114	HEC	CMB-C2B-C1B	-2.22	125.05	128.46
2	D	1110	HEC	CMD-C2D-C1D	-2.22	125.05	128.46
2	А	1105	HEC	CMA-C3A-C2A	2.21	129.11	124.94
2	В	1101	HEC	CMC-C2C-C3C	2.21	128.42	125.82
2	D	1102	HEC	CMC-C2C-C1C	-2.20	125.08	128.46
2	В	1107	HEC	C4B-C3B-C2B	2.20	108.73	106.35
2	A	1108	HEC	CMB-C2B-C1B	-2.20	125.09	128.46
2	B	1112	HEC	CMB-C2B-C3B	2.20	$128.4\overline{0}$	125.82
2	A	1108	HEC	CMD-C2D-C3D	2.19	129.08	124.94
2	A	1110	HEC	CMD-C2D-C3D	2.19	129.08	124.94
2	C	1108	HEC	CMB-C2B-C1B	-2.19	$125.1\overline{0}$	128.46
2	D	1109	HEC	CMB-C2B-C1B	-2.18	125.11	128.46
2	В	1108	HEC	CMC-C2C-C1C	-2.18	125.12	128.46
2	D	1109	HEC	CMC-C2C-C1C	-2.18	125.12	128.46
2	В	1114	HEC	CMB-C2B-C1B	-2.17	125.12	128.46
2	С	1108	HEC	CMC-C2C-C3C	2.17	128.37	125.82
2	D	1114	HEC	CBD-CAD-C3D	-2.16	108.50	112.49
2	D	1107	HEC	CMB-C2B-C3B	2.16	128.35	125.82
2	A	1107	HEC	CAA-CBA-CGA	-2.15	109.06	112.67



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1H	.29

Conti	Continued from previous page							
Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$	
2	D	1115	HEC	C4B-C3B-C2B	2.15	108.67	106.35	
2	А	1112	HEC	CMC-C2C-C1C	-2.14	125.17	128.46	
2	В	1110	HEC	CBA-CAA-C2A	-2.14	108.53	112.48	
2	В	1104	HEC	CMB-C2B-C3B	2.14	128.34	125.82	
2	D	1104	HEC	CMB-C2B-C1B	-2.14	125.18	128.46	
2	С	1111	HEC	CMB-C2B-C1B	-2.13	125.19	128.46	
2	С	1103	HEC	CMB-C2B-C3B	2.12	128.31	125.82	
2	В	1105	HEC	CAA-CBA-CGA	-2.12	109.12	112.67	
2	А	1106	HEC	C1D-C2D-C3D	-2.11	105.53	107.00	
2	С	1113	HEC	CMD-C2D-C3D	2.11	128.92	124.94	
2	D	1106	HEC	CMC-C2C-C3C	2.11	128.30	125.82	
2	D	1110	HEC	CMD-C2D-C3D	2.11	128.92	124.94	
2	С	1114	HEC	CAA-CBA-CGA	-2.11	109.13	112.67	
2	С	1105	HEC	CMB-C2B-C3B	2.11	128.30	125.82	
2	В	1109	HEC	CMB-C2B-C3B	2.10	128.29	125.82	
2	А	1111	HEC	C1D-C2D-C3D	-2.09	105.54	107.00	
2	А	1107	HEC	CBD-CAD-C3D	-2.08	108.65	112.49	
2	В	1101	HEC	CBD-CAD-C3D	-2.08	108.65	112.49	
2	С	1104	HEC	C1D-C2D-C3D	-2.08	105.55	107.00	
2	В	1115	HEC	CMB-C2B-C1B	-2.08	125.27	128.46	
2	С	1113	HEC	CMB-C2B-C3B	2.07	128.26	125.82	
2	D	1110	HEC	CAA-CBA-CGA	-2.07	109.19	112.67	
2	А	1101	HEC	CMB-C2B-C3B	2.07	128.25	125.82	
2	С	1110	HEC	CMB-C2B-C1B	-2.06	125.30	128.46	
2	С	1105	HEC	CAA-CBA-CGA	-2.06	109.22	112.67	
2	D	1104	HEC	CMA-C3A-C2A	2.05	128.80	124.94	
2	В	1114	HEC	CBA-CAA-C2A	-2.04	108.72	112.48	
2	А	1108	HEC	CBA-CAA-C2A	-2.04	108.72	112.48	
2	D	1106	HEC	CMB-C2B-C3B	2.04	128.22	125.82	
2	С	1110	HEC	CMA-C3A-C2A	2.04	128.78	124.94	
2	С	1112	HEC	CMC-C2C-C1C	-2.04	125.33	128.46	
2	А	1108	HEC	CAD-CBD-CGD	2.03	116.08	112.67	
2	D	1106	HEC	CAA-CBA-CGA	-2.03	109.27	112.67	
2	D	1105	HEC	CMB-C2B-C1B	-2.03	125.35	128.46	
2	А	1107	HEC	CMC-C2C-C1C	-2.03	125.35	128.46	
2	D	1111	HEC	CMB-C2B-C1B	-2.02	125.35	128.46	
2	С	1115	HEC	CMD-C2D-C3D	2.02	128.75	124.94	
2	D	1111	HEC	CAD-CBD-CGD	-2.00	109.31	112.67	
2	В	1108	HEC	CAA-CBA-CGA	-2.00	109.31	112.67	

There are no chirality outliers.

