



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 14, 2020 – 04:20 pm BST

PDB ID : 2M6Z  
Title : Refined solution structure of Human Adult Hemoglobin in the Carbonmonoxy Form  
Authors : Fan, J.S.; Yang, D.; Choy, W.Y.  
Deposited on : 2013-04-15

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

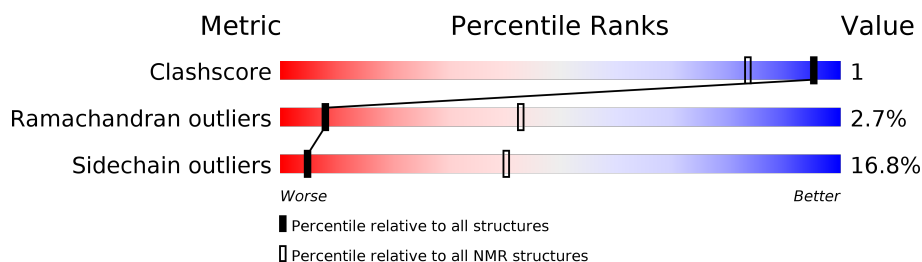
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 37%.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	141	87% 11% .
1	C	141	87% 11% .
2	B	146	84% 15% .
2	D	146	85% 15%

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:138, B:1-B:145 (283)	0.59	17
2	C:1-C:138, D:1-D:146 (284)	0.60	17

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	3, 4, 7, 9, 10, 11, 12, 13, 14, 15, 16, 17, 19, 20
2	1, 2, 5, 6, 8
Single-model clusters	18

### 3 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 9058 atoms, of which 4502 are hydrogens and 0 are deuteriums.

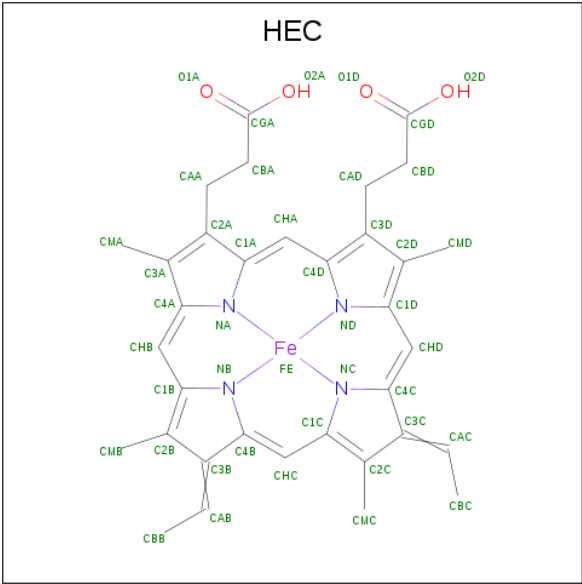
- Molecule 1 is a protein called Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms						Trace
1	A	141	Total	C	H	N	O	S	0
			2142	685	1073	187	194	3	
1	C	141	Total	C	H	N	O	S	0
			2142	685	1073	187	194	3	

- Molecule 2 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms						Trace
2	B	146	Total	C	H	N	O	S	0
			2241	724	1118	195	201	3	
2	D	146	Total	C	H	N	O	S	0
			2241	724	1118	195	201	3	

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



Mol	Chain	Residues	Atoms					
3	A	1	Total	C	Fe	H	N	O
			73	34	1	30	4	4
3	B	1	Total	C	Fe	H	N	O
			73	34	1	30	4	4

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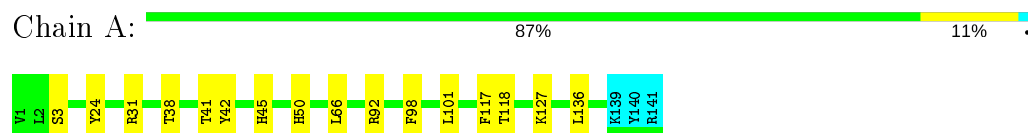
Mol	Chain	Residues	Atoms					
			Total	C	Fe	H	N	O
3	C	1	73	34	1	30	4	4
3	D	1	73	34	1	30	4	4

## 4 Residue-property plots [i](#)

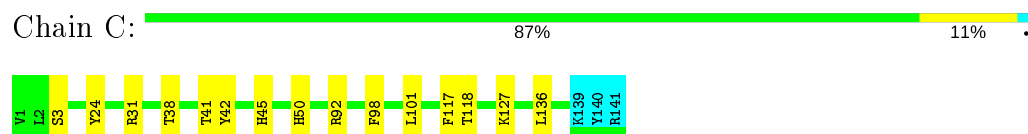
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

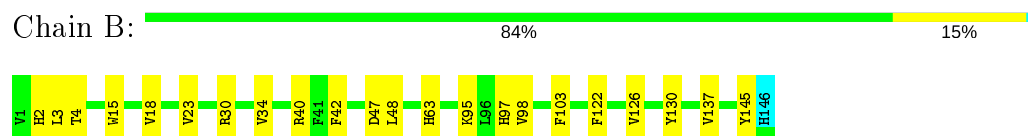
- Molecule 1: Hemoglobin subunit alpha



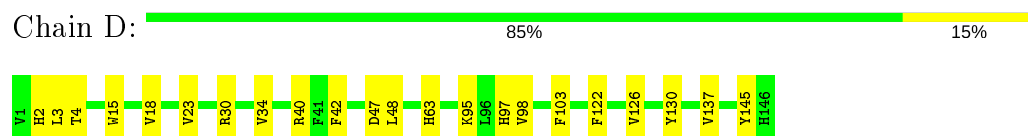
- Molecule 1: Hemoglobin subunit alpha



- Molecule 2: Hemoglobin subunit beta



- Molecule 2: Hemoglobin subunit beta

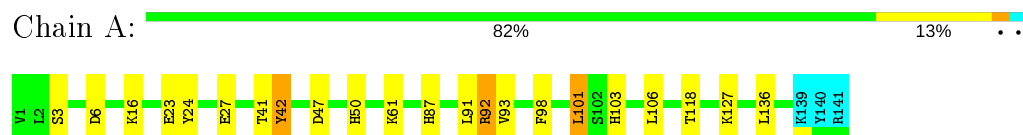


### 4.2 Scores per residue for each member of the ensemble

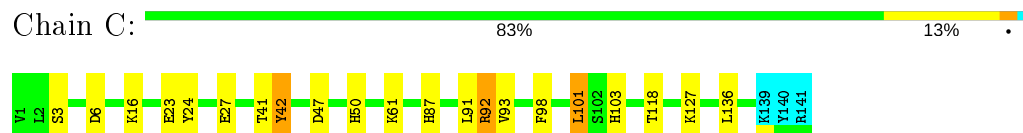
Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

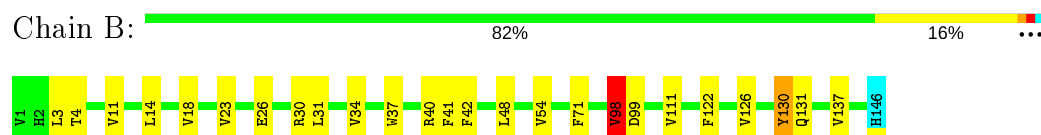
- Molecule 1: Hemoglobin subunit alpha



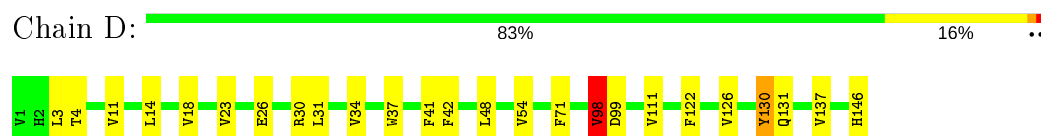
- Molecule 1: Hemoglobin subunit alpha



- Molecule 2: Hemoglobin subunit beta

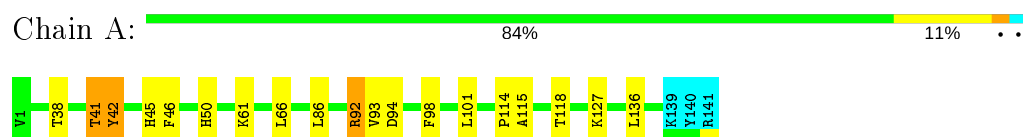


- Molecule 2: Hemoglobin subunit beta

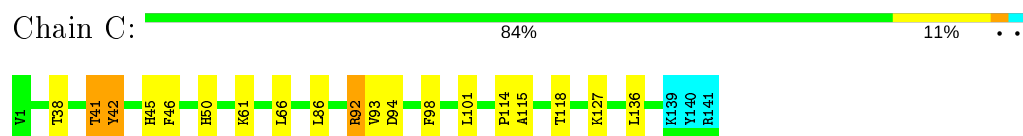


### 4.2.2 Score per residue for model 2

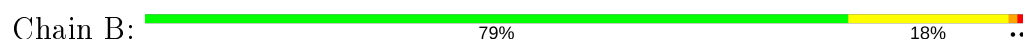
- Molecule 1: Hemoglobin subunit alpha



- Molecule 1: Hemoglobin subunit alpha

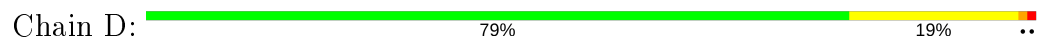


- Molecule 2: Hemoglobin subunit beta



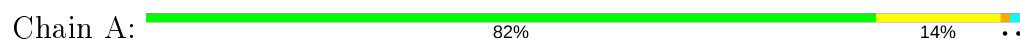


- Molecule 2: Hemoglobin subunit beta

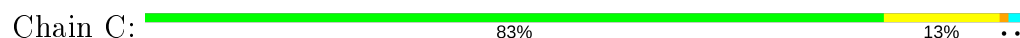


#### 4.2.3 Score per residue for model 3

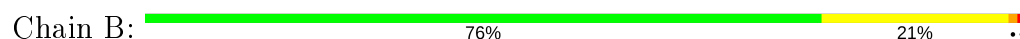
- Molecule 1: Hemoglobin subunit alpha



- Molecule 1: Hemoglobin subunit alpha



- Molecule 2: Hemoglobin subunit beta

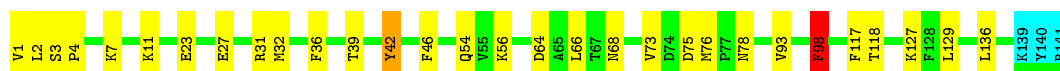
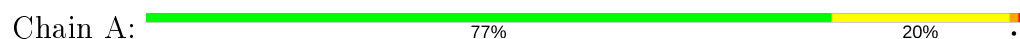


- Molecule 2: Hemoglobin subunit beta



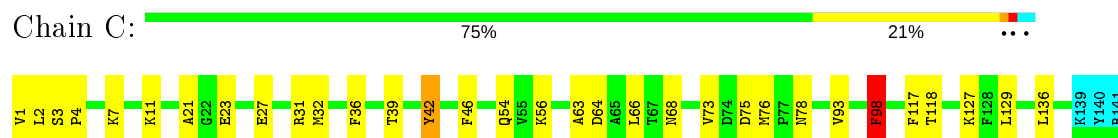
#### 4.2.4 Score per residue for model 4

