Full wwPDB NMR Structure Validation Report (i)

Feb 12, 2022 – 03:33 PM EST

PDB ID	:	1FI9
Title	:	SOLUTION STRUCTURE OF THE IMIDAZOLE COMPLEX OF CYTOCHROME C
Authors	:	Banci, L.; Bertini, I.; Liu, G.; Lu, J.; Reddig, T.; Tang, W.; Wu, Y.; Zhu, D.
Deposited on	:	2000-08-03

This is a Full wwPDB NMR 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

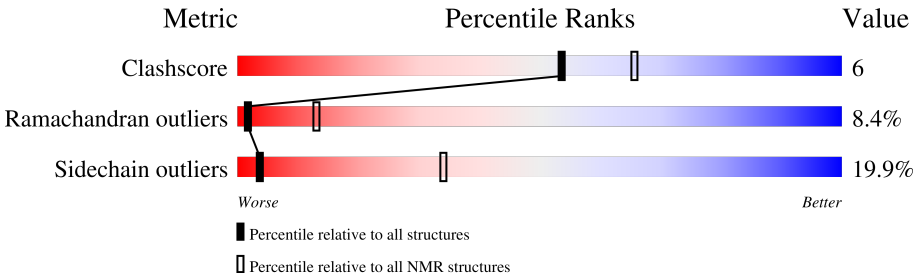
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	104	75% 23% •

2 Ensemble composition and analysis (i)

This entry contains 35 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:104 (104)	0.46	1

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 5 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 7, 9, 11, 12, 13, 15, 17, 19, 20, 21, 22, 23, 26, 28, 31, 34
2	5, 8, 14, 27, 29, 30
3	18, 25, 32
4	16, 35
5	10, 33
Single-model clusters	6; 24

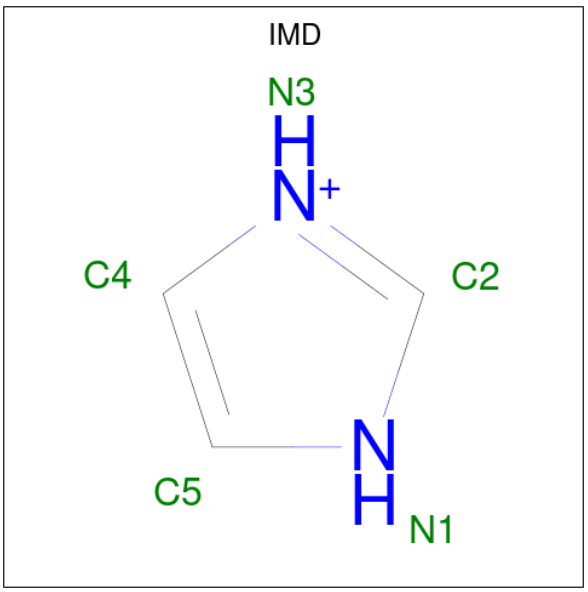
3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1754 atoms, of which 883 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CYTOCHROME C.

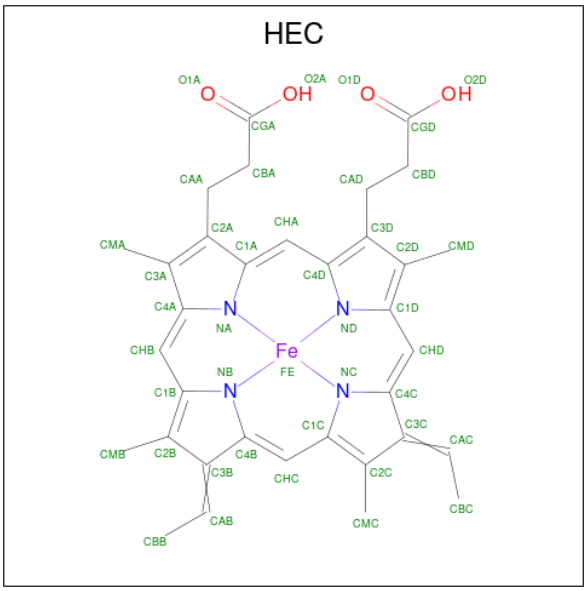
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	104	1670	524	847	144	151	4	0

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			
			Total	C	H	N
2	A	1	9	3	4	2

- Molecule 3 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					
			Total	C	Fe	H	N	O
3	A	1	75	34	1	32	4	4

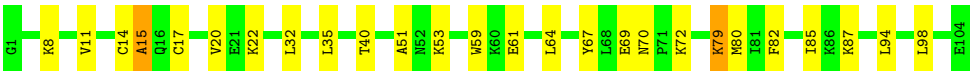
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: CYTOCHROME C