All (35) torsion outliers are listed below:



1	ТΤ	20
Т	п	Z9

Mol	Chain	\mathbf{Res}	Type	Atoms
2	В	1107	HEC	C1A-C2A-CAA-CBA
2	В	1107	HEC	C3A-C2A-CAA-CBA
2	D	1105	HEC	C1A-C2A-CAA-CBA
2	D	1105	HEC	C3A-C2A-CAA-CBA
2	А	1105	HEC	C1A-C2A-CAA-CBA
2	А	1105	HEC	C3A-C2A-CAA-CBA
2	С	1105	HEC	C1A-C2A-CAA-CBA
2	С	1105	HEC	C3A-C2A-CAA-CBA
2	С	1105	HEC	C2A-CAA-CBA-CGA
2	А	1107	HEC	C3A-C2A-CAA-CBA
2	В	1101	HEC	C3D-CAD-CBD-CGD
2	А	1109	HEC	C1A-C2A-CAA-CBA
2	А	1109	HEC	C3A-C2A-CAA-CBA
2	А	1109	HEC	C2A-CAA-CBA-CGA
2	D	1109	HEC	C1A-C2A-CAA-CBA
2	D	1109	HEC	C3A-C2A-CAA-CBA
2	D	1109	HEC	C2A-CAA-CBA-CGA
2	D	1109	HEC	C2D-C3D-CAD-CBD
2	D	1109	HEC	C4D-C3D-CAD-CBD
2	D	1101	HEC	C3D-CAD-CBD-CGD
2	С	1101	HEC	C3D-CAD-CBD-CGD
2	С	1110	HEC	C2A-CAA-CBA-CGA
2	В	1107	HEC	C2D-C3D-CAD-CBD
2	В	1107	HEC	C4D-C3D-CAD-CBD
2	А	1107	HEC	C1A-C2A-CAA-CBA
2	А	1109	HEC	C2D-C3D-CAD-CBD
2	А	1109	HEC	C4D-C3D-CAD-CBD
2	D	1110	HEC	C2D-C3D-CAD-CBD
2	D	1110	HEC	C4D-C3D-CAD-CBD
2	C	1111	HEC	C1A-C2A-CAA-CBA
2	С	1111	HEC	C3A-C2A-CAA-CBA
2	A	1101	HEC	C3D-CAD-CBD-CGD
2	С	1107	HEC	C3D-CAD-CBD-CGD
2	A	1111	HEC	C2A-CAA-CBA-CGA
2	A	1104	HEC	C2A-CAA-CBA-CGA

There are no ring outliers.

56 monomers are involved in 157 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1107	HEC	2	0
2	С	1107	HEC	3	0
2	В	1105	HEC	1	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	1114	HEC	1	0
2	В	1108	HEC	1	0
2	А	1113	HEC	5	0
2	В	1106	HEC	3	0
2	А	1111	HEC	2	0
2	D	1102	HEC	6	0
2	А	1102	HEC	5	0
2	D	1106	HEC	4	0
2	С	1105	HEC	2	0
2	А	1101	HEC	1	0
2	D	1107	HEC	2	0
2	В	1104	HEC	2	0
2	D	1104	HEC	6	0
2	D	1108	HEC	4	0
2	В	1101	HEC	1	0
2	А	1103	HEC	1	0
2	С	1102	HEC	4	0
2	В	1102	HEC	5	0
2	D	1114	HEC	2	0
2	А	1108	HEC	3	0
2	С	1106	HEC	2	0
2	С	1104	HEC	1	0
2	В	1110	HEC	2	0
2	С	1110	HEC	5	0
2	В	1112	HEC	3	0
2	D	1112	HEC	3	0
2	С	1103	HEC	2	0
2	А	1104	HEC	4	0
2	В	1111	HEC	4	0
2	А	1106	HEC	1	0
2	D	1115	HEC	1	0
2	А	1109	HEC	3	0
2	A	1115	HEC	3	0
2	D	1111	HEC	3	0
2	A	1112	HEC	5	0
2	С	1112	HEC	1	0
2	В	1114	HEC	2	0
2	D	1110	HEC	7	0
2	C	1101	HEC	3	0
2	D	1109	HEC	4	0
2	В	1113	HEC	2	0
2	D	1113	HEC	2	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	1110	HEC	4	0
2	В	1116	HEC	1	0
2	А	1114	HEC	1	0
2	С	1115	HEC	5	0
2	В	1115	HEC	6	0
2	В	1109	HEC	1	0
2	С	1109	HEC	4	0
2	D	1101	HEC	6	0
2	С	1108	HEC	3	0
2	С	1111	HEC	4	0
2	С	1113	HEC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.































































































































































































































































5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