- Molecule 1: Hemoglobin subunit alpha

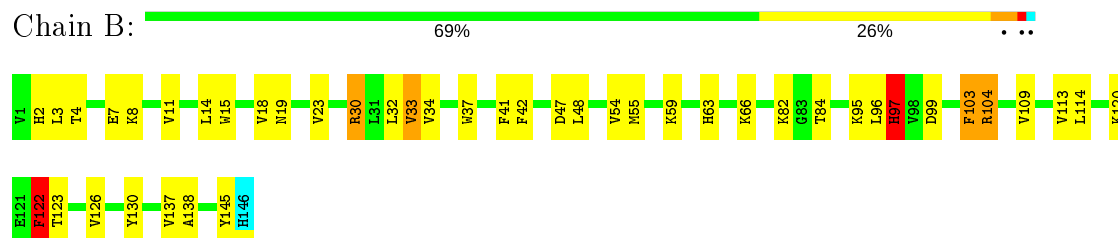




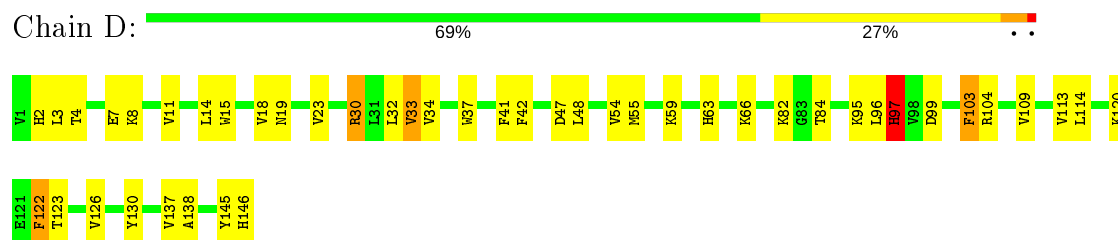
- Molecule 1: Hemoglobin subunit alpha



- Molecule 2: Hemoglobin subunit beta

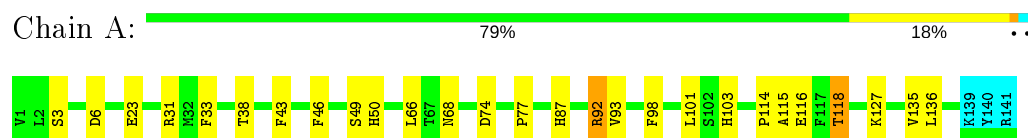


- Molecule 2: Hemoglobin subunit beta

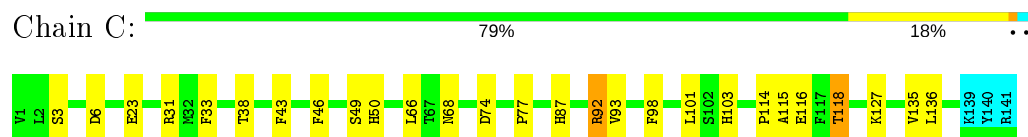


#### 4.2.5 Score per residue for model 5

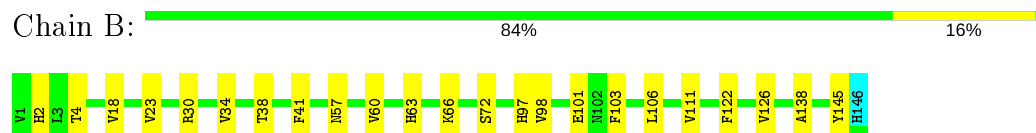
- Molecule 1: Hemoglobin subunit alpha



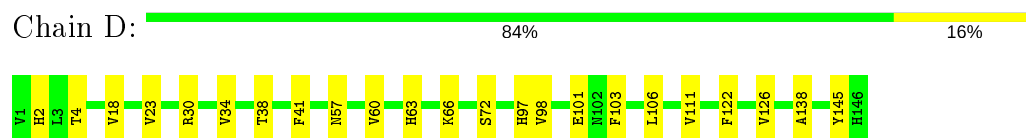
- Molecule 1: Hemoglobin subunit alpha



- Molecule 2: Hemoglobin subunit beta

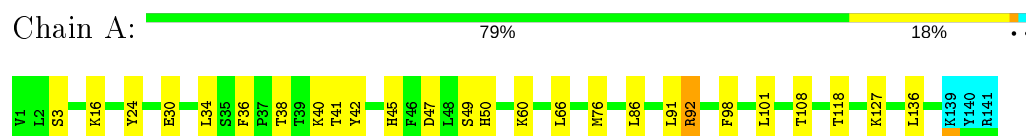


- Molecule 2: Hemoglobin subunit beta

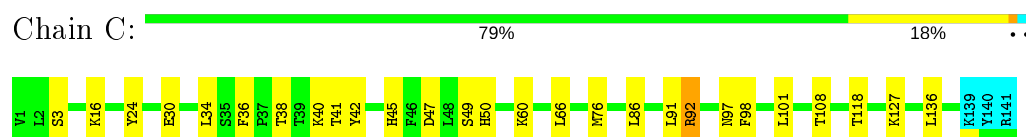


#### 4.2.6 Score per residue for model 6

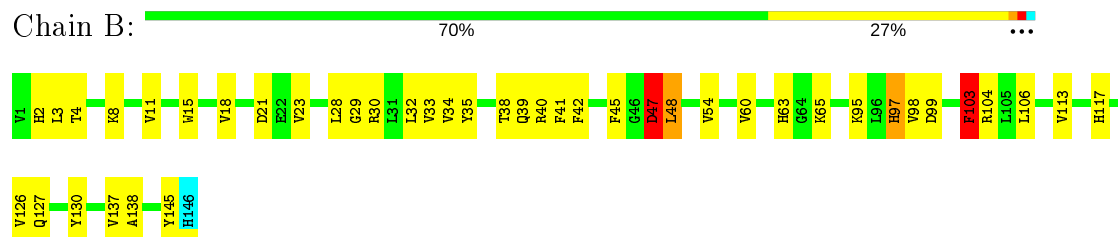
- Molecule 1: Hemoglobin subunit alpha



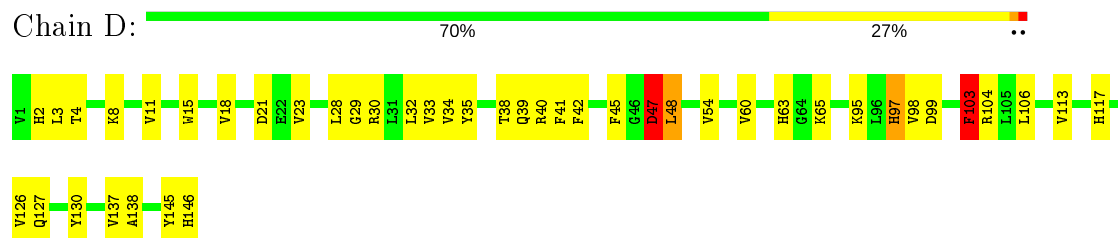
- Molecule 1: Hemoglobin subunit alpha



- Molecule 2: Hemoglobin subunit beta

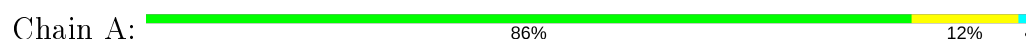


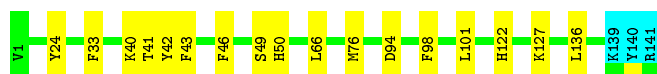
- Molecule 2: Hemoglobin subunit beta



#### 4.2.7 Score per residue for model 7

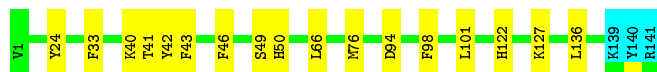
- Molecule 1: Hemoglobin subunit alpha





- Molecule 1: Hemoglobin subunit alpha

Chain C: 86% 12% .



- Molecule 2: Hemoglobin subunit beta

Chain B: 89% 9% ..



- Molecule 2: Hemoglobin subunit beta

Chain D: 90% 10% .



#### 4.2.8 Score per residue for model 8

- Molecule 1: Hemoglobin subunit alpha

Chain A: 82% 14% ..



- Molecule 1: Hemoglobin subunit alpha

Chain C: 82% 13% ..

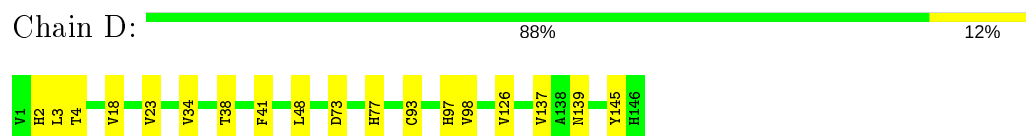


- Molecule 2: Hemoglobin subunit beta

Chain B: 87% 12% .

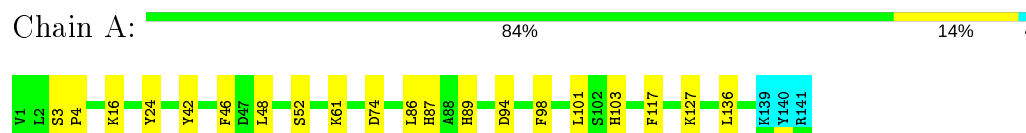


- Molecule 2: Hemoglobin subunit beta

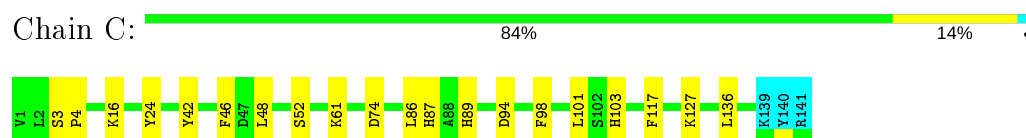


#### 4.2.9 Score per residue for model 9

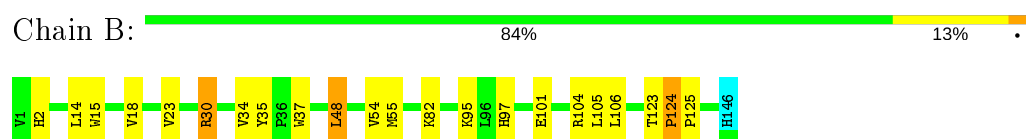
- Molecule 1: Hemoglobin subunit alpha



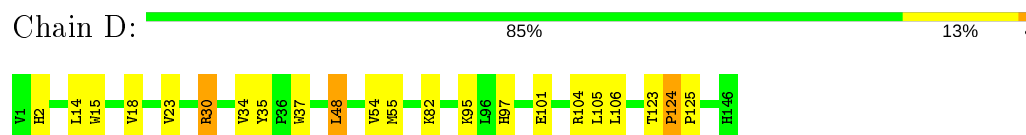
- Molecule 1: Hemoglobin subunit alpha



- Molecule 2: Hemoglobin subunit beta

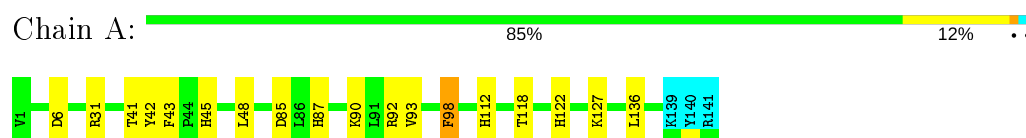


- Molecule 2: Hemoglobin subunit beta

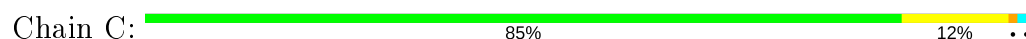


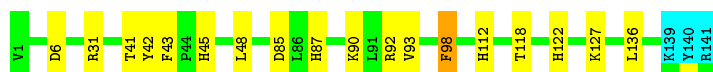
#### 4.2.10 Score per residue for model 10

- Molecule 1: Hemoglobin subunit alpha



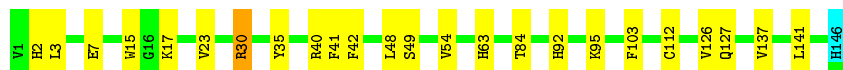
- Molecule 1: Hemoglobin subunit alpha





- Molecule 2: Hemoglobin subunit beta

Chain B: 83% 16% ..