Chain A: 75% 23% •



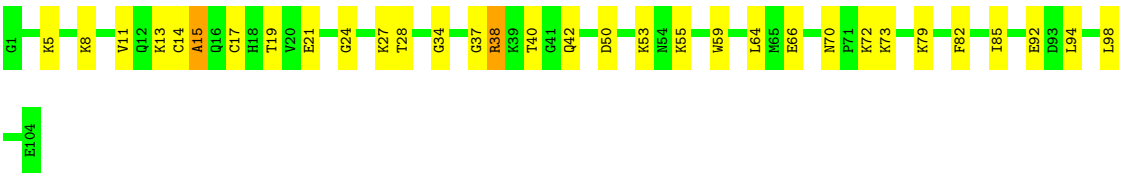
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: CYTOCHROME C

Chain A: 69% 29% •



4.2.2 Score per residue for model 2

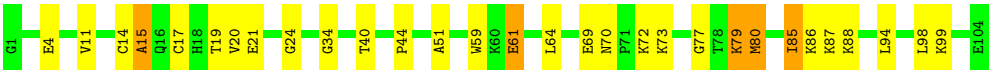
• Molecule 1: CYTOCHROME C

Chain A: 67% 28% 5%

4.2.3 Score per residue for model 3

• Molecule 1: CYTOCHROME C

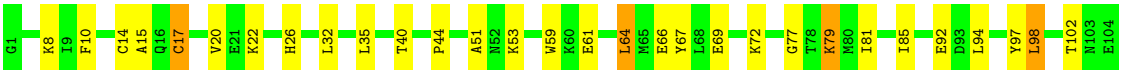
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: CYTOCHROME C

Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: CYTOCHROME C

Chain A:

4.2.6 Score per residue for model 6

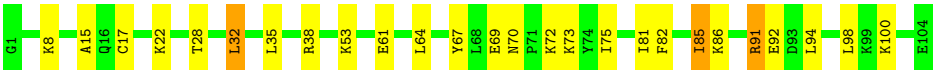
• Molecule 1: CYTOCHROME C

Chain A:

4.2.7 Score per residue for model 7

• Molecule 1: CYTOCHROME C

Chain A:



4.2.8 Score per residue for model 8

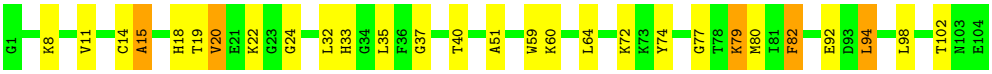
- Molecule 1: CYTOCHROME C

Chain A:

4.2.9 Score per residue for model 9

- Molecule 1: CYTOCHROME C

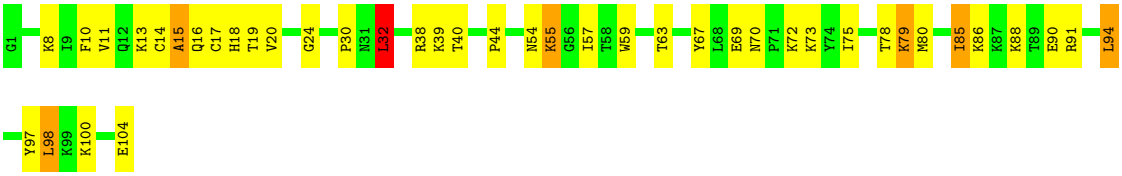
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: CYTOCHROME C

Chain A:



4.2.11 Score per residue for model 11

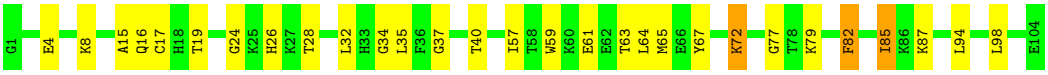
- Molecule 1: CYTOCHROME C

Chain A:

4.2.12 Score per residue for model 12

• Molecule 1: CYTOCHROME C

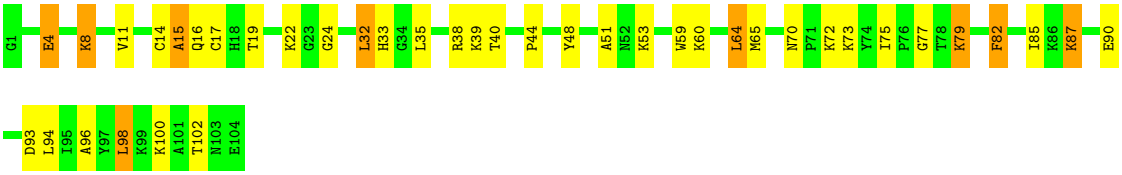
Chain A: 72% 25% •



4.2.13 Score per residue for model 13

• Molecule 1: CYTOCHROME C

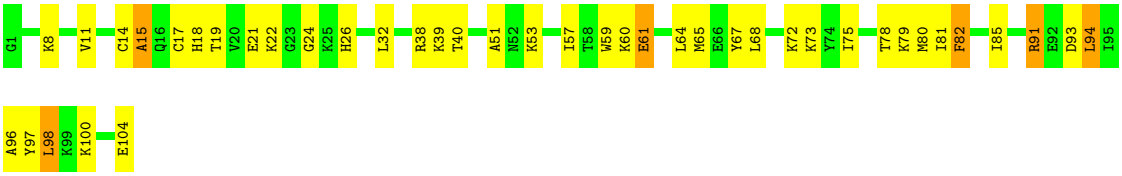
Chain A: 62% 30% 9%



4.2.14 Score per residue for model 14

• Molecule 1: CYTOCHROME C

Chain A: 60% 35% 6%



4.2.15 Score per residue for model 15

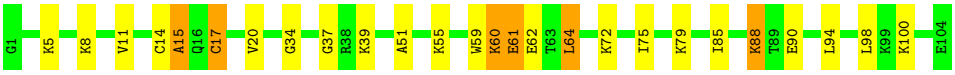
• Molecule 1: CYTOCHROME C

Chain A: 67% 27% 6%

4.2.16 Score per residue for model 16

- Molecule 1: CYTOCHROME C

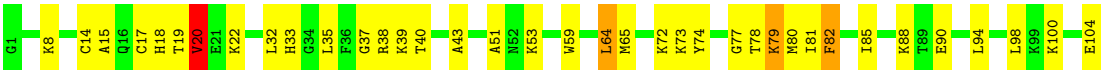
Chain A: 75% 19% 6%



4.2.17 Score per residue for model 17

- Molecule 1: CYTOCHROME C

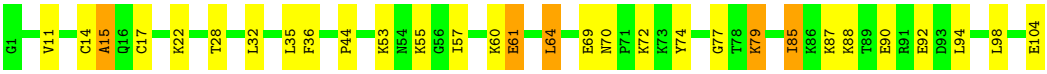
Chain A: 64% 32%



4.2.18 Score per residue for model 18

- Molecule 1: CYTOCHROME C

Chain A: 71% 24% 5%



4.2.19 Score per residue for model 19

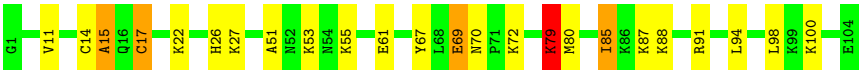
- Molecule 1: CYTOCHROME C

Chain A: 80% 17%

4.2.20 Score per residue for model 20

- Molecule 1: CYTOCHROME C

Chain A: 77% 18%



4.2.21 Score per residue for model 21

• Molecule 1: CYTOCHROME C

Chain A: 71% 26% •

4.2.22 Score per residue for model 22

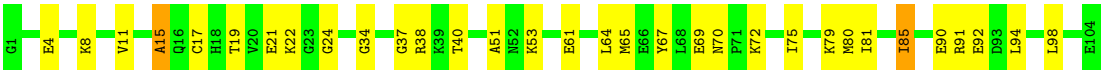
• Molecule 1: CYTOCHROME C

Chain A: 66% 29% 5%

4.2.23 Score per residue for model 23

• Molecule 1: CYTOCHROME C

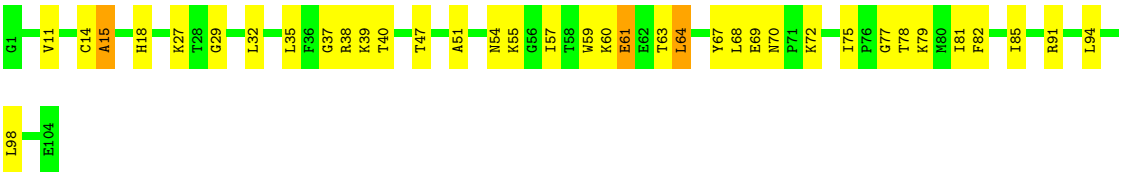
Chain A: 69% 29% •



4.2.24 Score per residue for model 24

• Molecule 1: CYTOCHROME C

Chain A: 64% 33% •



4.2.25 Score per residue for model 25

• Molecule 1: CYTOCHROME C

Chain A: 73% 23% •

4.2.26 Score per residue for model 26

- Molecule 1: CYTOCHROME C

Chain A:

4.2.27 Score per residue for model 27

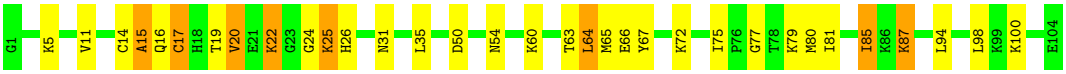
- Molecule 1: CYTOCHROME C

Chain A:

4.2.28 Score per residue for model 28

- Molecule 1: CYTOCHROME C

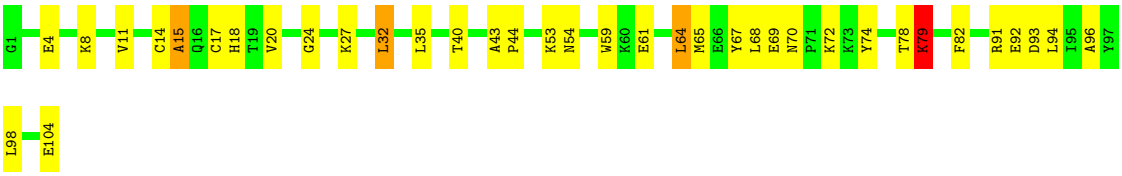
Chain A:



4.2.29 Score per residue for model 29

- Molecule 1: CYTOCHROME C

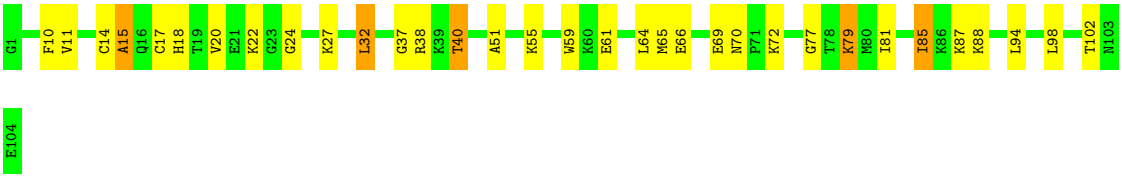
Chain A:



4.2.30 Score per residue for model 30

- Molecule 1: CYTOCHROME C

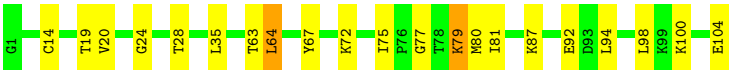
Chain A: 68% 27% 5%



4.2.31 Score per residue for model 31

- Molecule 1: CYTOCHROME C

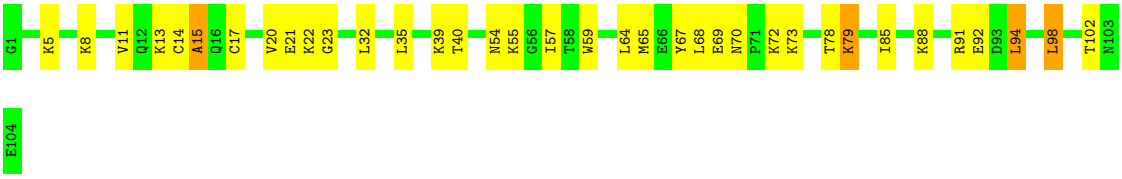
Chain A: 80% 18% •



4.2.32 Score per residue for model 32

- Molecule 1: CYTOCHROME C

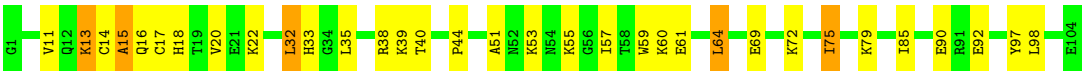
Chain A: 65% 31% •



4.2.33 Score per residue for model 33

- Molecule 1: CYTOCHROME C

Chain A: 68% 27% 5%



4.2.34 Score per residue for model 34

- Molecule 1: CYTOCHROME C

Chain A: 61% 36% •

G1 E4 K8 K13 C14 A15 Q16 T19 V20 E21 K22 G23 G24 T28 L32 H33 G34 L35 F36 G37 R38 K39 T40 A51 N52 K53 N54 K55 E61 E62 T63 L64 Y67 N70 P71 K72 K73 G77 T78 K79 M80 I81 F82 I85 K88 D93

L94 I95 A96 Y97 L98 K99 K100 E104

4.2.35 Score per residue for model 35

- Molecule 1: CYTOCHROME C

Chain A: 66% 26% 8%

G1 V11 C14 A15 Q16 C17 H18 T19 V20 E21 K22 G23 G24 K25 L32 H33 G34 L35 R38 K39 N52 K55 K60 E61 L64 L68 E69 K72 K73 Y74 I75 P76 G77 T78 K79 F82 I85 K86 K87 K88 E92 D93 L94 L98 A101

E104

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *AMBER*.

