



Full wwPDB NMR Structure Validation Report i

Jun 14, 2020 – 03:12 am BST

PDB ID : 1HKO
Title : NMR structure of bovine cytochrome b5
Authors : Muskett, F.W.; Whitford, D.
Deposited on : 2003-03-10

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](#) ①) were used in the production of this report:

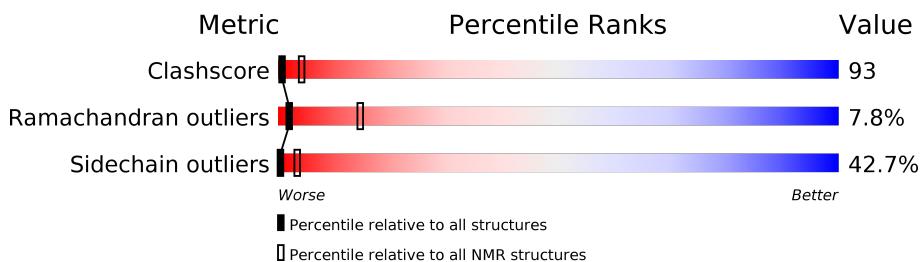
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
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 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain			
1	A	104	17%	50%	23%	• 8%

2 Ensemble composition and analysis i

This entry contains 42 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 6 as representative.

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:8-A:91 (84)	0.26	13
2	A:92-A:103 (12)	0.94	37

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 6 clusters and 3 single-model clusters were found.

Cluster number	Models
1	4, 6, 7, 13, 16, 18, 19, 23, 24, 27, 31, 40, 41
2	1, 8, 11, 12, 21, 22, 25, 28, 35, 37, 39, 42
3	9, 10, 14, 20, 29, 33, 34, 36
4	2, 32
5	15, 17
6	5, 26
Single-model clusters	3; 30; 38

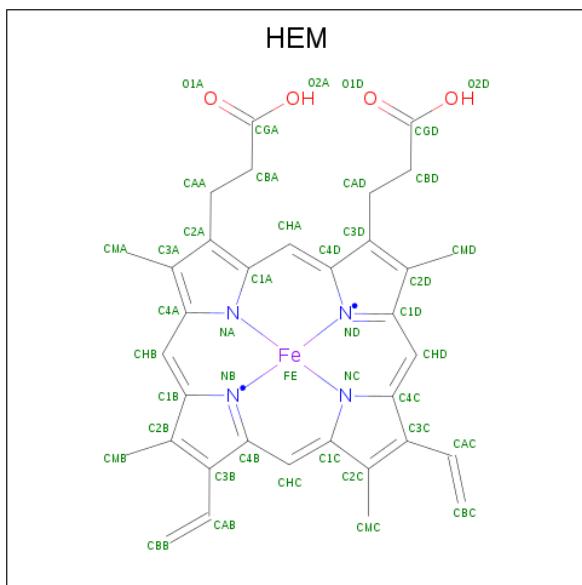
3 Entry composition [\(i\)](#)

There are 2 unique types of molecules in this entry. The entry contains 1699 atoms, of which 824 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CYTOCHROME B5.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	104	1636	520	804	138	174	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



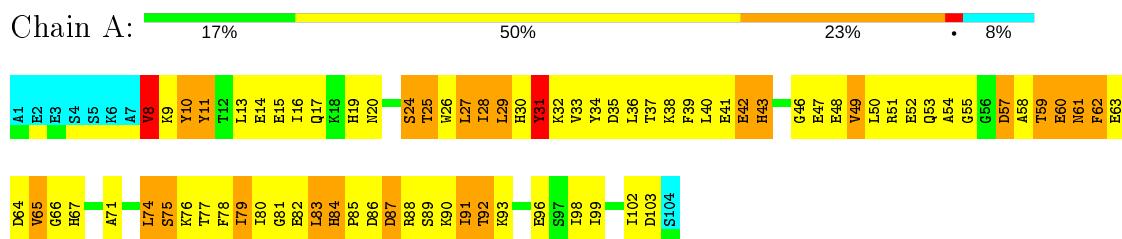
Mol	Chain	Residues	Atoms					
			Total	C	Fe	H	N	O
2	A	1	63	34	1	20	4	4