- Molecule 2: Hemoglobin subunit beta

Chain D: 84% 15% .



#### 4.2.11 Score per residue for model 11

- Molecule 1: Hemoglobin subunit alpha

Chain A: 83% 13% ..



- Molecule 1: Hemoglobin subunit alpha

Chain C: 83% 13% ..



- Molecule 2: Hemoglobin subunit beta

Chain B: 83% 15% ..



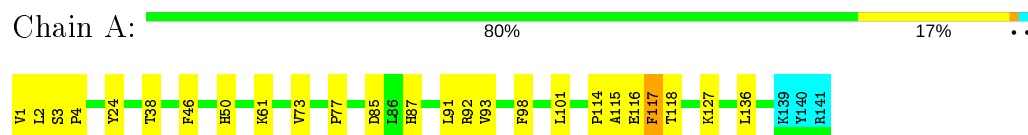
- Molecule 2: Hemoglobin subunit beta

Chain D: 83% 15% .

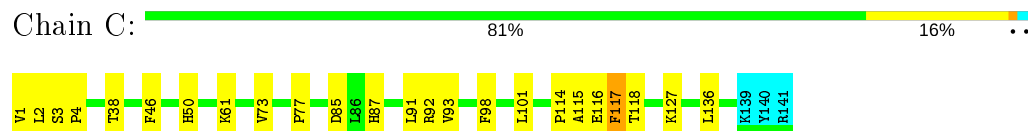


### 4.2.12 Score per residue for model 12

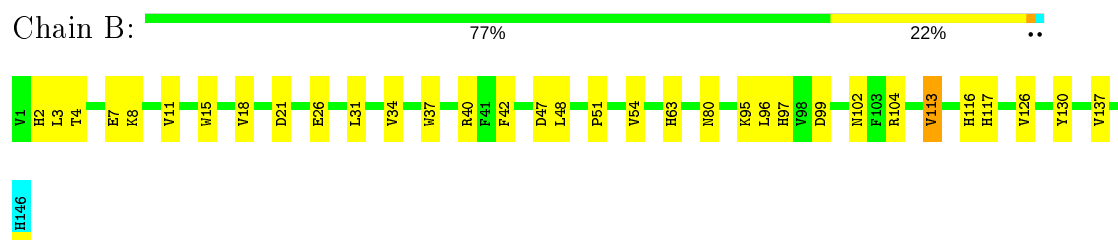
- Molecule 1: Hemoglobin subunit alpha



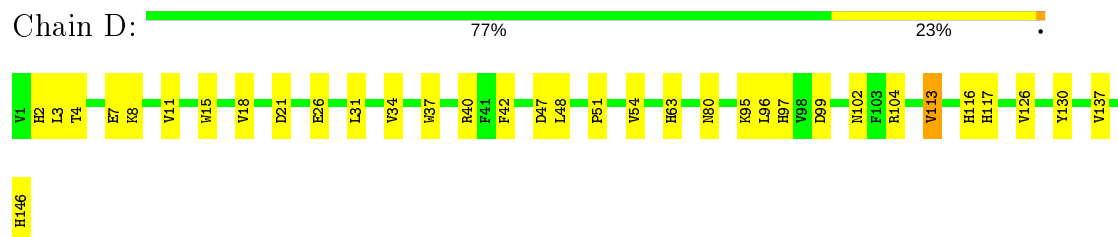
- Molecule 1: Hemoglobin subunit alpha



- Molecule 2: Hemoglobin subunit beta

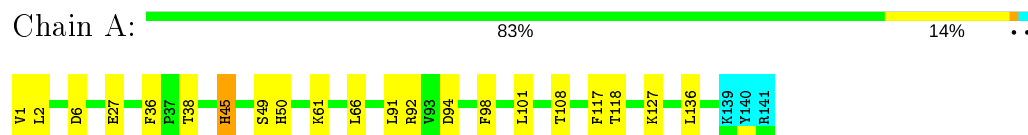


- Molecule 2: Hemoglobin subunit beta

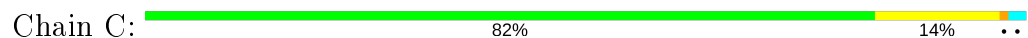


### 4.2.13 Score per residue for model 13

- Molecule 1: Hemoglobin subunit alpha



- Molecule 1: Hemoglobin subunit alpha





- Molecule 2: Hemoglobin subunit beta

Chain B: 82% 16% ...



- Molecule 2: Hemoglobin subunit beta

Chain D: 82% 16% ..



#### 4.2.14 Score per residue for model 14

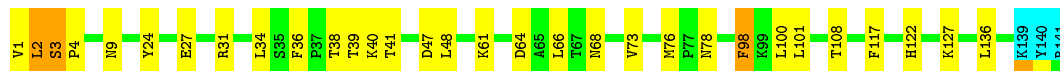
- Molecule 1: Hemoglobin subunit alpha

Chain A: 76% 20% ..



- Molecule 1: Hemoglobin subunit alpha

Chain C: 76% 20% ..



- Molecule 2: Hemoglobin subunit beta

Chain B: 77% 18% ..



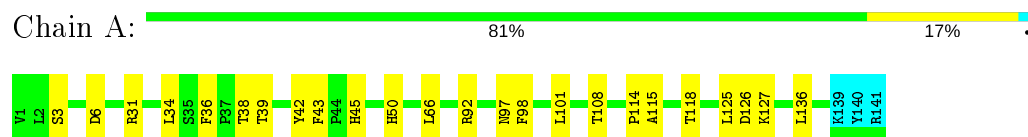
- Molecule 2: Hemoglobin subunit beta

Chain D: 78% 18% ..