Of the 400 calculated structures, 35 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
DYANA	structure solution	5.0
PSEUDODYANA	structure solution	5.0
Amber	refinement	5.0
PSEUDOREM	refinement	5.0

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

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	0.58±0.01	0±0/839 (0.0± 0.0%)	0.91±0.02	0±0/1118 (0.0± 0.0%)
All	All	0.58	0/29365 (0.0%)	0.91	11/39130 (0.0%)

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	1.3±0.9
All	All	0	45

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	32	LEU	CB-CG-CD2	8.23	124.98	111.00	34	1
1	A	20	VAL	CA-CB-CG2	6.04	119.96	110.90	32	5
1	A	32	LEU	CB-CG-CD1	5.69	120.67	111.00	35	2
1	A	91	ARG	NE-CZ-NH2	5.50	123.05	120.30	15	1
1	A	67	TYR	CB-CG-CD1	-5.32	117.81	121.00	2	1
1	A	17	CYS	CA-CB-SG	-5.10	104.82	114.00	29	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)
1	A	67	TYR	Sidechain	18
1	A	97	TYR	Sidechain	7
1	A	18	HIS	Sidechain	5
1	A	74	TYR	Sidechain	5
1	A	91	ARG	Sidechain	3
1	A	82	PHE	Sidechain	2
1	A	48	TYR	Sidechain	2
1	A	38	ARG	Sidechain	1
1	A	46	PHE	Sidechain	1
1	A	36	PHE	Sidechain	1

6.2 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 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	823	847	847	7±3
3	A	43	32	30	4±1
All	All	30485	30905	30835	340