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: CYTOCHROME B5

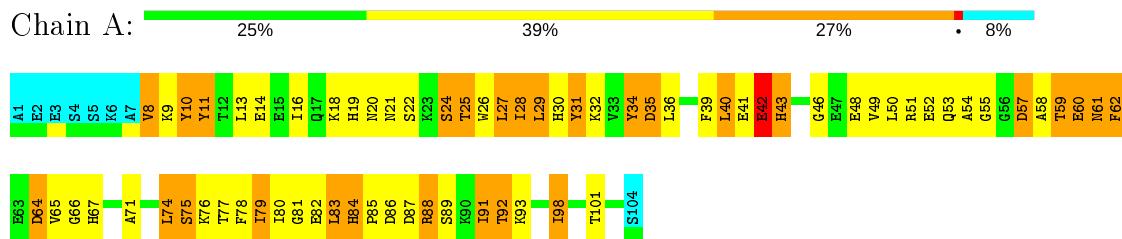


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

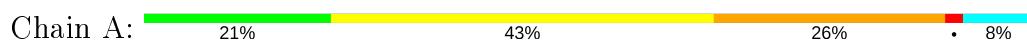
4.2.1 Score per residue for model 1

- Molecule 1: CYTOCHROME B5



4.2.2 Score per residue for model 2

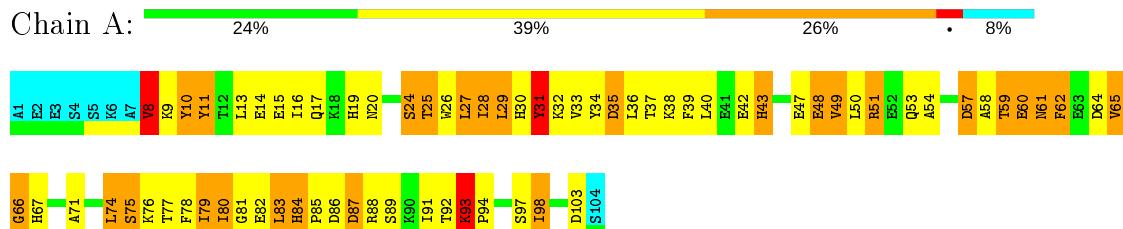
- Molecule 1: CYTOCHROME B5





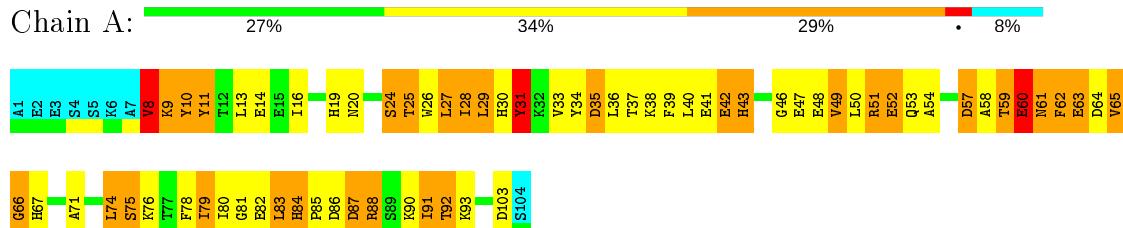
4.2.3 Score per residue for model 3

- Molecule 1: CYTOCHROME B5



4.2.4 Score per residue for model 4

- Molecule 1: CYTOCHROME B5



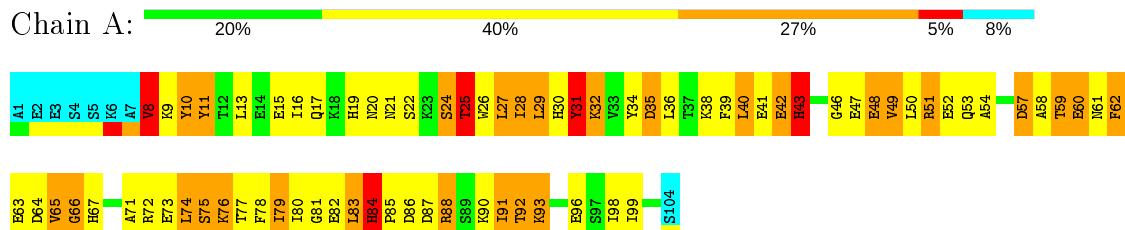
4.2.5 Score per residue for model 5

- Molecule 1: CYTOCHROME B5



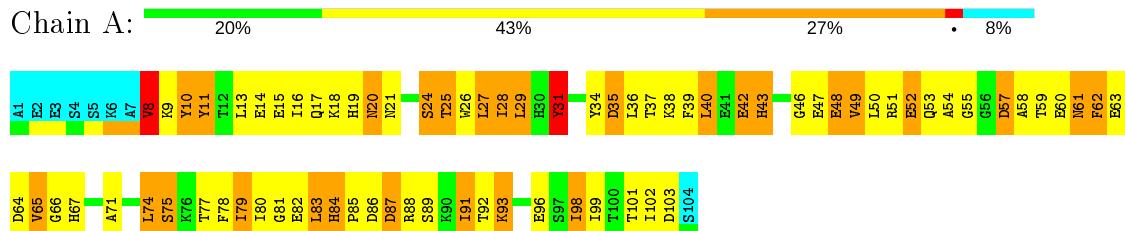
4.2.6 Score per residue for model 6

- Molecule 1: CYTOCHROME B5



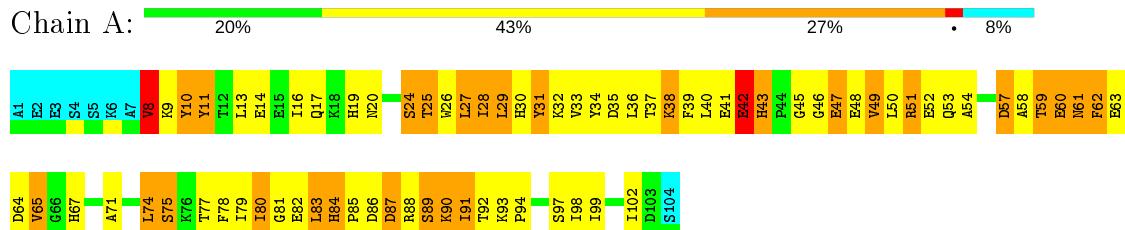
4.2.7 Score per residue for model 7

- Molecule 1: CYTOCHROME B5



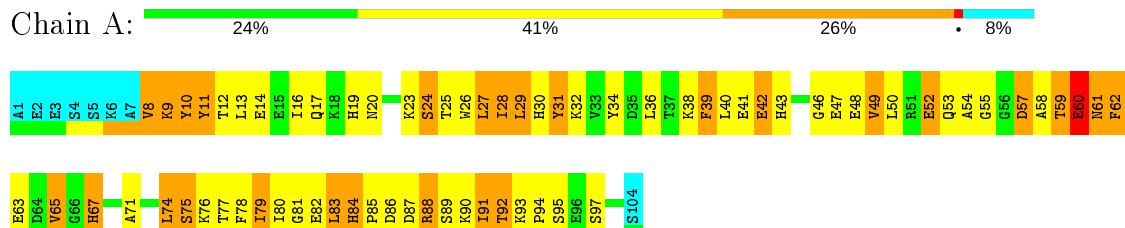
4.2.8 Score per residue for model 8

- Molecule 1: CYTOCHROME B5



4.2.9 Score per residue for model 9

- Molecule 1: CYTOCHROME B5



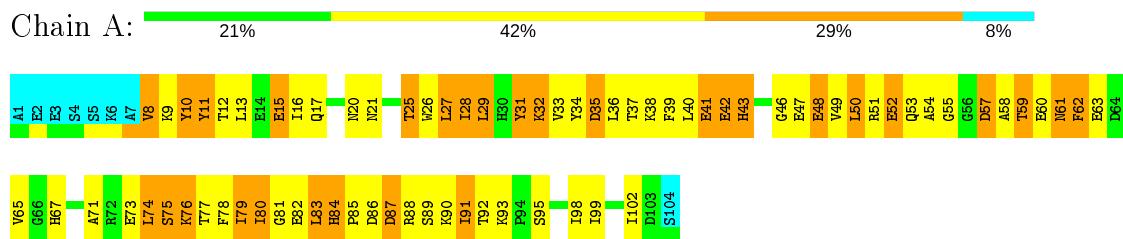
4.2.10 Score per residue for model 10

- Molecule 1: CYTOCHROME B5



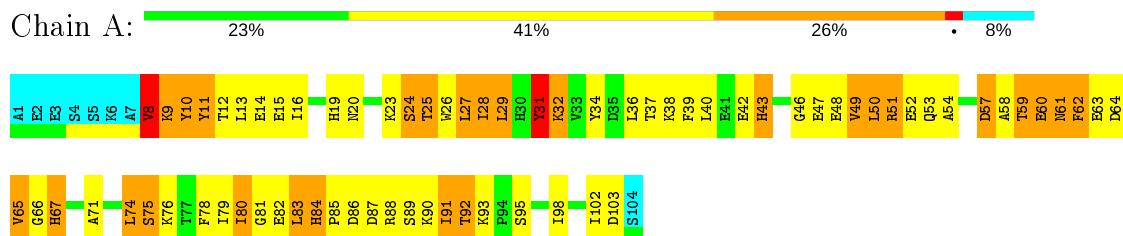
4.2.11 Score per residue for model 11

- Molecule 1: CYTOCHROME B5



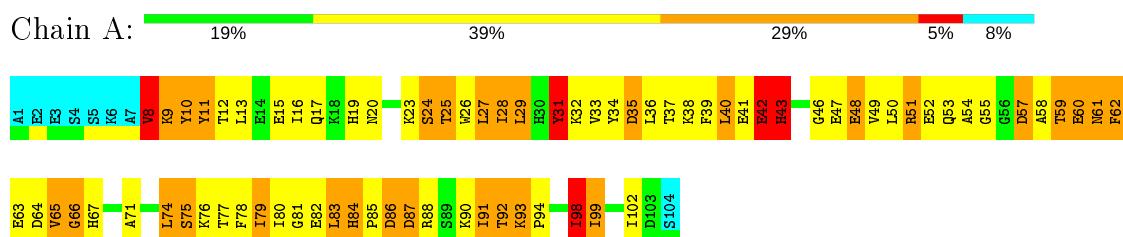
4.2.12 Score per residue for model 12

- Molecule 1: CYTOCHROME B5



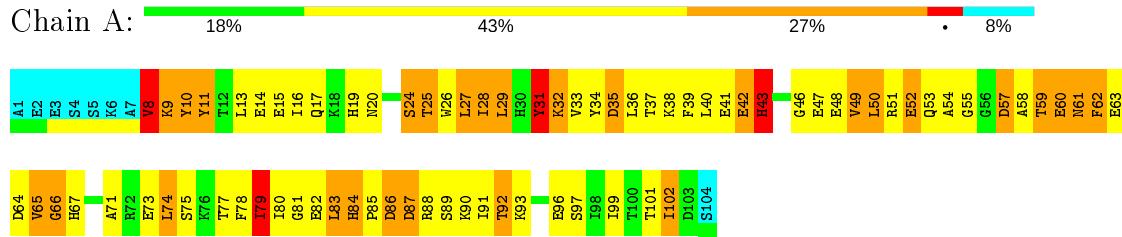
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: CYTOCHROME B5