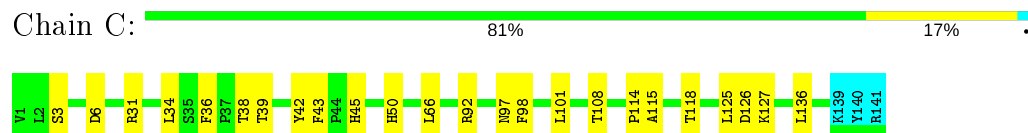


### 4.2.15 Score per residue for model 15

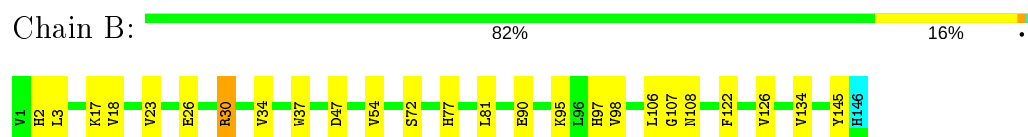
- Molecule 1: Hemoglobin subunit alpha



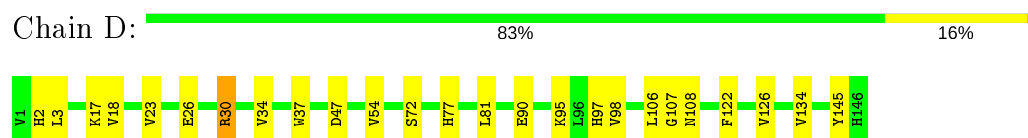
- Molecule 1: Hemoglobin subunit alpha



- Molecule 2: Hemoglobin subunit beta

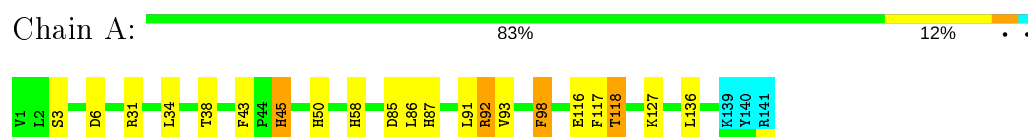


- Molecule 2: Hemoglobin subunit beta

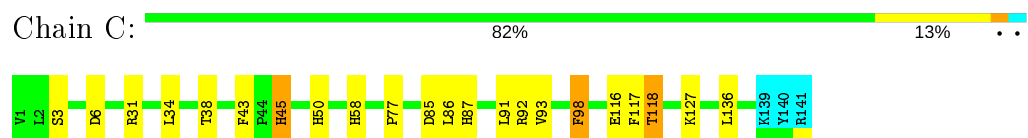


### 4.2.16 Score per residue for model 16

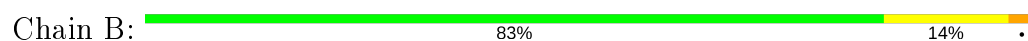
- Molecule 1: Hemoglobin subunit alpha



- Molecule 1: Hemoglobin subunit alpha



- Molecule 2: Hemoglobin subunit beta

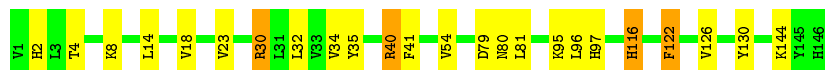






- Molecule 2: Hemoglobin subunit beta

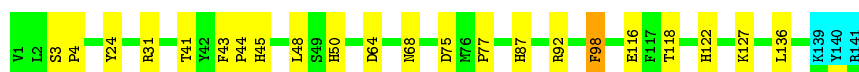
Chain D: 84% 14%



#### 4.2.17 Score per residue for model 17 (medoid)

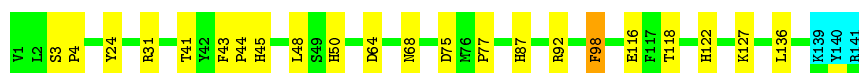
- Molecule 1: Hemoglobin subunit alpha

Chain A: 82% 15%



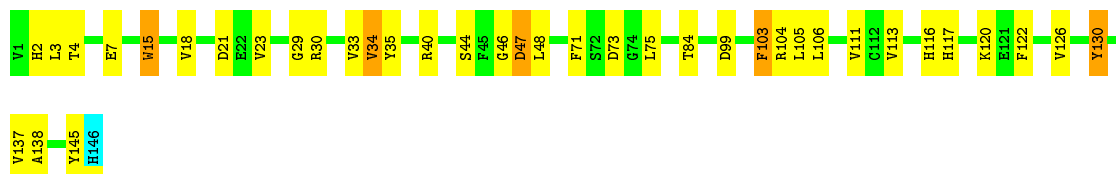
- Molecule 1: Hemoglobin subunit alpha

Chain C: 82% 15%



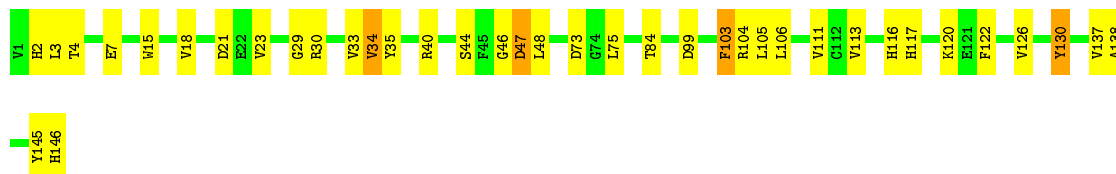
- Molecule 2: Hemoglobin subunit beta

Chain B: 73% 23%



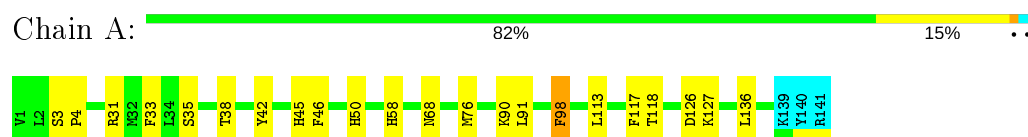
- Molecule 2: Hemoglobin subunit beta

Chain D: 74% 23%

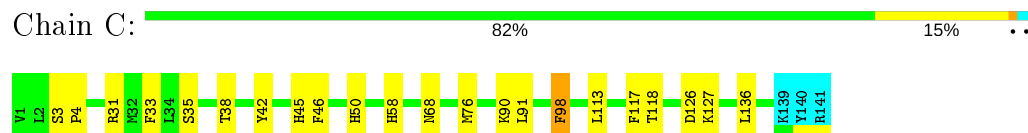


### 4.2.18 Score per residue for model 18

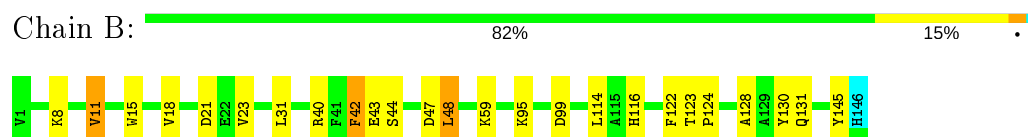
- Molecule 1: Hemoglobin subunit alpha



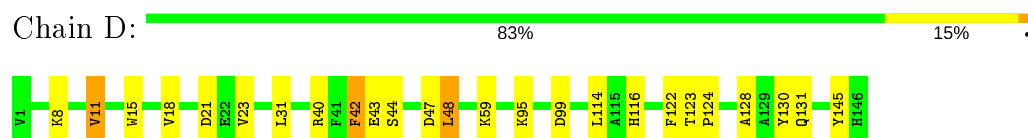
- Molecule 1: Hemoglobin subunit alpha



- Molecule 2: Hemoglobin subunit beta

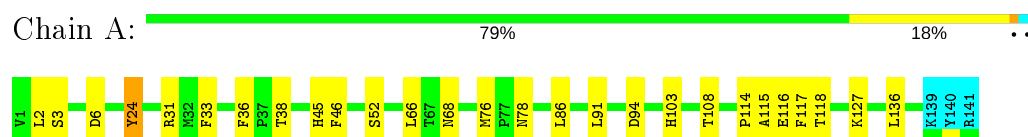


- Molecule 2: Hemoglobin subunit beta

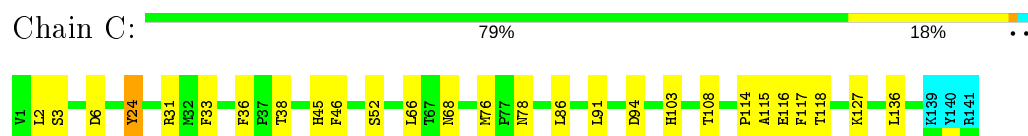


### 4.2.19 Score per residue for model 19

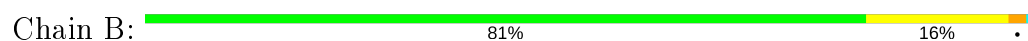
- Molecule 1: Hemoglobin subunit alpha

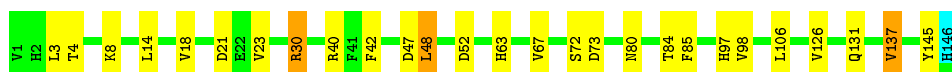


- Molecule 1: Hemoglobin subunit alpha



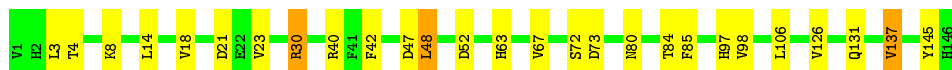
- Molecule 2: Hemoglobin subunit beta





- Molecule 2: Hemoglobin subunit beta

Chain D: 82% 16%



#### 4.2.20 Score per residue for model 20

- Molecule 1: Hemoglobin subunit alpha

Chain A: 87% 11%



- Molecule 1: Hemoglobin subunit alpha

Chain C: 87% 11%



- Molecule 2: Hemoglobin subunit beta

Chain B: 84% 14%



- Molecule 2: Hemoglobin subunit beta

Chain D: 84% 14%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR NIH	structure solution	2.30
X-PLOR NIH	refinement	2.30

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	2761
Number of shifts mapped to atoms	2761
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	37%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) 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	0.67±0.01	0±0/1064 ( 0.0± 0.0%)	0.99±0.02	1±1/1451 ( 0.1± 0.1%)
1	C	0.68±0.01	0±0/1064 ( 0.0± 0.0%)	0.99±0.02	1±1/1451 ( 0.1± 0.1%)
2	B	0.72±0.01	0±0/1142 ( 0.0± 0.0%)	1.06±0.02	1±1/1554 ( 0.1± 0.1%)
2	D	0.72±0.01	0±0/1153 ( 0.0± 0.0%)	1.05±0.02	1±1/1566 ( 0.1± 0.1%)
All	All	0.70	0/88460 ( 0.0%)	1.02	93/120440 ( 0.1%)

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	Planarity
1	A	0.0±0.0	0.5±0.5
1	C	0.0±0.0	0.5±0.5
2	B	0.0±0.0	0.8±0.7
2	D	0.0±0.0	0.8±0.7
All	All	0	50

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	D	30	ARG	NE-CZ-NH1	8.19	124.39	120.30	10	7
2	B	30	ARG	NE-CZ-NH1	7.87	124.24	120.30	10	7
2	D	145	TYR	CB-CG-CD2	-7.07	116.76	121.00	11	3
1	A	31	ARG	NE-CZ-NH1	7.06	123.83	120.30	20	6
2	B	145	TYR	CB-CG-CD2	-6.92	116.85	121.00	11	3
1	A	92	ARG	NE-CZ-NH1	6.91	123.76	120.30	1	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	31	ARG	NE-CZ-NH1	6.82	123.71	120.30	20	6
1	C	92	ARG	NE-CZ-NH1	6.72	123.66	120.30	1	4
2	B	40	ARG	NE-CZ-NH1	6.38	123.49	120.30	2	4
2	D	40	ARG	NE-CZ-NH1	6.26	123.43	120.30	2	3
2	B	97	HIS	CA-CB-CG	5.91	123.65	113.60	13	1
2	D	97	HIS	CA-CB-CG	5.91	123.65	113.60	13	1
1	A	31	ARG	NE-CZ-NH2	5.88	123.24	120.30	19	2
2	B	98	VAL	CA-CB-CG1	5.77	119.56	110.90	2	1
1	C	24	TYR	CB-CG-CD2	-5.77	117.54	121.00	17	11
2	D	98	VAL	CA-CB-CG1	5.77	119.55	110.90	2	1
2	B	103	PHE	CB-CG-CD1	5.75	124.82	120.80	3	1
1	A	24	TYR	CB-CG-CD2	-5.64	117.61	121.00	17	11
2	D	103	PHE	CB-CG-CD1	5.61	124.72	120.80	3	1
1	C	31	ARG	NE-CZ-NH2	5.59	123.09	120.30	19	2
2	D	30	ARG	CD-NE-CZ	5.33	131.07	123.60	7	1
1	A	118	THR	CA-CB-CG2	5.24	119.73	112.40	16	2
2	B	104	ARG	NE-CZ-NH1	5.24	122.92	120.30	4	1
1	C	118	THR	CA-CB-CG2	5.20	119.68	112.40	16	2
2	B	30	ARG	CD-NE-CZ	5.17	130.84	123.60	7	1
2	B	30	ARG	NE-CZ-NH2	-5.15	117.72	120.30	6	1
2	B	42	PHE	C-N-CA	5.15	134.59	121.70	18	1
2	D	42	PHE	C-N-CA	5.14	134.55	121.70	18	1
2	B	34	VAL	CG1-CB-CG2	-5.08	102.77	110.90	4	1
2	D	30	ARG	NE-CZ-NH2	-5.05	117.78	120.30	6	1
2	D	34	VAL	CG1-CB-CG2	-5.01	102.88	110.90	4	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	D	30	ARG	Sidechain	8
2	B	30	ARG	Sidechain	8
1	A	42	TYR	Sidechain	4
1	C	42	TYR	Sidechain	4
2	D	130	TYR	Sidechain	2
2	B	130	TYR	Sidechain	2
1	C	24	TYR	Sidechain	1
1	C	31	ARG	Sidechain	1
2	D	92	HIS	Sidechain	1
2	B	40	ARG	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
2	B	103	PHE	Sidechain	1
1	C	117	PHE	Sidechain	1
2	B	49	SER	Peptide	1
1	A	117	PHE	Sidechain	1
1	A	24	TYR	Sidechain	1
2	D	104	ARG	Sidechain	1
2	D	40	ARG	Sidechain	1
2	D	103	PHE	Sidechain	1
1	C	98	PHE	Sidechain	1
1	A	31	ARG	Sidechain	1
1	A	137	THR	Peptide	1
2	D	49	SER	Peptide	1
1	C	137	THR	Peptide	1
2	B	104	ARG	Sidechain	1
1	A	98	PHE	Sidechain	1
2	B	92	HIS	Sidechain	1
2	B	97	HIS	Sidechain	1
2	D	97	HIS	Sidechain	1

## 6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1036	1038	1038	2±2
1	C	1036	1038	1038	2±2
2	B	1112	1111	1111	3±2
2	D	1123	1118	1118	3±2
3	A	43	30	32	0±1
3	B	43	30	32	0±1
3	C	43	30	32	0±1
3	D	43	30	32	0±1
All	All	89580	88500	88660	176