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LEU:CD2	1:A:35:LEU:HD22	0.80	2.06	2	6
1:A:35:LEU:HD21	1:A:64:LEU:HD11	0.78	1.54	13	17
3:A:110:HEC:HMC1	3:A:110:HEC:HBC3	0.77	1.55	20	32
1:A:57:ILE:HD12	1:A:63:THR:HG21	0.77	1.54	22	3
3:A:110:HEC:HBB3	3:A:110:HEC:HMB1	0.73	1.58	14	28
1:A:11:VAL:HA	1:A:15:ALA:HB2	0.71	1.63	13	26
1:A:32:LEU:HD22	1:A:35:LEU:HD22	0.70	1.59	4	6
1:A:68:LEU:HD13	1:A:91:ARG:CZ	0.69	2.17	32	1
1:A:64:LEU:HD21	3:A:110:HEC:HMA1	0.69	1.64	29	13
1:A:40:THR:HG22	1:A:59:TRP:CZ2	0.68	2.24	9	10
1:A:40:THR:HG22	1:A:59:TRP:NE1	0.66	2.05	3	10
1:A:32:LEU:HD23	1:A:35:LEU:HD13	0.65	1.68	33	1
1:A:19:THR:HG21	1:A:24:GLY:HA3	0.63	1.70	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:THR:O	3:A:110:HEC:HMD3	0.62	1.94	22	9
1:A:85:ILE:HD11	3:A:110:HEC:CBB	0.62	2.24	15	14
1:A:32:LEU:CD2	1:A:35:LEU:HD13	0.61	2.26	33	1
1:A:19:THR:HG21	1:A:24:GLY:CA	0.60	2.26	34	6
1:A:85:ILE:HD11	3:A:110:HEC:HBB1	0.60	1.74	3	11
3:A:110:HEC:HMC1	3:A:110:HEC:CBC	0.59	2.26	16	24
1:A:32:LEU:O	1:A:102:THR:HG22	0.59	1.98	4	4
1:A:40:THR:HG22	1:A:59:TRP:CE2	0.59	2.32	14	7
1:A:18:HIS:CE1	1:A:32:LEU:CD1	0.58	2.86	10	1
1:A:19:THR:HG21	1:A:24:GLY:HA2	0.57	1.76	1	8
1:A:20:VAL:HB	1:A:102:THR:HG22	0.57	1.76	9	1
1:A:57:ILE:CD1	1:A:63:THR:HG21	0.56	2.31	10	2
1:A:98:LEU:HD23	1:A:102:THR:HG21	0.56	1.75	4	5
1:A:43:ALA:HB1	1:A:44:PRO:HD2	0.55	1.77	29	1
1:A:20:VAL:HG12	1:A:32:LEU:HB3	0.55	1.77	29	6
1:A:35:LEU:HD21	1:A:64:LEU:CD1	0.55	2.31	24	2
1:A:91:ARG:NH2	1:A:94:LEU:HD13	0.55	2.17	32	2
1:A:32:LEU:HD21	1:A:35:LEU:HD22	0.54	1.79	2	2
1:A:32:LEU:HD23	1:A:35:LEU:HB2	0.54	1.80	2	1
1:A:18:HIS:CG	1:A:32:LEU:HD12	0.54	2.38	29	2
1:A:19:THR:HG22	1:A:21:GLU:HG2	0.53	1.81	34	2
1:A:68:LEU:HD21	3:A:110:HEC:CHB	0.53	2.34	14	1
1:A:13:LYS:HB3	3:A:110:HEC:HBB1	0.53	1.79	33	3
1:A:75:ILE:HD12	1:A:75:ILE:O	0.52	2.03	10	1
1:A:32:LEU:HD22	1:A:35:LEU:HD13	0.52	1.80	5	6
1:A:68:LEU:HD13	1:A:91:ARG:NH2	0.52	2.19	32	1
1:A:78:THR:HG22	1:A:79:LYS:HD2	0.52	1.83	29	1
1:A:29:GLY:CA	3:A:110:HEC:HMD3	0.51	2.35	24	1
1:A:35:LEU:HD23	1:A:36:PHE:CE1	0.51	2.41	22	1
1:A:79:LYS:NZ	3:A:110:HEC:O1D	0.51	2.44	19	1
1:A:51:ALA:HB1	1:A:75:ILE:HD12	0.50	1.82	15	1
1:A:40:THR:HG23	1:A:57:ILE:O	0.49	2.07	15	4
3:A:110:HEC:HMB1	3:A:110:HEC:CBB	0.48	2.37	6	1
1:A:19:THR:O	1:A:20:VAL:HG22	0.48	2.08	5	3
1:A:30:PRO:O	1:A:32:LEU:HD12	0.48	2.09	10	1
1:A:94:LEU:CD2	1:A:98:LEU:HD12	0.47	2.39	10	2
1:A:10:PHE:CZ	1:A:20:VAL:HG13	0.47	2.43	30	3
1:A:91:ARG:HH22	1:A:94:LEU:HD13	0.47	1.69	32	2
1:A:40:THR:HG21	1:A:55:LYS:HD2	0.47	1.85	34	1
1:A:18:HIS:CE1	1:A:32:LEU:HD13	0.46	2.45	10	3
1:A:40:THR:HG21	1:A:55:LYS:HB3	0.46	1.87	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:ILE:HD12	1:A:78:THR:CB	0.46	2.39	24	1
1:A:4:GLU:OE1	1:A:8:LYS:NZ	0.46	2.48	13	2
1:A:20:VAL:HG12	1:A:32:LEU:CB	0.46	2.41	10	1
1:A:93:ASP:O	1:A:96:ALA:HB3	0.45	2.10	29	4
1:A:20:VAL:CG2	1:A:101:ALA:HB1	0.45	2.42	35	1
1:A:32:LEU:CD1	1:A:35:LEU:HD22	0.45	2.42	7	1
1:A:75:ILE:HD13	1:A:78:THR:OG1	0.45	2.12	10	1
1:A:100:LYS:NZ	1:A:104:GLU:OXT	0.45	2.50	22	1
1:A:51:ALA:HB1	1:A:75:ILE:HG12	0.44	1.88	16	1
1:A:35:LEU:HD23	1:A:36:PHE:CZ	0.44	2.47	18	1
1:A:68:LEU:HB3	1:A:91:ARG:CZ	0.44	2.42	29	1
1:A:64:LEU:HD23	1:A:68:LEU:HD11	0.43	1.90	35	1
1:A:79:LYS:HE2	3:A:110:HEC:HMD2	0.43	1.89	20	1
1:A:20:VAL:HG12	1:A:32:LEU:HB2	0.43	1.90	33	1
3:A:110:HEC:HBB3	3:A:110:HEC:CMB	0.43	2.41	1	1
1:A:60:LYS:CG	1:A:60:LYS:O	0.42	2.67	9	1
1:A:22:LYS:H	1:A:22:LYS:CD	0.42	2.28	19	1
1:A:13:LYS:CB	3:A:110:HEC:HBB1	0.42	2.45	22	1
1:A:85:ILE:HG22	1:A:86:LYS:N	0.42	2.29	7	1
1:A:64:LEU:HD23	1:A:68:LEU:HG	0.42	1.92	24	1
1:A:75:ILE:HD12	1:A:75:ILE:N	0.41	2.30	13	1
1:A:18:HIS:ND1	1:A:32:LEU:HD13	0.41	2.30	35	1
1:A:69:GLU:OE1	1:A:91:ARG:NH2	0.41	2.53	20	1
1:A:59:TRP:CZ2	3:A:110:HEC:HAA1	0.41	2.51	16	1
1:A:94:LEU:HD11	3:A:110:HEC:HBB3	0.41	1.90	9	1
1:A:19:THR:HG21	1:A:24:GLY:N	0.41	2.31	28	1
1:A:32:LEU:HD11	3:A:110:HEC:CHB	0.41	2.46	30	1
1:A:75:ILE:HD12	1:A:78:THR:HG21	0.41	1.92	24	1
1:A:55:LYS:NZ	3:A:110:HEC:O2D	0.40	2.55	16	1