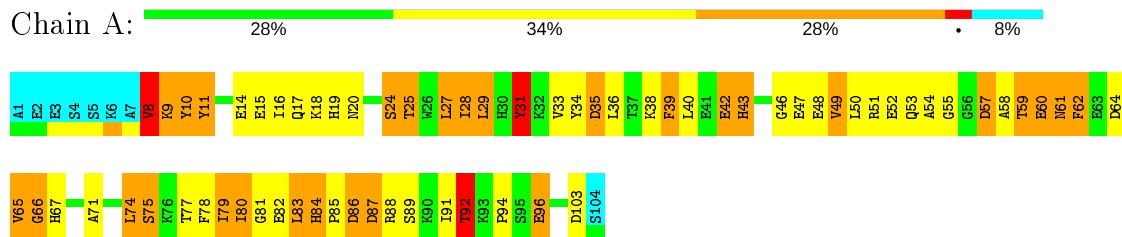
4.2.14 Score per residue for model 14

- Molecule 1: CYTOCHROME B5



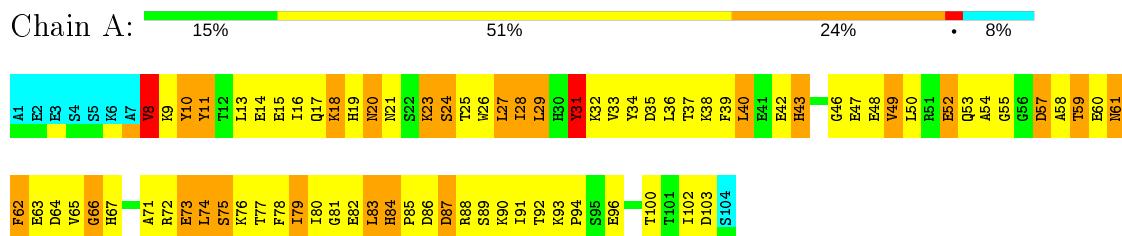
4.2.15 Score per residue for model 15

- Molecule 1: CYTOCHROME B5



4.2.16 Score per residue for model 16

- Molecule 1: CYTOCHROME B5



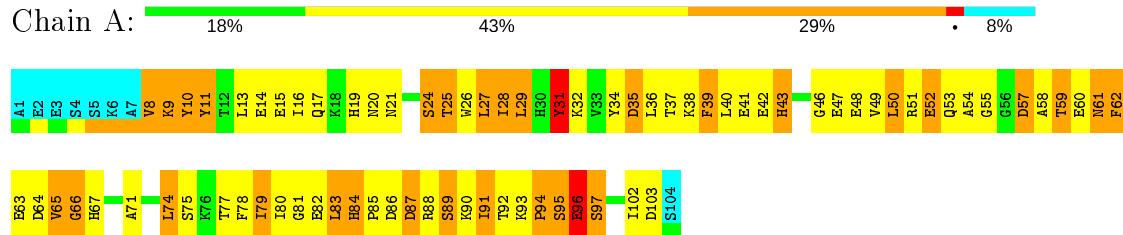
4.2.17 Score per residue for model 17

- Molecule 1: CYTOCHROME B5



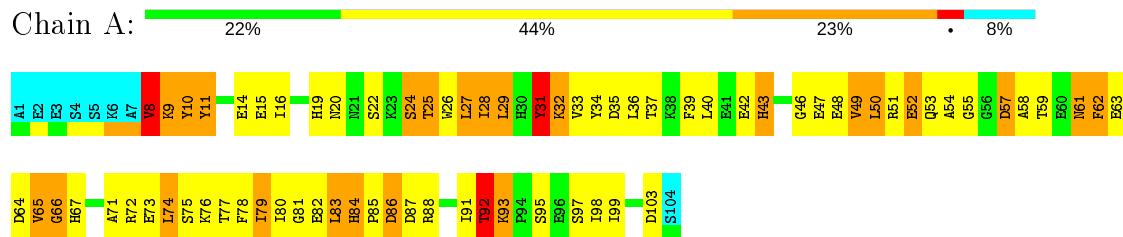
4.2.18 Score per residue for model 18

- Molecule 1: CYTOCHROME B5



4.2.19 Score per residue for model 19

- Molecule 1: CYTOCHROME B5



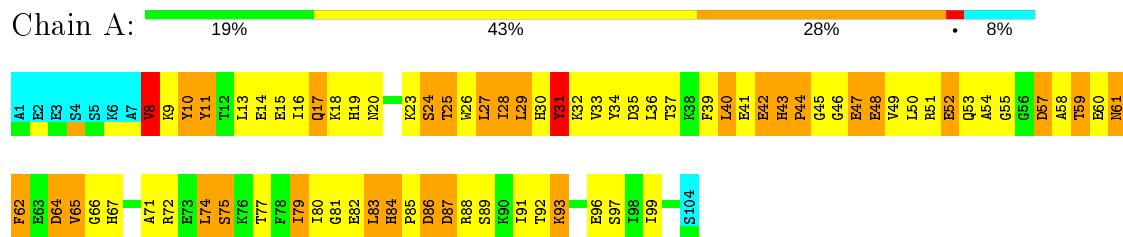
4.2.20 Score per residue for model 20

- Molecule 1: CYTOCHROME B5



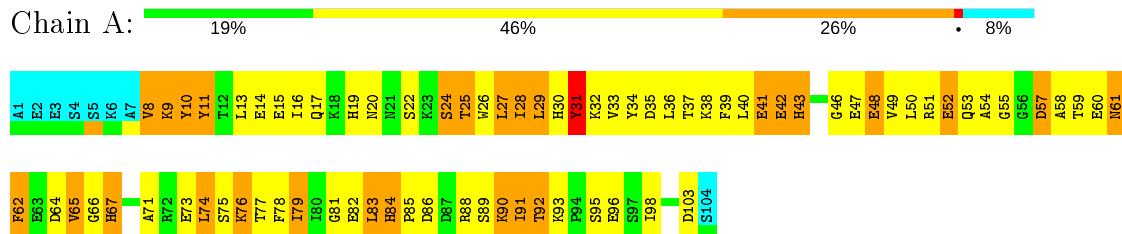
4.2.21 Score per residue for model 21

- Molecule 1: CYTOCHROME B5



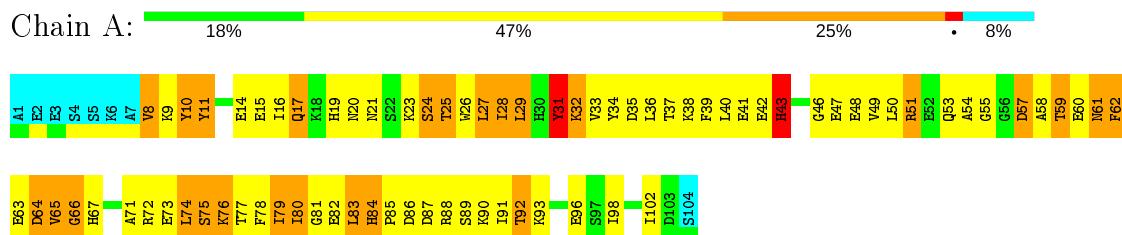
4.2.22 Score per residue for model 22

- Molecule 1: CYTOCHROME B5



4.2.23 Score per residue for model 23

- Molecule 1: CYTOCHROME B5



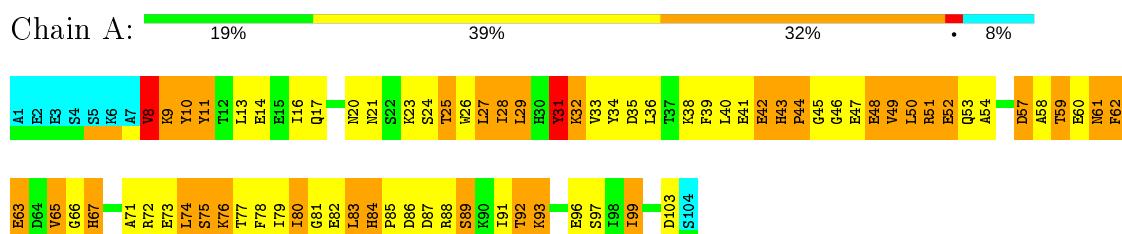
4.2.24 Score per residue for model 24

- Molecule 1: CYTOCHROME B5



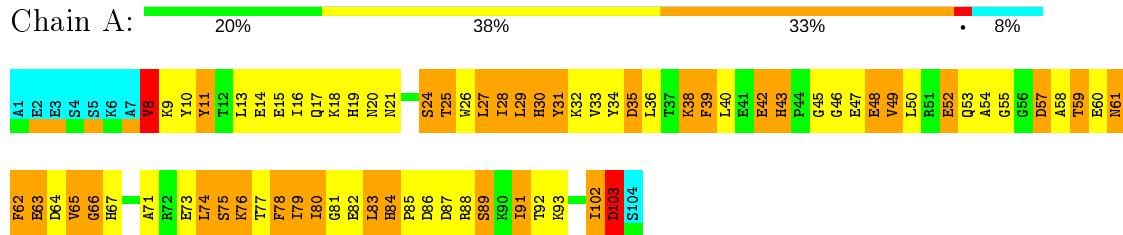
4.2.25 Score per residue for model 25

- Molecule 1: CYTOCHROME B5



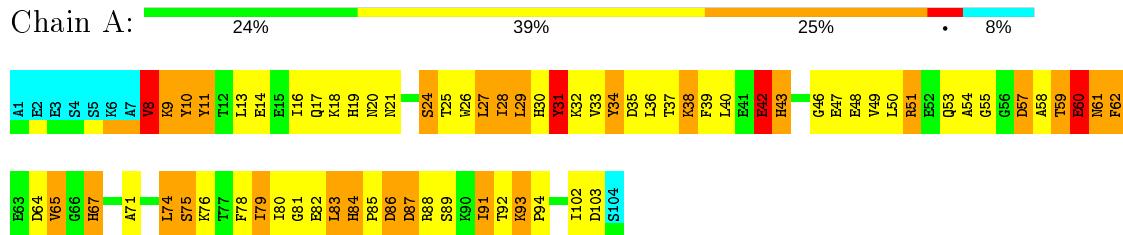
4.2.26 Score per residue for model 26

- Molecule 1: CYTOCHROME B5



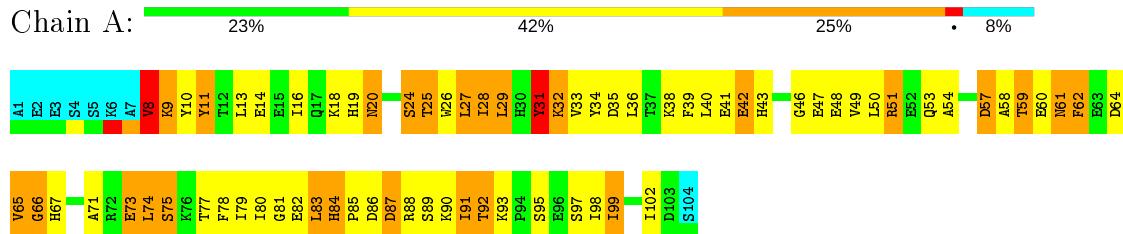
4.2.27 Score per residue for model 27