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 1.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:103:PHE:CE1	2:D:138:ALA:HB1	0.61	2.31	6	2
2:B:103:PHE:CE1	2:B:138:ALA:HB1	0.61	2.31	6	2
2:B:11:VAL:HG23	2:B:130:TYR:CE1	0.59	2.32	12	3
2:D:29:GLY:O	2:D:33:VAL:HG13	0.58	1.98	17	3
2:D:11:VAL:HG23	2:D:130:TYR:CE1	0.58	2.32	12	3
2:B:29:GLY:O	2:B:33:VAL:HG13	0.58	1.98	17	3
2:D:97:HIS:H	2:D:97:HIS:CD2	0.55	2.20	4	1
2:D:57:ASN:HD22	2:D:60:VAL:HG23	0.53	1.63	5	1
2:B:57:ASN:HD22	2:B:60:VAL:HG23	0.53	1.63	5	1
2:B:97:HIS:H	2:B:97:HIS:CD2	0.53	2.20	4	1
2:B:45:PHE:HB2	2:B:48:LEU:HD11	0.53	1.80	6	1
2:D:102:ASN:HD22	3:D:201:HEC:HMC1	0.52	1.64	12	1
2:D:45:PHE:HB2	2:D:48:LEU:HD11	0.52	1.80	6	1
2:B:102:ASN:HD22	3:B:201:HEC:HMC1	0.51	1.65	12	1
1:C:2:LEU:HD13	1:C:73:VAL:HG22	0.51	1.82	4	2
2:B:93:CYS:SG	1:C:41:THR:HG21	0.51	2.46	2	2
1:C:38:THR:O	1:C:41:THR:HG22	0.50	2.05	8	2
3:B:201:HEC:HHD	3:B:201:HEC:HBC3	0.50	1.82	4	1
1:A:38:THR:O	1:A:41:THR:HG22	0.50	2.06	8	2
2:B:111:VAL:HG12	2:B:130:TYR:HB3	0.50	1.84	17	2
1:A:41:THR:HG21	2:D:93:CYS:SG	0.50	2.46	2	2
1:A:2:LEU:HD13	1:A:73:VAL:HG22	0.49	1.82	4	2
3:D:201:HEC:HBC3	3:D:201:HEC:HHD	0.49	1.83	4	1
1:C:98:PHE:C	1:C:98:PHE:CD1	0.49	2.87	14	9
3:B:201:HEC:HBD1	3:B:201:HEC:HMD1	0.49	1.85	10	1
1:A:98:PHE:C	1:A:98:PHE:CD1	0.48	2.87	14	4
2:B:32:LEU:HD21	2:B:45:PHE:CE2	0.48	2.44	13	2
2:D:32:LEU:HD21	2:D:45:PHE:CE2	0.48	2.44	13	2
2:B:32:LEU:HD13	2:B:48:LEU:HD12	0.48	1.85	3	1
1:C:42:TYR:CE2	1:C:93:VAL:HG22	0.48	2.44	2	1
2:D:111:VAL:HG12	2:D:130:TYR:HB3	0.48	1.84	17	2
2:B:42:PHE:CG	2:B:43:GLU:N	0.47	2.82	14	1
2:D:32:LEU:HD13	2:D:48:LEU:HD12	0.47	1.85	3	1
1:A:42:TYR:CE2	1:A:93:VAL:HG22	0.47	2.44	2	1
3:D:201:HEC:HMD1	3:D:201:HEC:HBD1	0.47	1.85	10	1
2:D:42:PHE:CG	2:D:43:GLU:N	0.47	2.82	14	1
1:A:35:SER:HA	2:B:128:ALA:HB2	0.47	1.87	18	1
1:C:117:PHE:CE2	2:D:113:VAL:HG12	0.46	2.45	12	1
2:B:113:VAL:HA	2:B:116:HIS:CD2	0.46	2.45	7	1
1:A:98:PHE:CD1	1:A:98:PHE:C	0.46	2.89	3	6
2:D:113:VAL:HA	2:D:116:HIS:CD2	0.46	2.45	7	1
1:C:117:PHE:CE2	2:D:116:HIS:CG	0.46	3.04	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:HIS:CD2	2:B:30:ARG:HH21	0.46	2.29	10	1
1:C:35:SER:HA	2:D:128:ALA:HB2	0.46	1.87	18	1
2:B:47:ASP:C	2:B:48:LEU:HD12	0.46	2.31	6	1
2:B:103:PHE:CD1	2:B:138:ALA:HB1	0.46	2.46	4	2
2:D:28:LEU:HD21	2:D:63:HIS:CD2	0.46	2.46	14	1
1:C:122:HIS:CD2	2:D:30:ARG:HH21	0.46	2.29	10	1
2:B:102:ASN:ND2	3:B:201:HEC:HBC2	0.46	2.26	3	1
2:D:103:PHE:CD1	2:D:138:ALA:HB1	0.45	2.46	4	2
2:D:15:TRP:CZ2	2:D:72:SER:HB3	0.45	2.47	14	1
1:A:117:PHE:CE2	2:B:113:VAL:HG12	0.45	2.45	12	1
1:A:117:PHE:CE2	2:B:116:HIS:CG	0.45	3.04	16	1
2:D:47:ASP:C	2:D:48:LEU:HD12	0.45	2.31	6	1
1:C:101:LEU:HD21	3:C:201:HEC:HBB3	0.45	1.88	1	1
1:A:101:LEU:HD23	3:A:201:HEC:HMC3	0.45	1.88	8	1
3:C:201:HEC:HBB2	3:C:201:HEC:HMB1	0.45	1.88	2	1
2:D:102:ASN:ND2	3:D:201:HEC:HBC2	0.45	2.26	3	1
1:A:101:LEU:HD21	3:A:201:HEC:HBB3	0.45	1.88	1	1
2:B:28:LEU:HD21	2:B:63:HIS:CD2	0.45	2.46	14	1
2:B:15:TRP:CZ2	2:B:72:SER:HB3	0.44	2.47	14	1
2:B:103:PHE:CZ	2:B:138:ALA:HB1	0.44	2.47	6	1
3:A:201:HEC:HBB2	3:A:201:HEC:HMB1	0.44	1.88	2	1
2:B:71:PHE:CE2	2:B:130:TYR:CE1	0.44	3.06	1	1
1:C:97:ASN:HB3	3:C:201:HEC:HMC1	0.44	1.89	8	2
2:B:30:ARG:CD	2:B:113:VAL:HG22	0.44	2.43	20	1
2:D:71:PHE:CE2	2:D:130:TYR:CE1	0.44	3.06	1	1
2:D:57:ASN:ND2	2:D:60:VAL:HG23	0.44	2.28	5	1
2:B:103:PHE:CE1	2:B:138:ALA:CB	0.44	3.01	6	1
2:D:103:PHE:CE1	2:D:138:ALA:CB	0.44	3.01	6	1
2:D:114:LEU:CD2	2:D:130:TYR:CZ	0.44	3.01	2	1
1:C:101:LEU:HD23	3:C:201:HEC:HMC3	0.44	1.88	8	1
2:D:27:ALA:HA	2:D:113:VAL:HG11	0.43	1.89	3	1
2:B:27:ALA:HA	2:B:113:VAL:HG11	0.43	1.89	3	1
1:A:97:ASN:HB3	3:A:201:HEC:HMC1	0.43	1.89	8	1
2:B:103:PHE:CD1	2:B:138:ALA:CB	0.43	3.01	4	1
1:C:32:MET:HG2	1:C:39:THR:HG21	0.43	1.90	4	1
2:B:98:VAL:CG1	3:B:201:HEC:HBC2	0.43	2.44	1	1
1:C:122:HIS:CE1	2:D:34:VAL:HG22	0.43	2.49	17	1
2:D:124:PRO:CB	2:D:125:PRO:HD3	0.43	2.44	9	1
2:B:114:LEU:CD2	2:B:130:TYR:CZ	0.43	3.01	2	1
2:D:30:ARG:CD	2:D:113:VAL:HG22	0.43	2.44	20	1
2:B:124:PRO:CB	2:B:125:PRO:HD3	0.43	2.44	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:98:VAL:CG1	3:D:201:HEC:HBC2	0.43	2.43	1	1
1:A:122:HIS:CE1	2:B:34:VAL:HG22	0.43	2.49	17	1
2:B:32:LEU:HD22	2:B:32:LEU:H	0.43	1.74	4	1
2:D:103:PHE:CD1	2:D:138:ALA:CB	0.43	3.01	4	1
2:D:103:PHE:CZ	2:D:138:ALA:HB1	0.43	2.47	6	1
2:B:57:ASN:ND2	2:B:60:VAL:HG23	0.42	2.28	5	1
1:C:42:TYR:CE1	1:C:93:VAL:HA	0.42	2.49	4	1
2:D:11:VAL:HG23	2:D:130:TYR:CE2	0.42	2.49	1	1
2:D:71:PHE:CE2	2:D:110:LEU:HD23	0.42	2.49	20	1
2:D:85:PHE:CE2	2:D:137:VAL:HG23	0.42	2.50	19	1
2:B:71:PHE:CE2	2:B:110:LEU:HD23	0.42	2.49	20	1
2:D:32:LEU:HD22	2:D:32:LEU:H	0.42	1.74	4	1
3:B:201:HEC:HMD1	3:B:201:HEC:CBD	0.42	2.44	10	1
3:D:201:HEC:HMD1	3:D:201:HEC:CBD	0.42	2.44	10	1
1:C:98:PHE:CD1	1:C:98:PHE:C	0.42	2.93	16	2
1:C:77:PRO:HA	1:C:135:VAL:HG13	0.42	1.92	5	1
2:B:11:VAL:HG23	2:B:130:TYR:CE2	0.42	2.49	1	1
2:D:103:PHE:CD1	2:D:104:ARG:N	0.42	2.88	4	3
2:B:85:PHE:CE2	2:B:137:VAL:HG23	0.42	2.50	19	1
2:D:107:GLY:CA	2:D:134:VAL:HG11	0.42	2.45	15	1
1:A:42:TYR:CE1	1:A:93:VAL:HA	0.41	2.49	4	1
1:A:2:LEU:HD13	1:A:73:VAL:CG2	0.41	2.46	12	1
1:A:32:MET:HG2	1:A:39:THR:HG21	0.41	1.91	4	1
2:B:103:PHE:CD1	2:B:104:ARG:N	0.41	2.88	4	3
2:B:11:VAL:HG23	2:B:130:TYR:CZ	0.41	2.50	4	1
1:C:98:PHE:CD1	1:C:133:SER:CB	0.41	3.03	3	1
2:B:107:GLY:CA	2:B:134:VAL:HG11	0.41	2.45	15	1
2:B:122:PHE:CG	2:B:122:PHE:O	0.41	2.73	4	1
3:A:201:HEC:HMC1	3:A:201:HEC:HBC2	0.41	1.92	12	1
1:A:98:PHE:CD1	1:A:133:SER:CB	0.41	3.03	3	1
1:C:110:ALA:CB	2:D:116:HIS:CE1	0.41	3.04	11	1
2:B:48:LEU:C	2:B:48:LEU:HD23	0.41	2.36	3	1
1:A:36:PHE:CE2	1:A:100:LEU:HD22	0.41	2.51	14	1
1:C:36:PHE:CE2	1:C:100:LEU:HD22	0.41	2.51	14	1
1:C:32:MET:CE	3:C:201:HEC:HBC2	0.41	2.46	8	1
2:D:48:LEU:C	2:D:48:LEU:HD23	0.41	2.36	3	1
1:A:77:PRO:HA	1:A:135:VAL:HG13	0.40	1.92	5	1
2:B:103:PHE:CD1	2:B:103:PHE:C	0.40	2.95	6	1
2:D:11:VAL:HG23	2:D:130:TYR:CZ	0.40	2.51	4	1
1:A:36:PHE:O	1:A:39:THR:HG22	0.40	2.17	4	1
1:A:32:MET:CE	3:A:201:HEC:HBC2	0.40	2.46	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:114:LEU:CD1	2:D:130:TYR:CE2	0.40	3.04	11	1
1:C:36:PHE:O	1:C:39:THR:HG22	0.40	2.16	4	1
2:B:98:VAL:HG11	3:B:201:HEC:HBC2	0.40	1.94	1	1
2:D:103:PHE:CD1	2:D:103:PHE:C	0.40	2.94	6	1
1:C:21:ALA:HB1	1:C:63:ALA:HB1	0.40	1.93	4	1
2:B:15:TRP:CZ2	2:B:71:PHE:CD1	0.40	3.10	17	1
1:C:2:LEU:HD13	1:C:73:VAL:CG2	0.40	2.46	12	1
1:A:110:ALA:CB	2:B:116:HIS:CE1	0.40	3.04	11	1