6.3 Torsion angles (i)

6.3.1 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 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	102/104 (98%)	68±4 (67±4%)	25±4 (25±4%)	9±2 (8±2%)	2 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3570/3640 (98%)	2393 (67%)	877 (25%)	300 (8%)	2 13

All 41 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	15	ALA	32
1	A	17	CYS	25
1	A	79	LYS	23
1	A	85	ILE	18
1	A	77	GLY	17
1	A	51	ALA	16
1	A	61	GLU	15
1	A	70	ASN	13
1	A	87	LYS	13
1	A	37	GLY	12
1	A	34	GLY	11
1	A	80	MET	11
1	A	81	ILE	10
1	A	44	PRO	9
1	A	20	VAL	8
1	A	82	PHE	6
1	A	27	LYS	5
1	A	75	ILE	5
1	A	33	HIS	5
1	A	88	LYS	5
1	A	31	ASN	4
1	A	53	LYS	3
1	A	62	GLU	3
1	A	24	GLY	3
1	A	60	LYS	3
1	A	40	THR	3
1	A	22	LYS	3
1	A	50	ASP	2
1	A	28	THR	2
1	A	47	THR	2
1	A	23	GLY	2
1	A	25	LYS	2
1	A	42	GLN	1
1	A	41	GLY	1
1	A	48	TYR	1
1	A	26	HIS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	72	LYS	1
1	A	73	LYS	1
1	A	78	THR	1
1	A	43	ALA	1
1	A	71	PRO	1

6.3.2 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 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	86/86 (100%)	69±3 (80±4%)	17±3 (20±4%)	4 34
All	All	3010/3010 (100%)	2412 (80%)	598 (20%)	4 34

All 56 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	72	LYS	35
1	A	98	LEU	35
1	A	94	LEU	33
1	A	64	LEU	31
1	A	79	LYS	31
1	A	14	CYS	29
1	A	69	GLU	21
1	A	22	LYS	21
1	A	8	LYS	19
1	A	92	GLU	17
1	A	61	GLU	17
1	A	53	LYS	16
1	A	100	LYS	15
1	A	38	ARG	14
1	A	73	LYS	14
1	A	82	PHE	14
1	A	85	ILE	13
1	A	65	MET	13
1	A	39	LYS	12
1	A	88	LYS	12

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Mol	Chain	Res	Type	Models (Total)
1	A	32	LEU	11
1	A	13	LYS	10
1	A	21	GLU	10
1	A	55	LYS	10
1	A	60	LYS	10
1	A	17	CYS	9
1	A	104	GLU	9
1	A	16	GLN	9
1	A	80	MET	8
1	A	87	LYS	8
1	A	91	ARG	8
1	A	90	GLU	8
1	A	4	GLU	7
1	A	54	ASN	7
1	A	75	ILE	6
1	A	86	LYS	5
1	A	70	ASN	5
1	A	5	LYS	4
1	A	50	ASP	4
1	A	66	GLU	4
1	A	26	HIS	4
1	A	27	LYS	3
1	A	78	THR	3
1	A	57	ILE	3
1	A	63	THR	3
1	A	42	GLN	2
1	A	47	THR	2
1	A	99	LYS	2
1	A	40	THR	2
1	A	52	ASN	2
1	A	81	ILE	2
1	A	25	LYS	2
1	A	62	GLU	1
1	A	74	TYR	1
1	A	49	THR	1
1	A	103	ASN	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

2 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
2	IMD	A	105	3	3,5,5	0.36±0.03	0±0 (0±0%)
3	HEC	A	110	2,1	26,50,50	1.03±0.03	2±0 (7±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
2	IMD	A	105	3	4,5,5	0.43±0.02	0±0 (0±0%)
3	HEC	A	110	2,1	18,82,82	1.07±0.14	1±1 (6±6%)

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	IMD	A	105	3	-	-	0±0,1,1,1
3	HEC	A	110	2,1	-	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	110	HEC	C3C-C2C	3.05	1.37	1.40	5	35
3	A	110	HEC	C2B-C3B	2.83	1.37	1.40	20	35