- Molecule 1: CYTOCHROME B5



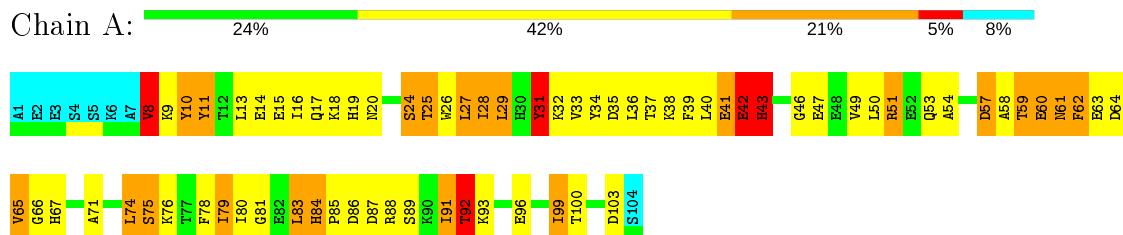
4.2.28 Score per residue for model 28

- Molecule 1: CYTOCHROME B5



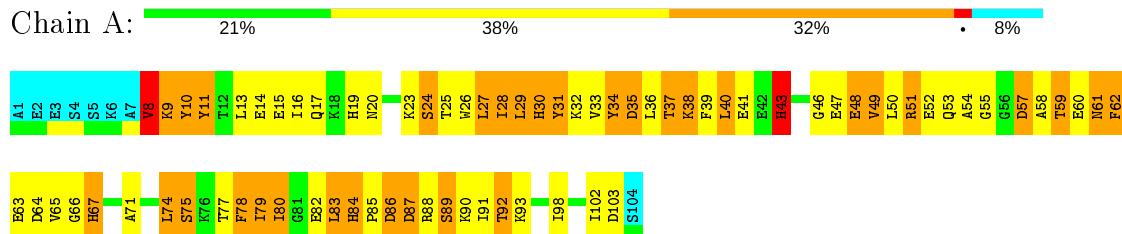
4.2.29 Score per residue for model 29

- Molecule 1: CYTOCHROME B5



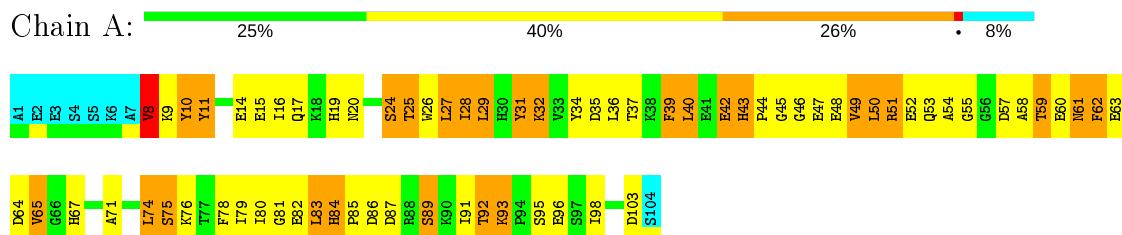
4.2.30 Score per residue for model 30

- Molecule 1: CYTOCHROME B5



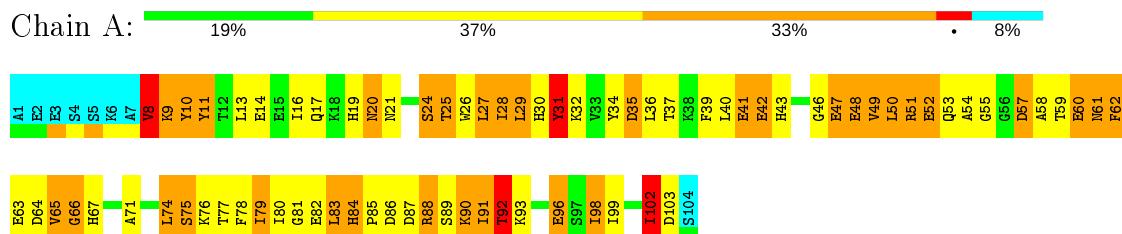
4.2.31 Score per residue for model 31

- Molecule 1: CYTOCHROME B5



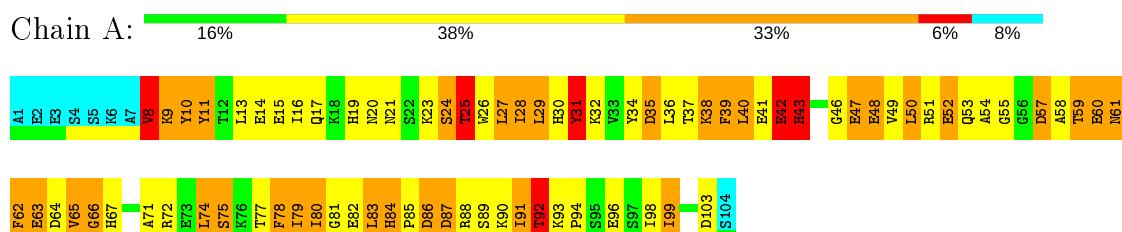
4.2.32 Score per residue for model 32

- Molecule 1: CYTOCHROME B5



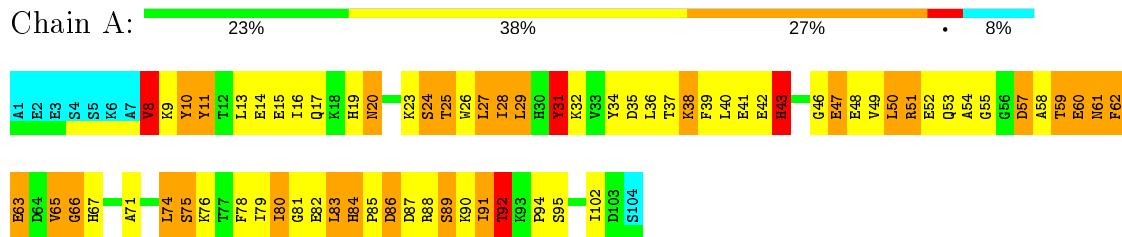
4.2.33 Score per residue for model 33

- Molecule 1: CYTOCHROME B5



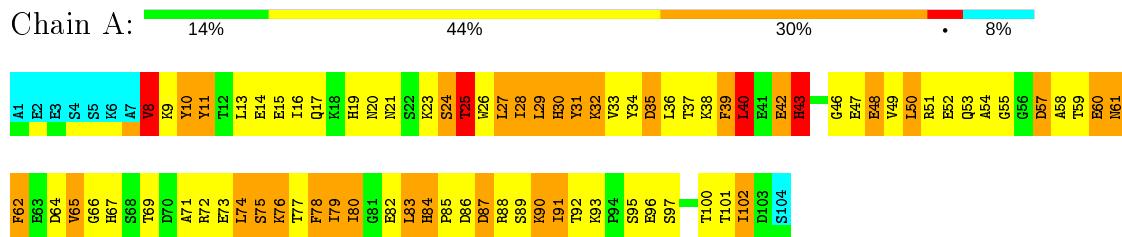
4.2.34 Score per residue for model 34

- Molecule 1: CYTOCHROME B5



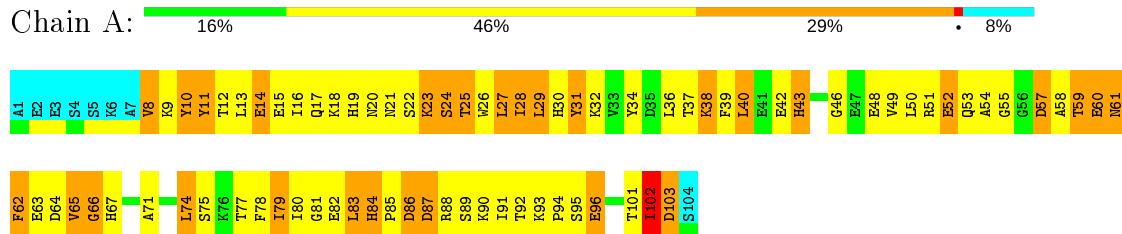
4.2.35 Score per residue for model 35

- Molecule 1: CYTOCHROME B5



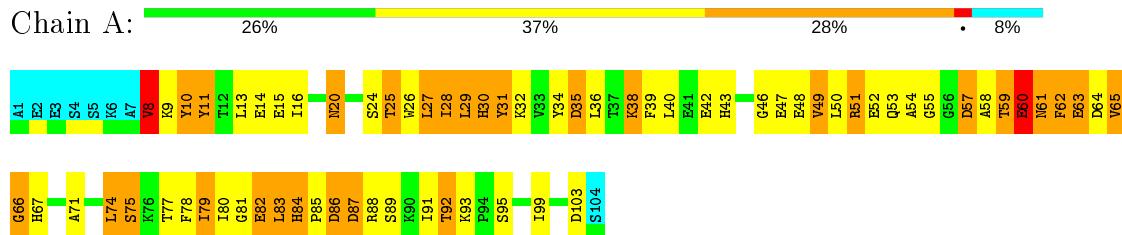
4.2.36 Score per residue for model 36

- Molecule 1: CYTOCHROME B5



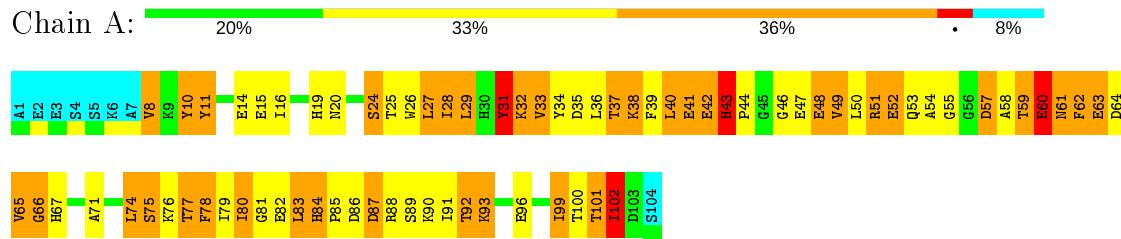
4.2.37 Score per residue for model 37

- Molecule 1: CYTOCHROME B5



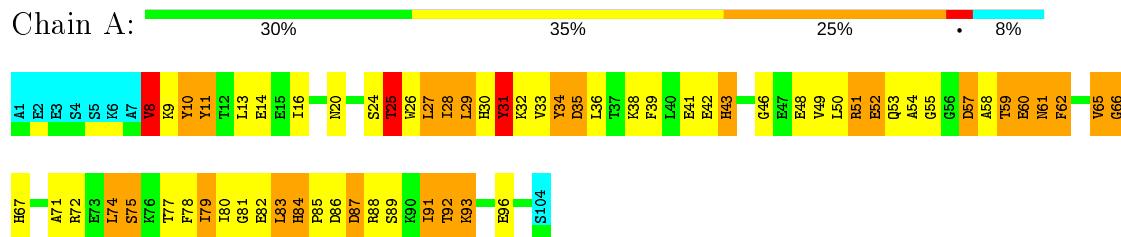
4.2.38 Score per residue for model 38

- Molecule 1: CYTOCHROME B5



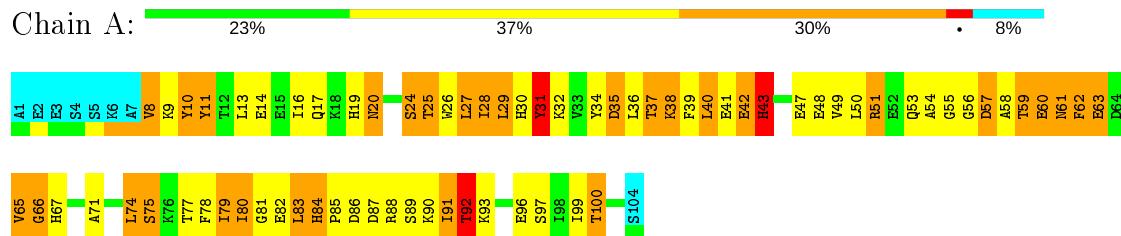
4.2.39 Score per residue for model 39

- Molecule 1: CYTOCHROME B5