## 6.3 Torsion angles

### 6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	137/141 (97%)	121±2 (88±2%)	12±2 (9±2%)	4±1 (3±1%)	8	42
1	C	137/141 (97%)	121±2 (88±2%)	12±2 (9±2%)	4±1 (3±1%)	7	41
2	B	144/146 (99%)	130±2 (90±2%)	11±3 (7±2%)	4±1 (2±1%)	9	45
2	D	144/146 (99%)	130±2 (90±2%)	10±3 (7±2%)	4±1 (2±1%)	9	45
All	All	11240/11480 (98%)	10038 (89%)	902 (8%)	300 (3%)	8	43

All 71 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	2	HIS	15
2	D	2	HIS	15
1	C	50	HIS	11
2	B	47	ASP	11
2	B	48	LEU	11
2	D	97	HIS	11
2	B	97	HIS	11
2	D	47	ASP	11
1	A	50	HIS	11
2	D	48	LEU	11

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Mol	Chain	Res	Type	Models (Total)
1	C	114	PRO	7
1	A	4	PRO	7
1	A	114	PRO	7
1	A	93	VAL	7
1	C	93	VAL	7
1	C	4	PRO	7
2	B	122	PHE	6
2	D	122	PHE	6
1	A	115	ALA	6
1	C	115	ALA	6
1	C	49	SER	5
1	A	49	SER	5
2	D	98	VAL	4
1	C	76	MET	4
2	B	98	VAL	4
1	A	76	MET	4
1	C	92	ARG	4
1	C	3	SER	4
1	A	45	HIS	4
1	A	3	SER	4
1	C	45	HIS	4
1	A	92	ARG	4
1	C	77	PRO	3
2	D	81	LEU	3
1	C	117	PHE	3
2	B	81	LEU	3
1	C	91	LEU	3
1	A	91	LEU	3
1	A	117	PHE	3
1	C	43	PHE	2
1	A	77	PRO	2
2	B	43	GLU	2
1	A	48	LEU	2
1	C	116	GLU	2
1	A	43	PHE	2
1	A	116	GLU	2
1	C	44	PRO	2
1	C	48	LEU	2
1	A	44	PRO	2
2	D	124	PRO	2
2	D	43	GLU	2
2	B	124	PRO	2

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Mol	Chain	Res	Type	Models (Total)
1	C	95	PRO	1
2	B	33	VAL	1
2	B	99	ASP	1
2	D	99	ASP	1
2	D	44	SER	1
2	B	120	LYS	1
1	A	95	PRO	1
2	D	46	GLY	1
1	C	2	LEU	1
2	B	44	SER	1
2	B	42	PHE	1
2	D	33	VAL	1
2	D	42	PHE	1
2	D	120	LYS	1
1	C	19	ALA	1
1	A	2	LEU	1
2	B	46	GLY	1
2	B	34	VAL	1
2	D	34	VAL	1

### 6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	110/113 (97%)	93±3 (85±3%)	17±3 (15±3%)	6	44
1	C	110/113 (97%)	94±3 (85±3%)	17±3 (15±3%)	6	44
2	B	117/118 (99%)	96±6 (82±5%)	22±6 (18±5%)	4	37
2	D	118/118 (100%)	96±6 (82±5%)	22±6 (18±5%)	4	37
All	All	9100/9240 (98%)	7571 (83%)	1529 (17%)	5	40

All 302 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	136	LEU	20
1	C	127	LYS	20

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Mol	Chain	Res	Type	Models (Total)
1	A	127	LYS	20
1	C	136	LEU	20
2	B	18	VAL	19
2	D	18	VAL	19
2	D	23	VAL	18
2	B	23	VAL	18
1	A	98	PHE	17
1	C	98	PHE	17
1	C	118	THR	14
2	B	126	VAL	14
2	D	3	LEU	14
2	B	3	LEU	14
1	A	118	THR	14
2	D	126	VAL	13
1	C	101	LEU	13
1	A	101	LEU	13
2	B	137	VAL	13
2	D	137	VAL	13
2	B	34	VAL	12
2	B	4	THR	12
1	A	66	LEU	12
2	D	4	THR	12
2	D	34	VAL	12
2	D	95	LYS	11
2	B	95	LYS	11
2	D	42	PHE	11
1	C	3	SER	11
2	B	42	PHE	11
1	A	3	SER	11
2	B	54	VAL	10
1	C	38	THR	10
2	D	15	TRP	10
2	D	54	VAL	10
1	A	38	THR	10
2	B	15	TRP	10
1	C	66	LEU	10
2	B	41	PHE	9
1	C	6	ASP	9
2	B	63	HIS	9
1	A	41	THR	9
2	D	63	HIS	9
2	B	97	HIS	9

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Mol	Chain	Res	Type	Models (Total)
1	C	41	THR	9
2	D	146	HIS	9
1	A	6	ASP	9
2	D	41	PHE	9
1	C	42	TYR	8
2	B	122	PHE	8
2	D	122	PHE	8
1	C	46	PHE	8
2	B	8	LYS	8
1	A	42	TYR	8
2	D	145	TYR	8
1	A	46	PHE	8
2	D	8	LYS	8
2	B	145	TYR	8
1	A	68	ASN	8
2	B	48	LEU	8
2	D	97	HIS	8
2	B	30	ARG	8
1	C	68	ASN	8
2	D	48	LEU	8
2	D	106	LEU	8
1	A	45	HIS	8
2	D	30	ARG	8
2	B	106	LEU	8
1	C	45	HIS	8
2	B	40	ARG	7
1	A	87	HIS	7
2	B	35	TYR	7
1	C	87	HIS	7
2	B	37	TRP	7
2	D	37	TRP	7
2	D	40	ARG	7
1	A	61	LYS	7
2	D	84	THR	7
2	B	14	LEU	7
1	C	61	LYS	7
1	A	92	ARG	7
2	B	84	THR	7
1	C	92	ARG	7
2	D	35	TYR	7
2	D	14	LEU	7
2	B	116	HIS	6

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Mol	Chain	Res	Type	Models (Total)
1	C	108	THR	6
1	C	91	LEU	6
2	B	98	VAL	6
2	D	116	HIS	6
2	D	98	VAL	6
1	C	94	ASP	6
1	A	108	THR	6
2	B	99	ASP	6
2	B	38	THR	6
1	A	116	GLU	6
2	D	38	THR	6
1	A	91	LEU	6
1	A	94	ASP	6
2	D	99	ASP	6
1	C	116	GLU	6
2	B	17	LYS	5
2	D	80	ASN	5
2	B	113	VAL	5
1	A	122	HIS	5
1	A	117	PHE	5
2	D	7	GLU	5
1	A	33	PHE	5
1	C	34	LEU	5
2	B	80	ASN	5
2	B	103	PHE	5
1	C	86	LEU	5
2	B	31	LEU	5
1	A	36	PHE	5
2	B	7	GLU	5
1	C	122	HIS	5
1	C	36	PHE	5
1	A	34	LEU	5
2	B	32	LEU	5
2	B	72	SER	5
2	D	32	LEU	5
1	C	117	PHE	5
1	A	27	GLU	5
1	C	27	GLU	5
1	A	86	LEU	5
2	B	21	ASP	5
2	D	113	VAL	5
1	C	33	PHE	5

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Mol	Chain	Res	Type	Models (Total)
2	D	21	ASP	5
2	D	17	LYS	5
1	A	1	VAL	5
2	D	31	LEU	5
1	C	1	VAL	5
2	D	72	SER	5
1	C	40	LYS	4
2	B	33	VAL	4
1	C	78	ASN	4
1	A	47	ASP	4
2	D	104	ARG	4
2	D	55	MET	4
1	A	43	PHE	4
2	D	66	LYS	4
2	B	55	MET	4
2	B	66	LYS	4
1	C	47	ASP	4
2	D	26	GLU	4
1	A	103	HIS	4
2	B	59	LYS	4
2	D	103	PHE	4
1	A	23	GLU	4
1	C	103	HIS	4
2	B	104	ARG	4
2	B	96	LEU	4
1	C	23	GLU	4
1	A	40	LYS	4
2	B	26	GLU	4
2	B	73	ASP	4
2	D	131	GLN	4
2	D	33	VAL	4
2	D	96	LEU	4
1	A	31	ARG	4
2	B	131	GLN	4
1	A	78	ASN	4
1	C	43	PHE	4
2	D	59	LYS	4
2	D	114	LEU	4
1	C	31	ARG	4
2	B	114	LEU	4
2	D	73	ASP	4
1	A	58	HIS	3

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Mol	Chain	Res	Type	Models (Total)
2	D	120	LYS	3
2	B	127	GLN	3
1	C	56	LYS	3
2	D	127	GLN	3
1	C	58	HIS	3
1	C	74	ASP	3
2	B	39	GLN	3
1	C	64	ASP	3
2	B	102	ASN	3
1	C	90	LYS	3
1	A	64	ASP	3
1	A	16	LYS	3
1	A	90	LYS	3
1	C	48	LEU	3
2	D	102	ASN	3
2	D	39	GLN	3
2	D	47	ASP	3
1	A	85	ASP	3
2	D	117	HIS	3
1	A	48	LEU	3
2	B	47	ASP	3
2	B	120	LYS	3
1	C	16	LYS	3
1	A	74	ASP	3
2	B	117	HIS	3
2	D	123	THR	3
2	B	101	GLU	3
1	A	56	LYS	3
2	B	123	THR	3
1	C	85	ASP	3
2	D	101	GLU	3
1	C	50	HIS	2
2	D	1	VAL	2
2	D	81	LEU	2
2	D	139	ASN	2
2	B	109	VAL	2
1	C	126	ASP	2
1	A	76	MET	2
1	A	2	LEU	2
2	D	109	VAL	2
2	B	19	ASN	2
2	D	75	LEU	2

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Mol	Chain	Res	Type	Models (Total)
2	B	82	LYS	2
2	B	90	GLU	2
2	D	90	GLU	2
2	B	77	HIS	2
2	B	105	LEU	2
1	A	39	THR	2
1	C	30	GLU	2
2	B	139	ASN	2
2	D	82	LYS	2
2	B	111	VAL	2
2	B	1	VAL	2
1	A	75	ASP	2
1	A	30	GLU	2
1	C	39	THR	2
2	D	111	VAL	2
1	C	60	LYS	2
2	B	81	LEU	2
2	B	130	TYR	2
2	D	130	TYR	2
1	C	2	LEU	2
1	C	76	MET	2
1	A	60	LYS	2
2	D	19	ASN	2
1	A	126	ASP	2
2	D	105	LEU	2
1	A	50	HIS	2
2	D	77	HIS	2
1	C	52	SER	2
1	C	75	ASP	2
2	B	75	LEU	2
1	A	52	SER	2
2	B	141	LEU	1
1	C	7	LYS	1
1	A	11	LYS	1
2	B	65	LYS	1
1	A	54	GLN	1
1	A	112	HIS	1
2	B	52	ASP	1
2	D	67	VAL	1
2	B	51	PRO	1
2	D	49	SER	1
2	D	144	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	C	125	LEU	1
2	B	61	LYS	1
2	D	51	PRO	1
1	C	89	HIS	1
2	D	28	LEU	1
2	B	108	ASN	1
2	B	44	SER	1
2	D	65	LYS	1
1	A	125	LEU	1
1	A	9	ASN	1
2	B	49	SER	1
2	B	67	VAL	1
2	D	57	ASN	1
2	B	9	SER	1
2	D	94	ASP	1
1	C	54	GLN	1
1	A	113	LEU	1
2	D	9	SER	1
2	B	28	LEU	1
1	A	97	ASN	1
1	C	112	HIS	1
1	A	129	LEU	1
2	D	44	SER	1
1	A	7	LYS	1
2	D	108	ASN	1
2	B	94	ASP	1
1	A	89	HIS	1
2	B	79	ASP	1
1	C	97	ASN	1
2	D	121	GLU	1
2	D	11	VAL	1
1	A	106	LEU	1
2	B	11	VAL	1
2	D	141	LEU	1
1	C	11	LYS	1
1	C	113	LEU	1
2	D	79	ASP	1
2	B	57	ASN	1
2	D	112	CYS	1
1	C	129	LEU	1
2	D	61	LYS	1
2	D	60	VAL	1