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	110	HEC	CBD-CAD-C3D	3.57	119.08	112.49	4	2
3	A	110	HEC	CBA-CAA-C2A	3.29	118.54	112.48	28	12
3	A	110	HEC	CMC-C2C-C1C	2.59	124.49	128.46	3	7
3	A	110	HEC	CMD-C2D-C1D	2.58	124.50	128.46	4	1
3	A	110	HEC	CAD-CBD-CGD	2.58	117.00	112.67	12	3
3	A	110	HEC	CMC-C2C-C3C	2.46	128.71	125.82	28	6
3	A	110	HEC	CMB-C2B-C1B	2.29	124.94	128.46	21	8
3	A	110	HEC	CAA-CBA-CGA	2.15	116.29	112.67	28	1

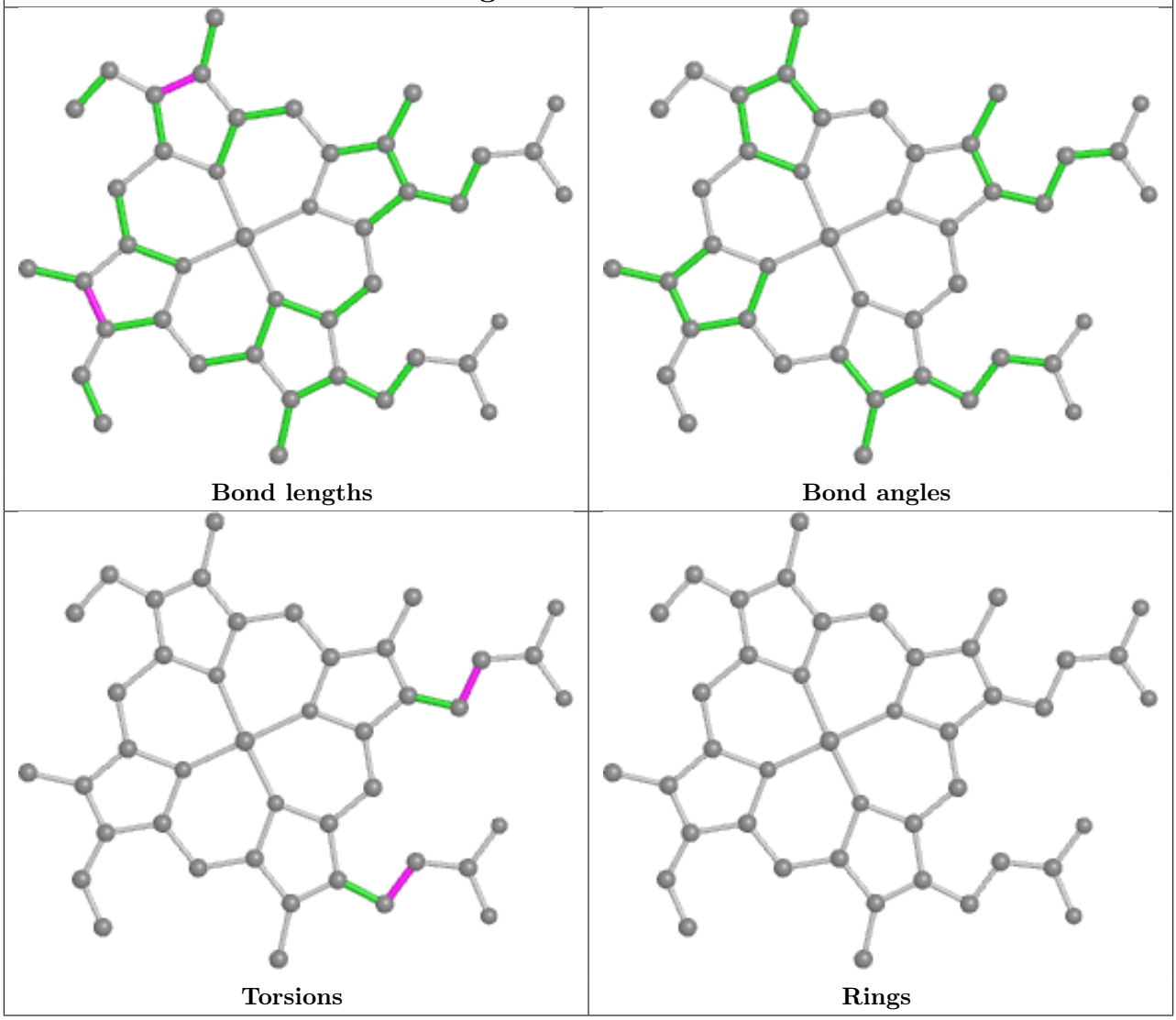
There are no chirality outliers.

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 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.

Ligand HEC A 110



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)

No chemical shift data were provided