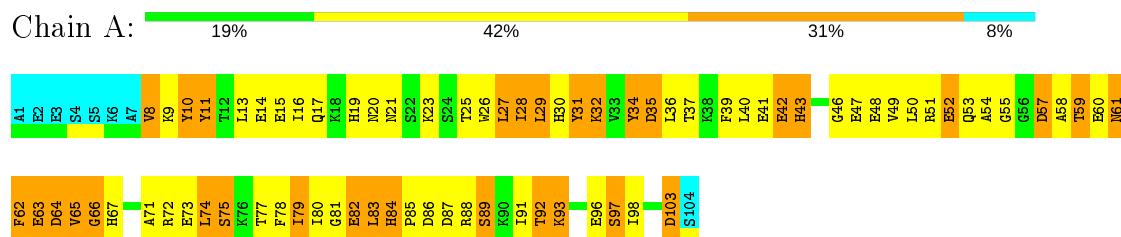
4.2.40 Score per residue for model 40

- Molecule 1: CYTOCHROME B5



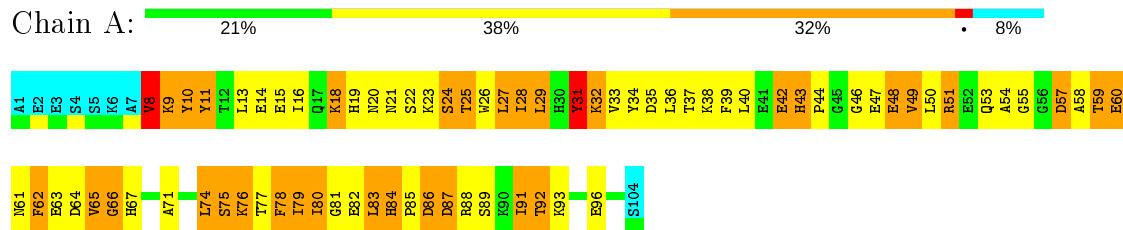
4.2.41 Score per residue for model 41

- Molecule 1: CYTOCHROME B5



4.2.42 Score per residue for model 42

- Molecule 1: CYTOCHROME B5



5 Refinement protocol and experimental data overview i

The models were refined using the following method: ?.

Of the 100 calculated structures, 42 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
DYANA	refinement	
DYANA	structure solution	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

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:
HEM

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	777	754	749	148±12
2	A	43	20	30	13±3
All	All	34440	32508	32718	6256

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 93.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:ILE:HD13	1:A:28:ILE:CD1	1.13	1.73	35	37
1:A:16:ILE:HD13	1:A:28:ILE:HD11	1.11	1.15	16	35
1:A:83:LEU:HD23	1:A:91:ILE:HD13	1.11	1.21	40	28
1:A:26:TRP:CH2	1:A:80:ILE:HD13	1.04	1.87	39	3
1:A:28:ILE:HG21	1:A:91:ILE:HD11	1.01	1.32	22	30
1:A:29:LEU:HD21	1:A:62:PHE:CG	0.99	1.92	1	32
1:A:36:LEU:HD13	1:A:50:LEU:HB3	0.98	1.35	20	42
1:A:36:LEU:HD22	1:A:50:LEU:HD23	0.97	1.35	30	7
1:A:39:PHE:O	1:A:50:LEU:HD13	0.97	1.60	26	8
1:A:83:LEU:HD23	1:A:91:ILE:CD1	0.96	1.90	34	32
1:A:27:LEU:HD23	1:A:58:ALA:HB3	0.95	1.37	3	42