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Mol	Chain	Res	Type	Models (Total)
2	D	52	ASP	1
2	B	112	CYS	1
1	C	9	ASN	1
2	B	121	GLU	1
2	B	60	VAL	1
2	B	144	LYS	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	HEC	C	201	-	26,50,50	1.80±0.03	0±0 (0±0%)
3	HEC	B	201	2	26,50,50	1.80±0.02	0±0 (0±0%)
3	HEC	A	201	-	26,50,50	1.80±0.03	0±0 (0±0%)
3	HEC	D	201	2	26,50,50	1.80±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	HEC	C	201	-	18,82,82	1.19±0.08	0±0 (0±0%)
3	HEC	B	201	2	18,82,82	1.32±0.10	0±0 (0±0%)
3	HEC	A	201	-	18,82,82	1.19±0.08	0±0 (0±0%)
3	HEC	D	201	2	18,82,82	1.32±0.10	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	C	201	-	-	0±0,6,54,54	-
3	HEC	D	201	2	-	0±0,6,54,54	-
3	HEC	A	201	-	-	0±0,6,54,54	-
3	HEC	B	201	2	-	0±0,6,54,54	-

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	201	HEC	C3B-C2B	5.42	1.35	1.40	1	1
3	C	201	HEC	C3B-C2B	5.34	1.35	1.40	1	1

There are no bond-angle outliers.

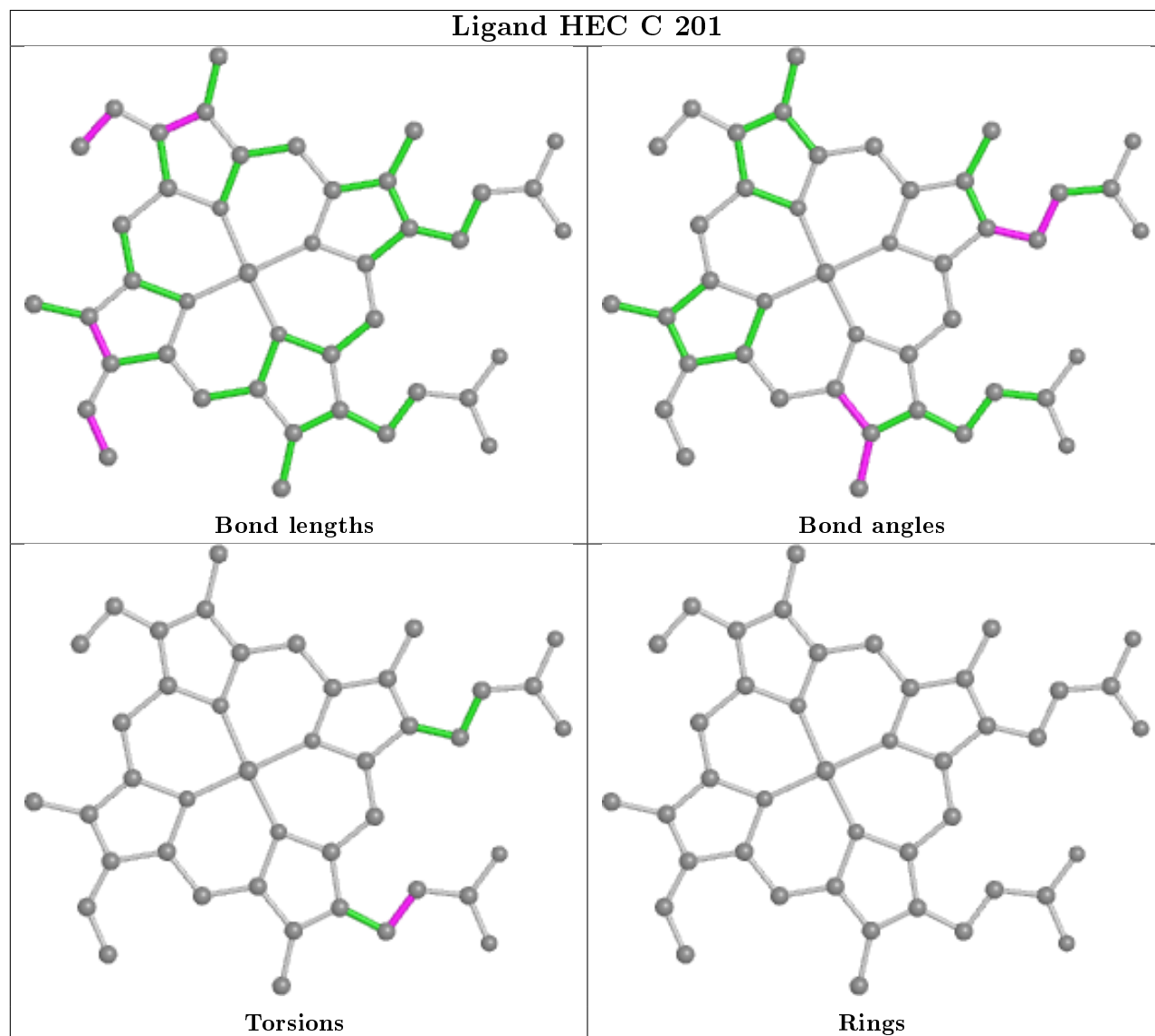
There are no chirality outliers.

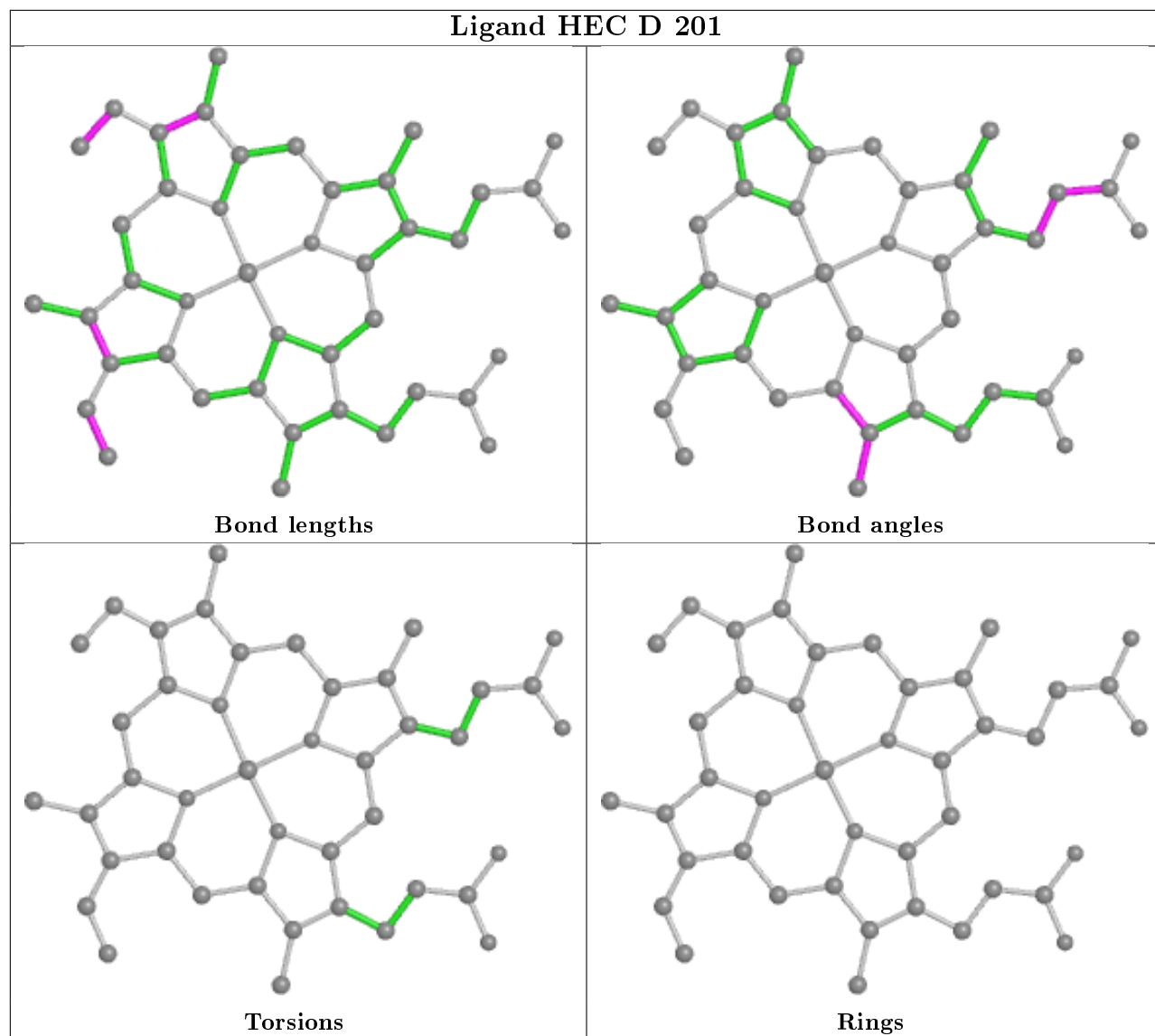
There are no torsion outliers.

There are no ring outliers.

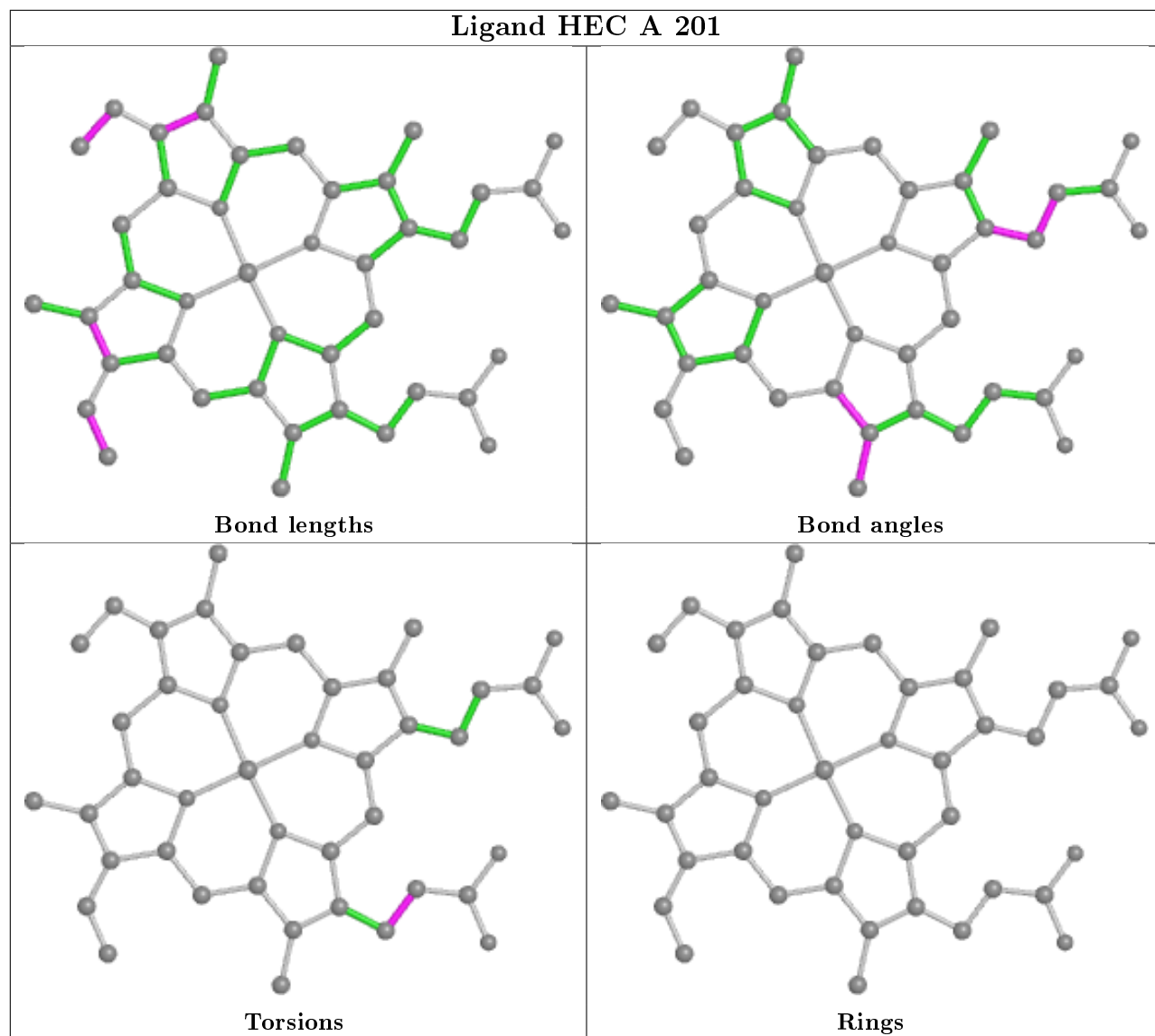
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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

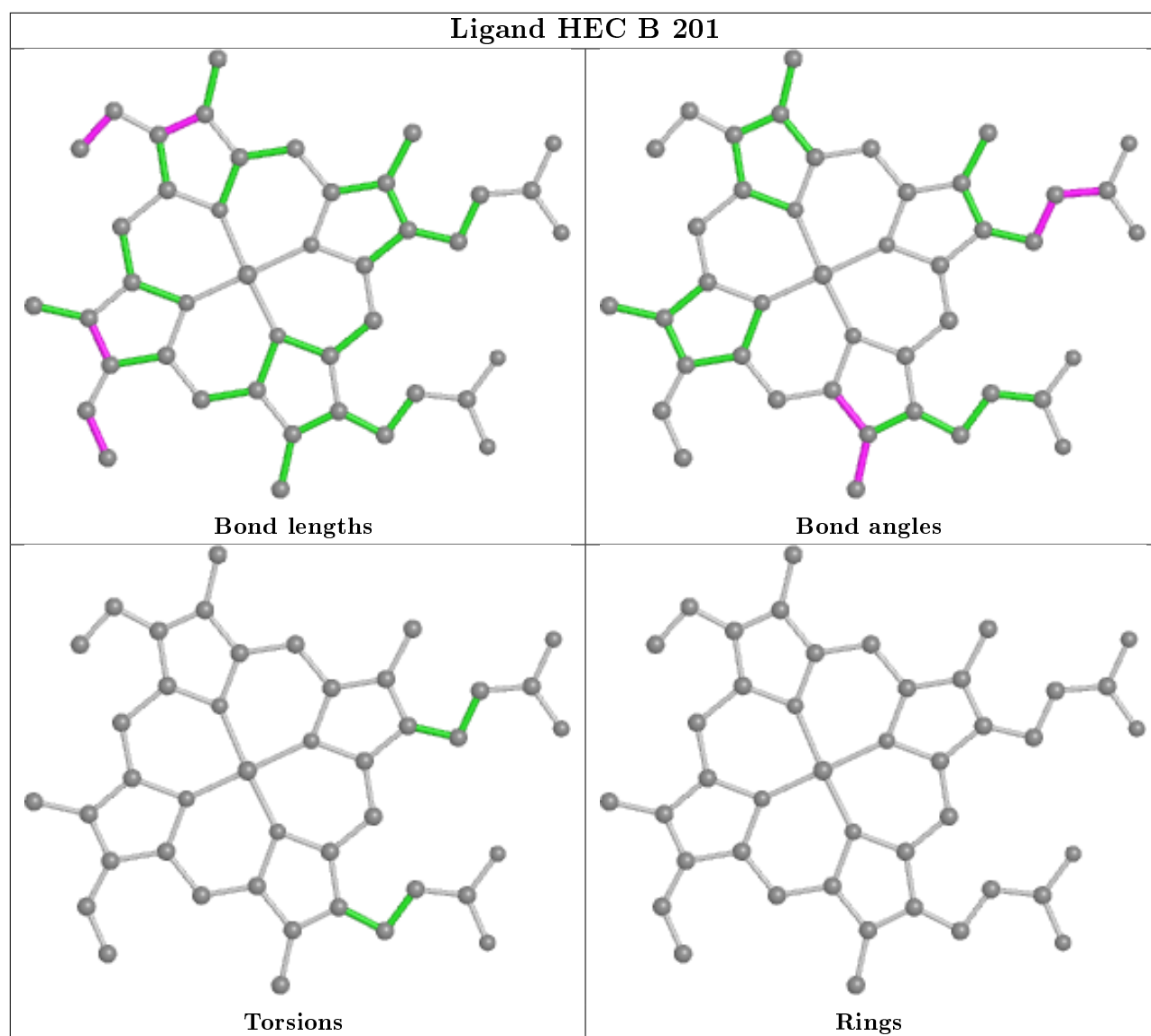
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 37% for the well-defined parts and 37% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2761
Number of shifts mapped to atoms	2761
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	29

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	275	$-0.95 \pm 0.11$	Should be applied
$^{13}\text{C}_\beta$	228	$0.20 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	259	$0.55 \pm 0.29$	None needed (imprecise)

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 37%, i.e. 2492 atoms were assigned a chemical shift out of a possible 6651. 1 out of 134 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	1057/2779 (38%)	527/1106 (48%)	273/1134 (24%)	257/539 (48%)
Sidechain	1226/3189 (38%)	734/1852 (40%)	488/1237 (39%)	4/100 (4%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	209/683 (31%)	106/374 (28%)	96/264 (36%)	7/45 (16%)
Overall	2492/6651 (37%)	1367/3332 (41%)	857/2635 (33%)	268/684 (39%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 37%, i.e. 2516 atoms were assigned a chemical shift out of a possible 6780. 1 out of 134 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	1065/2814 (38%)	531/1120 (47%)	275/1148 (24%)	259/546 (47%)
Sidechain	1238/3260 (38%)	742/1896 (39%)	492/1256 (39%)	4/108 (4%)
Aromatic	213/706 (30%)	108/386 (28%)	98/274 (36%)	7/46 (15%)
Overall	2516/6780 (37%)	1381/3402 (41%)	865/2678 (32%)	270/700 (39%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	92	HIS	HD2	0.89	9.28 – 4.78	-13.6
1	A	87	HIS	HD2	1.00	9.28 – 4.78	-13.4
2	B	92	HIS	HE1	1.41	10.53 – 5.43	-12.9
1	A	87	HIS	HE1	1.44	10.53 – 5.43	-12.8
2	B	67	VAL	HG11	-1.83	2.13 – -0.47	-10.2
2	B	67	VAL	HG13	-1.83	2.13 – -0.47	-10.2
2	B	67	VAL	HG12	-1.83	2.13 – -0.47	-10.2
1	A	62	VAL	HG13	-1.76	2.13 – -0.47	-10.0
1	A	62	VAL	HG12	-1.76	2.13 – -0.47	-10.0
1	A	62	VAL	HG11	-1.76	2.13 – -0.47	-10.0
2	B	141	LEU	HD21	-1.05	2.14 – -0.66	-6.4
2	B	141	LEU	HD23	-1.05	2.14 – -0.66	-6.4
2	B	141	LEU	HD22	-1.05	2.14 – -0.66	-6.4
1	A	29	LEU	HD23	-0.85	2.14 – -0.66	-5.7
1	A	29	LEU	HD22	-0.85	2.14 – -0.66	-5.7
1	A	29	LEU	HD21	-0.85	2.14 – -0.66	-5.7
2	B	141	LEU	HD12	-0.83	2.16 – -0.64	-5.7
2	B	141	LEU	HD11	-0.83	2.16 – -0.64	-5.7
2	B	141	LEU	HD13	-0.83	2.16 – -0.64	-5.7
1	A	58	HIS	HD2	4.50	9.28 – 4.78	-5.6
2	B	63	HIS	HD2	4.57	9.28 – 4.78	-5.5
2	B	28	LEU	HD12	-0.72	2.16 – -0.64	-5.3

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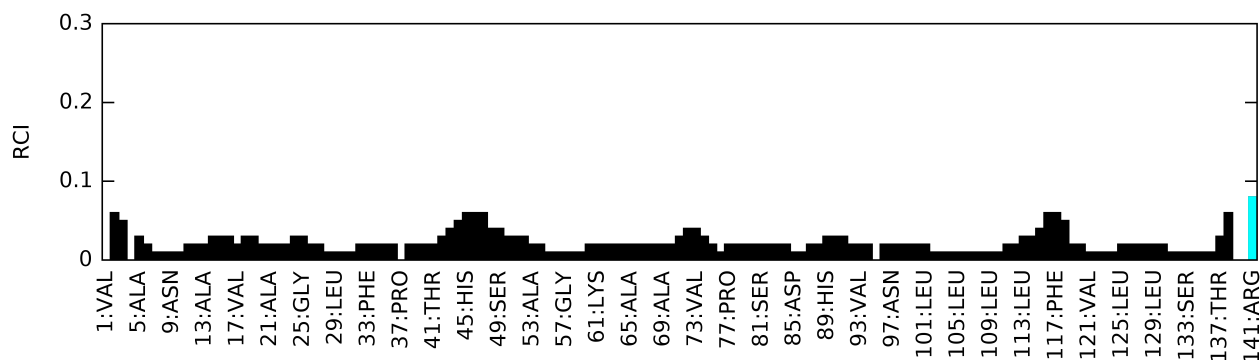
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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	28	LEU	HD13	-0.72	2.16 – -0.64	-5.3
2	B	28	LEU	HD11	-0.72	2.16 – -0.64	-5.3
2	B	141	LEU	HB3	-0.36	3.34 – -0.26	-5.3
2	B	96	LEU	HD21	-0.69	2.14 – -0.66	-5.1
2	B	96	LEU	HD22	-0.69	2.14 – -0.66	-5.1
2	B	96	LEU	HD23	-0.69	2.14 – -0.66	-5.1
1	A	86	LEU	HG	-0.15	3.16 – -0.14	-5.0

### 7.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