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:PHE:CE2	1:A:74:LEU:HD11	0.95	1.97	15	3
1:A:39:PHE:CE1	1:A:78:PHE:CD1	0.95	2.55	22	1
1:A:39:PHE:CZ	1:A:74:LEU:HD21	0.94	1.97	10	19
1:A:43:HIS:CE1	1:A:49:VAL:HG11	0.94	1.98	12	13
1:A:46:GLY:O	1:A:49:VAL:HG12	0.93	1.62	38	39
1:A:8:VAL:HG23	1:A:11:TYR:CD1	0.93	1.98	39	25
1:A:28:ILE:HD13	1:A:83:LEU:HD23	0.93	1.41	20	8
1:A:74:LEU:HD11	1:A:78:PHE:CZ	0.92	1.98	22	4
1:A:39:PHE:CE1	1:A:74:LEU:HD11	0.92	2.00	20	10
1:A:29:LEU:HD22	1:A:30:HIS:CD2	0.92	1.99	35	2
1:A:74:LEU:O	1:A:77:THR:HG22	0.92	1.63	24	24
1:A:43:HIS:ND1	1:A:49:VAL:HG11	0.92	1.80	31	25
1:A:33:VAL:HG12	1:A:80:ILE:HD11	0.91	1.39	27	8
1:A:21:ASN:O	1:A:25:THR:HG23	0.90	1.65	7	6
1:A:36:LEU:HD22	1:A:50:LEU:HD22	0.89	1.44	38	28
1:A:8:VAL:HG13	1:A:80:ILE:O	0.89	1.67	24	38
1:A:83:LEU:CD2	1:A:91:ILE:HD13	0.89	1.98	23	12
1:A:28:ILE:HD13	1:A:83:LEU:CD2	0.89	1.97	20	12
1:A:25:THR:HG22	1:A:54:ALA:HB2	0.88	1.46	35	34
1:A:25:THR:HG22	1:A:54:ALA:CB	0.88	1.99	39	33
1:A:26:TRP:CH2	1:A:35:ASP:HB3	0.88	2.04	41	3
1:A:39:PHE:CE2	1:A:74:LEU:HD21	0.86	2.05	35	5
1:A:57:ASP:HB2	1:A:91:ILE:HD12	0.86	1.47	13	40
1:A:13:LEU:HG	1:A:83:LEU:HD21	0.86	1.47	17	28
1:A:27:LEU:HD22	1:A:28:ILE:N	0.86	1.86	39	42
1:A:83:LEU:HD12	1:A:84:HIS:N	0.85	1.86	38	28
1:A:19:HIS:CE1	1:A:26:TRP:CH2	0.84	2.66	13	9
1:A:39:PHE:CG	1:A:78:PHE:CE2	0.84	2.65	14	8
1:A:43:HIS:CG	1:A:49:VAL:HG11	0.83	2.08	22	24
1:A:77:THR:HG22	1:A:78:PHE:CD1	0.83	2.09	9	3
1:A:71:ALA:HA	1:A:74:LEU:HD23	0.83	1.51	20	40
1:A:43:HIS:CE1	1:A:49:VAL:HG21	0.83	2.09	16	19
1:A:19:HIS:CD2	1:A:26:TRP:CZ3	0.82	2.67	16	2
1:A:39:PHE:CZ	1:A:78:PHE:CD1	0.82	2.68	22	1
1:A:26:TRP:CZ3	1:A:35:ASP:CB	0.82	2.62	39	3
1:A:35:ASP:OD1	1:A:80:ILE:HD13	0.81	1.75	4	3
1:A:13:LEU:HD12	1:A:87:ASP:OD1	0.81	1.76	35	10
1:A:74:LEU:O	1:A:77:THR:HG23	0.81	1.75	14	6
1:A:19:HIS:CE1	1:A:26:TRP:CZ2	0.81	2.69	17	9
1:A:33:VAL:HG23	1:A:80:ILE:CD1	0.81	2.05	25	3
1:A:98:ILE:HD13	1:A:99:ILE:N	0.81	1.90	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:VAL:HG23	1:A:80:ILE:HD12	0.81	1.52	25	3
1:A:58:ALA:HB1	2:A:105:HEM:CMC	0.80	2.06	16	41
1:A:13:LEU:HD21	1:A:91:ILE:HD13	0.80	1.52	24	1
1:A:39:PHE:CD2	1:A:74:LEU:HD11	0.80	2.10	15	2
1:A:11:TYR:CE2	1:A:26:TRP:CZ3	0.80	2.70	32	17
1:A:33:VAL:HG12	1:A:81:GLY:C	0.80	1.96	39	2
1:A:102:ILE:HD13	1:A:103:ASP:N	0.79	1.91	26	2
1:A:26:TRP:CH2	1:A:80:ILE:CD1	0.79	2.64	37	2
1:A:43:HIS:CD2	1:A:49:VAL:HG11	0.79	2.13	22	15
1:A:19:HIS:CE1	1:A:26:TRP:CZ3	0.79	2.71	6	4
1:A:19:HIS:CG	1:A:26:TRP:CE3	0.79	2.71	17	9
1:A:39:PHE:CE1	1:A:78:PHE:CE1	0.78	2.71	22	1
1:A:39:PHE:CD1	1:A:78:PHE:CE1	0.78	2.72	22	1
1:A:13:LEU:HD11	1:A:91:ILE:HG21	0.78	1.54	2	16
1:A:28:ILE:HG21	1:A:91:ILE:CD1	0.78	2.09	16	15
1:A:43:HIS:ND1	1:A:50:LEU:HD11	0.78	1.93	5	14
1:A:33:VAL:HG22	1:A:81:GLY:C	0.77	2.00	25	8
1:A:40:LEU:HD13	1:A:47:GLU:HB3	0.77	1.57	33	2
1:A:40:LEU:HD22	1:A:47:GLU:HB3	0.77	1.56	29	13
1:A:36:LEU:HD13	1:A:50:LEU:CB	0.76	2.10	24	42
1:A:27:LEU:HD23	1:A:58:ALA:CB	0.76	2.11	2	40
1:A:26:TRP:CZ2	1:A:80:ILE:HD13	0.76	2.15	37	3
1:A:50:LEU:O	1:A:53:GLN:HG2	0.76	1.80	37	42
1:A:8:VAL:HG11	1:A:80:ILE:HD12	0.76	1.58	39	4
1:A:30:HIS:CE1	1:A:62:PHE:CZ	0.75	2.74	30	3
1:A:39:PHE:CD2	1:A:78:PHE:CD2	0.75	2.75	34	5
1:A:16:ILE:HG23	1:A:26:TRP:HB3	0.75	1.56	40	10
1:A:30:HIS:CE1	1:A:31:TYR:CE2	0.75	2.74	4	1
1:A:39:PHE:CE2	1:A:78:PHE:CB	0.74	2.70	22	1
1:A:35:ASP:OD1	1:A:80:ILE:HG21	0.74	1.82	13	3
1:A:58:ALA:HB1	2:A:105:HEM:HMC2	0.74	1.59	23	18
1:A:39:PHE:CE1	1:A:78:PHE:CB	0.74	2.71	40	5
1:A:13:LEU:HD12	1:A:87:ASP:CG	0.74	2.03	35	15
1:A:43:HIS:HD1	1:A:50:LEU:HD11	0.74	1.42	42	13
1:A:29:LEU:HD21	1:A:62:PHE:CD2	0.74	2.17	1	12
1:A:8:VAL:HG21	1:A:11:TYR:CD2	0.74	2.18	37	16
1:A:39:PHE:CE2	1:A:78:PHE:CD2	0.73	2.76	34	2
1:A:29:LEU:CB	1:A:34:TYR:CE1	0.73	2.72	22	27
1:A:34:TYR:CE2	1:A:79:ILE:CG1	0.73	2.71	30	40
1:A:49:VAL:O	1:A:53:GLN:NE2	0.73	2.21	29	22
1:A:38:LYS:CD	1:A:78:PHE:CZ	0.73	2.72	38	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:ILE:HD13	1:A:28:ILE:HD12	0.73	1.58	35	16
1:A:28:ILE:HD12	1:A:57:ASP:N	0.73	1.98	19	15
1:A:13:LEU:HD12	1:A:87:ASP:HB3	0.73	1.61	2	9
1:A:26:TRP:CH2	1:A:80:ILE:HG21	0.73	2.18	41	2
1:A:39:PHE:CD1	1:A:74:LEU:HD11	0.73	2.18	16	3
1:A:28:ILE:CG2	1:A:91:ILE:HD11	0.72	2.14	22	12
1:A:27:LEU:HD12	1:A:36:LEU:HG	0.72	1.61	22	40
1:A:27:LEU:HD21	2:A:105:HEM:HBB1	0.72	1.60	15	6
1:A:19:HIS:CD2	1:A:26:TRP:CD1	0.72	2.77	12	1
1:A:65:VAL:HG11	1:A:67:HIS:CE1	0.72	2.18	1	1
1:A:74:LEU:HD11	1:A:78:PHE:CE2	0.72	2.18	22	7
1:A:13:LEU:HD12	1:A:87:ASP:CB	0.72	2.13	37	7
1:A:35:ASP:OD2	1:A:80:ILE:HD13	0.71	1.84	26	3
1:A:19:HIS:CD2	1:A:26:TRP:CE3	0.71	2.79	16	2
1:A:30:HIS:CE1	1:A:62:PHE:CE1	0.71	2.78	30	1
1:A:29:LEU:HD12	2:A:105:HEM:CBB	0.71	2.15	25	30
1:A:58:ALA:HB1	2:A:105:HEM:HMC1	0.71	1.62	15	10
1:A:35:ASP:O	1:A:35:ASP:CG	0.70	2.29	15	3
1:A:19:HIS:ND1	1:A:26:TRP:CZ3	0.70	2.59	6	1
1:A:19:HIS:CD2	1:A:26:TRP:NE1	0.70	2.59	12	1
1:A:84:HIS:CG	1:A:85:PRO:CD	0.70	2.74	35	42
1:A:13:LEU:CG	1:A:83:LEU:HD21	0.70	2.16	14	13
1:A:29:LEU:HD21	1:A:62:PHE:CD1	0.70	2.22	14	21
1:A:39:PHE:CE2	1:A:78:PHE:CG	0.70	2.79	34	5
1:A:31:TYR:CE1	1:A:88:ARG:CZ	0.70	2.74	40	3
1:A:20:ASN:O	1:A:20:ASN:CG	0.70	2.30	9	18
1:A:19:HIS:CD2	1:A:24:SER:HG	0.70	2.04	12	1
1:A:26:TRP:CZ3	1:A:35:ASP:OD1	0.70	2.45	28	9
1:A:20:ASN:ND2	1:A:54:ALA:O	0.70	2.24	40	35
1:A:53:GLN:HE22	2:A:105:HEM:CHC	0.70	2.00	9	17
1:A:57:ASP:OD2	1:A:59:THR:HG22	0.69	1.87	19	8
1:A:10:TYR:CB	1:A:84:HIS:CE1	0.69	2.75	38	10
1:A:74:LEU:CD1	1:A:78:PHE:CZ	0.69	2.75	22	6
1:A:39:PHE:CZ	1:A:75:SER:HA	0.69	2.22	42	7
1:A:19:HIS:CD2	1:A:24:SER:CB	0.69	2.76	12	1
1:A:89:SER:HA	1:A:92:THR:HG22	0.69	1.62	12	9
1:A:8:VAL:CG2	1:A:11:TYR:CD1	0.69	2.75	38	24
1:A:25:THR:HG22	1:A:36:LEU:HB2	0.69	1.63	16	1
1:A:16:ILE:CD1	1:A:28:ILE:HD11	0.69	2.15	12	23
1:A:39:PHE:CD2	1:A:78:PHE:CG	0.69	2.80	22	1
1:A:20:ASN:CG	1:A:20:ASN:O	0.68	2.31	1	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:PHE:CZ	1:A:78:PHE:CG	0.68	2.81	40	2
1:A:8:VAL:CG2	1:A:11:TYR:CD2	0.68	2.76	37	10
1:A:39:PHE:CD2	1:A:50:LEU:CD2	0.68	2.77	12	9
1:A:26:TRP:NE1	1:A:80:ILE:HD12	0.68	2.04	34	2
1:A:39:PHE:CD1	1:A:78:PHE:CZ	0.68	2.81	14	4
1:A:34:TYR:CD2	1:A:79:ILE:HG13	0.68	2.24	26	15
1:A:26:TRP:CZ3	1:A:80:ILE:CD1	0.68	2.77	41	4
1:A:34:TYR:CD2	1:A:79:ILE:CG1	0.68	2.76	30	25
1:A:39:PHE:CE1	1:A:78:PHE:CG	0.68	2.81	40	1
1:A:31:TYR:O	1:A:31:TYR:CD1	0.68	2.47	14	12
1:A:101:THR:O	1:A:102:ILE:HG22	0.68	1.89	14	2
1:A:38:LYS:CD	1:A:78:PHE:CD1	0.68	2.77	33	1
1:A:43:HIS:CE1	2:A:105:HEM:ND	0.67	2.62	16	17
1:A:34:TYR:CE2	1:A:79:ILE:HG13	0.67	2.25	39	40
1:A:71:ALA:HB2	2:A:105:HEM:O1A	0.67	1.90	30	8
1:A:25:THR:HG23	1:A:54:ALA:CB	0.67	2.19	16	2
1:A:50:LEU:O	1:A:53:GLN:CG	0.67	2.42	34	42
1:A:36:LEU:HD22	1:A:50:LEU:CD2	0.67	2.19	37	28
1:A:83:LEU:HD23	1:A:91:ILE:HD11	0.67	1.64	11	4
1:A:31:TYR:CD1	1:A:31:TYR:N	0.67	2.60	30	2
1:A:35:ASP:O	1:A:39:PHE:CD2	0.67	2.48	22	1
1:A:43:HIS:CE1	1:A:49:VAL:CG2	0.67	2.77	8	14
1:A:13:LEU:HD11	1:A:91:ILE:CG2	0.67	2.19	18	13
1:A:30:HIS:ND1	1:A:31:TYR:CE2	0.67	2.62	4	1
1:A:25:THR:HG21	1:A:40:LEU:HD21	0.67	1.64	22	5
2:A:105:HEM:C2A	2:A:105:HEM:O1A	0.67	2.48	23	6
1:A:39:PHE:CD2	1:A:50:LEU:HD21	0.67	2.25	12	11
1:A:26:TRP:CZ3	1:A:80:ILE:HD13	0.67	2.24	41	1
1:A:29:LEU:HD22	1:A:30:HIS:NE2	0.67	2.05	35	1
1:A:10:TYR:CB	1:A:84:HIS:CD2	0.67	2.78	39	26
1:A:26:TRP:HH2	1:A:80:ILE:HG21	0.67	1.49	39	3
1:A:26:TRP:CZ3	1:A:35:ASP:HB3	0.66	2.24	39	3
1:A:30:HIS:NE2	1:A:62:PHE:CZ	0.66	2.63	9	6
1:A:57:ASP:CB	1:A:91:ILE:HD12	0.66	2.20	32	7
1:A:26:TRP:CZ3	1:A:80:ILE:HD12	0.66	2.24	4	5
1:A:62:PHE:C	1:A:62:PHE:CD1	0.66	2.68	1	13
1:A:39:PHE:CG	1:A:78:PHE:CD2	0.66	2.83	22	1
1:A:24:SER:O	1:A:26:TRP:CD1	0.66	2.48	36	9
1:A:26:TRP:CE3	1:A:80:ILE:CD1	0.66	2.78	4	3
1:A:71:ALA:HB2	2:A:105:HEM:O2A	0.66	1.90	31	6
1:A:43:HIS:CE1	2:A:105:HEM:C4D	0.66	2.83	31	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LYS:CB	1:A:78:PHE:CE2	0.66	2.79	38	2
1:A:26:TRP:CZ2	1:A:35:ASP:OD2	0.66	2.48	20	8
1:A:49:VAL:CG2	2:A:105:HEM:CHD	0.66	2.74	34	9
1:A:13:LEU:HA	1:A:16:ILE:HD12	0.66	1.67	5	25
1:A:29:LEU:HD22	1:A:30:HIS:CE1	0.66	2.26	30	3
1:A:80:ILE:HD12	1:A:81:GLY:N	0.65	2.05	28	5
1:A:27:LEU:HG	1:A:36:LEU:HD11	0.65	1.68	42	13
1:A:26:TRP:CH2	1:A:35:ASP:CB	0.65	2.79	39	3
1:A:67:HIS:CE1	2:A:105:HEM:NC	0.65	2.64	38	10
1:A:31:TYR:CD1	1:A:31:TYR:O	0.65	2.50	38	8
1:A:28:ILE:HD13	1:A:33:VAL:HG12	0.65	1.66	22	5
1:A:69:THR:HG23	1:A:72:ARG:NH2	0.65	2.06	35	1
1:A:29:LEU:HD22	1:A:30:HIS:ND1	0.65	2.06	9	2
1:A:26:TRP:CD1	1:A:80:ILE:CD1	0.65	2.80	35	5
1:A:26:TRP:CZ3	1:A:35:ASP:CA	0.65	2.79	39	3
1:A:39:PHE:CZ	1:A:78:PHE:HB2	0.64	2.28	32	7
1:A:30:HIS:C	1:A:31:TYR:CG	0.64	2.68	30	3
1:A:33:VAL:CG1	1:A:80:ILE:HD11	0.64	2.22	28	2
1:A:39:PHE:CZ	2:A:105:HEM:CHB	0.64	2.81	35	2
1:A:34:TYR:CE2	1:A:75:SER:HB2	0.64	2.26	38	29
1:A:26:TRP:CD2	1:A:80:ILE:CD1	0.64	2.80	36	6
1:A:38:LYS:CG	1:A:78:PHE:CZ	0.64	2.81	38	1
1:A:27:LEU:HD13	1:A:27:LEU:C	0.64	2.13	34	19
1:A:84:HIS:CB	1:A:85:PRO:CD	0.64	2.75	35	42
1:A:8:VAL:HG11	1:A:26:TRP:CZ3	0.64	2.28	5	3
1:A:39:PHE:CD1	1:A:78:PHE:CE2	0.64	2.86	19	7
1:A:19:HIS:ND1	1:A:26:TRP:CE2	0.64	2.66	1	8
1:A:31:TYR:CD1	1:A:88:ARG:NH1	0.64	2.66	40	1
1:A:39:PHE:CZ	1:A:78:PHE:CB	0.64	2.81	24	5
1:A:84:HIS:CG	1:A:85:PRO:HD2	0.64	2.28	19	42
1:A:19:HIS:CE1	1:A:24:SER:OG	0.63	2.51	34	17
1:A:34:TYR:CD2	1:A:75:SER:OG	0.63	2.51	35	6
1:A:19:HIS:CE1	1:A:24:SER:HG	0.63	2.11	4	10
1:A:26:TRP:NE1	1:A:80:ILE:CD1	0.63	2.62	34	2
1:A:31:TYR:CE2	1:A:92:THR:OG1	0.63	2.52	13	5
2:A:105:HEM:O2A	2:A:105:HEM:C2A	0.63	2.52	21	5
1:A:26:TRP:CZ2	1:A:35:ASP:OD1	0.63	2.51	20	1
1:A:65:VAL:CG1	1:A:67:HIS:CE1	0.63	2.81	1	1
1:A:25:THR:CG2	1:A:54:ALA:HB2	0.63	2.24	16	8
2:A:105:HEM:O1A	2:A:105:HEM:C2A	0.63	2.52	17	8
1:A:61:ASN:O	1:A:65:VAL:HG12	0.63	1.94	15	27

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:VAL:HG11	1:A:80:ILE:CD1	0.63	2.24	39	3
1:A:19:HIS:CG	1:A:26:TRP:CD2	0.62	2.87	17	5
1:A:46:GLY:O	1:A:49:VAL:CG1	0.62	2.46	25	34
1:A:26:TRP:CH2	1:A:35:ASP:OD1	0.62	2.52	19	10
1:A:30:HIS:O	1:A:31:TYR:CB	0.62	2.47	41	10
1:A:88:ARG:O	1:A:92:THR:N	0.62	2.32	17	8
1:A:8:VAL:HG22	1:A:9:LYS:N	0.62	2.10	26	29
1:A:26:TRP:CH2	1:A:35:ASP:CG	0.62	2.72	21	9
1:A:16:ILE:HG21	1:A:28:ILE:CD1	0.62	2.24	30	7
1:A:62:PHE:CD2	1:A:67:HIS:ND1	0.62	2.67	10	13
1:A:11:TYR:CE1	1:A:15:GLU:CD	0.62	2.73	26	4
1:A:19:HIS:ND1	1:A:26:TRP:CD2	0.62	2.67	42	7
1:A:34:TYR:CD2	1:A:75:SER:CB	0.62	2.83	26	7
1:A:77:THR:OG1	1:A:78:PHE:CD1	0.62	2.53	40	2
1:A:32:LYS:HA	1:A:82:GLU:HA	0.62	1.71	42	30
1:A:25:THR:HG23	1:A:54:ALA:HB2	0.62	1.72	16	1
1:A:39:PHE:CE2	1:A:78:PHE:HB3	0.62	2.30	22	1
1:A:39:PHE:CE2	2:A:105:HEM:HMB3	0.62	2.30	10	11
1:A:33:VAL:HG12	1:A:80:ILE:CD1	0.61	2.25	8	4
1:A:19:HIS:CD2	1:A:24:SER:OG	0.61	2.53	12	1
1:A:26:TRP:CZ2	1:A:35:ASP:CG	0.61	2.74	20	9
1:A:77:THR:CG2	1:A:78:PHE:CD1	0.61	2.83	9	5
1:A:96:GLU:O	1:A:98:ILE:HG22	0.61	1.94	32	1
1:A:19:HIS:CG	1:A:26:TRP:CZ3	0.61	2.87	6	2
1:A:26:TRP:CE2	1:A:80:ILE:CD1	0.61	2.83	36	3
1:A:29:LEU:HB3	1:A:34:TYR:CE1	0.61	2.30	11	23
1:A:16:ILE:CD1	1:A:28:ILE:CD1	0.61	2.78	12	13
1:A:39:PHE:CZ	1:A:78:PHE:HA	0.61	2.30	22	1
1:A:13:LEU:HD21	1:A:91:ILE:CD1	0.61	2.26	24	3
1:A:34:TYR:CD1	1:A:34:TYR:N	0.61	2.69	41	29
1:A:53:GLN:OE1	1:A:58:ALA:CB	0.61	2.48	5	21
1:A:27:LEU:HD13	1:A:27:LEU:O	0.61	1.94	34	14
1:A:39:PHE:CZ	2:A:105:HEM:HMB3	0.61	2.30	31	2
1:A:40:LEU:HD22	1:A:47:GLU:CB	0.61	2.26	10	6
1:A:30:HIS:O	1:A:31:TYR:CD2	0.61	2.54	3	1
1:A:33:VAL:O	1:A:80:ILE:HD12	0.61	1.96	23	4
1:A:26:TRP:CE3	1:A:35:ASP:HA	0.61	2.31	41	3
1:A:27:LEU:O	1:A:27:LEU:HD13	0.61	1.96	17	19
1:A:74:LEU:O	1:A:77:THR:CG2	0.61	2.47	38	20
1:A:38:LYS:HG3	1:A:78:PHE:CE2	0.61	2.31	35	1
1:A:13:LEU:HD23	1:A:28:ILE:CD1	0.60	2.26	36	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:TYR:CE1	1:A:15:GLU:OE2	0.60	2.54	33	1
1:A:20:ASN:O	1:A:20:ASN:ND2	0.60	2.33	39	11
1:A:26:TRP:CZ3	1:A:80:ILE:HG12	0.60	2.31	37	3
1:A:58:ALA:HB1	2:A:105:HEM:HMC3	0.60	1.72	16	8
1:A:10:TYR:HB3	1:A:84:HIS:CD2	0.60	2.32	39	27
1:A:8:VAL:HG21	1:A:11:TYR:CD1	0.60	2.31	38	1
1:A:36:LEU:HD13	1:A:50:LEU:CA	0.60	2.26	39	37
1:A:31:TYR:CG	1:A:31:TYR:O	0.60	2.55	38	3
1:A:40:LEU:HD23	1:A:50:LEU:HB2	0.60	1.72	22	1
1:A:26:TRP:CH2	1:A:35:ASP:OD2	0.60	2.55	2	9
1:A:29:LEU:CD1	2:A:105:HEM:CAB	0.60	2.80	26	39
1:A:38:LYS:O	1:A:78:PHE:CE2	0.60	2.55	28	2
1:A:77:THR:HG23	1:A:78:PHE:CD1	0.60	2.32	25	5
1:A:11:TYR:CD2	1:A:15:GLU:OE1	0.60	2.55	14	2
1:A:39:PHE:CB	1:A:50:LEU:HD22	0.60	2.27	40	4
1:A:38:LYS:HB2	1:A:78:PHE:CE2	0.60	2.31	38	7
2:A:105:HEM:C2A	2:A:105:HEM:O2A	0.60	2.54	25	2
1:A:39:PHE:CE1	1:A:74:LEU:CD1	0.59	2.83	4	5
1:A:13:LEU:HD23	1:A:28:ILE:HD11	0.59	1.74	37	3
1:A:39:PHE:CD1	1:A:39:PHE:N	0.59	2.68	38	4
1:A:38:LYS:HG2	1:A:78:PHE:CE1	0.59	2.33	38	2
1:A:13:LEU:CD2	1:A:83:LEU:HD21	0.59	2.27	14	5
1:A:39:PHE:HB2	1:A:78:PHE:CE2	0.59	2.33	7	15
1:A:39:PHE:CE2	1:A:74:LEU:CD1	0.59	2.83	15	2
1:A:39:PHE:CE2	2:A:105:HEM:HMB2	0.59	2.31	1	5
1:A:33:VAL:HG23	1:A:82:GLU:CA	0.59	2.27	26	3
1:A:30:HIS:CD2	1:A:62:PHE:CZ	0.59	2.91	36	3
1:A:62:PHE:CD1	1:A:62:PHE:C	0.59	2.75	22	13
1:A:12:THR:O	1:A:16:ILE:HD12	0.59	1.98	36	5
1:A:48:GLU:O	1:A:52:GLU:N	0.59	2.36	35	30
1:A:39:PHE:CD1	1:A:78:PHE:CD1	0.59	2.90	22	1
1:A:49:VAL:HG13	1:A:50:LEU:HG	0.59	1.74	24	11
1:A:36:LEU:CD1	1:A:50:LEU:O	0.59	2.51	40	29
1:A:74:LEU:HD12	1:A:78:PHE:CE1	0.59	2.33	9	5
1:A:34:TYR:CD2	1:A:75:SER:HB2	0.58	2.33	33	17
1:A:20:ASN:ND2	1:A:55:GLY:CA	0.58	2.66	16	1
1:A:11:TYR:CD2	1:A:26:TRP:CZ3	0.58	2.91	11	5
1:A:25:THR:CG2	1:A:54:ALA:CB	0.58	2.81	41	14
1:A:11:TYR:CE2	1:A:15:GLU:CG	0.58	2.85	41	5
1:A:16:ILE:O	1:A:55:GLY:HA2	0.58	1.98	36	29
1:A:29:LEU:HB2	1:A:34:TYR:CE1	0.58	2.32	22	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LYS:NZ	1:A:74:LEU:CD1	0.58	2.66	35	1
1:A:11:TYR:CD1	1:A:15:GLU:CB	0.58	2.85	13	4
1:A:77:THR:OG1	1:A:78:PHE:CE1	0.58	2.57	40	1
1:A:26:TRP:CE3	1:A:80:ILE:HD12	0.58	2.33	32	4
1:A:43:HIS:CE1	1:A:50:LEU:HD21	0.58	2.33	5	2
1:A:38:LYS:HD3	1:A:78:PHE:CZ	0.58	2.33	38	1
1:A:74:LEU:CD1	1:A:78:PHE:CE2	0.58	2.86	14	8
1:A:34:TYR:CD2	1:A:75:SER:HB3	0.58	2.34	26	3
1:A:34:TYR:N	1:A:34:TYR:CD1	0.58	2.71	13	12
1:A:67:HIS:CE1	2:A:105:HEM:C1C	0.58	2.92	31	28
1:A:65:VAL:O	1:A:65:VAL:CG2	0.58	2.52	18	16
1:A:28:ILE:HB	1:A:57:ASP:HA	0.57	1.74	36	19
1:A:43:HIS:NE2	2:A:105:HEM:NA	0.57	2.52	30	6
1:A:88:ARG:O	1:A:92:THR:HG22	0.57	1.99	35	5
1:A:77:THR:HG22	1:A:78:PHE:CE1	0.57	2.34	9	2
1:A:91:ILE:O	1:A:92:THR:C	0.57	2.43	19	39
1:A:38:LYS:HB2	1:A:78:PHE:CZ	0.57	2.35	42	5
1:A:36:LEU:O	1:A:40:LEU:N	0.57	2.38	42	17
1:A:27:LEU:HD22	1:A:28:ILE:O	0.57	2.00	24	10
1:A:61:ASN:O	1:A:65:VAL:HG13	0.57	2.00	12	7
1:A:36:LEU:HA	1:A:39:PHE:CD1	0.57	2.35	28	6
1:A:48:GLU:O	1:A:51:ARG:N	0.57	2.38	8	18
1:A:19:HIS:NE2	1:A:26:TRP:CZ3	0.57	2.71	16	1
1:A:65:VAL:CG2	1:A:65:VAL:O	0.57	2.52	17	16
1:A:43:HIS:CD2	2:A:105:HEM:C4A	0.57	2.93	20	3
1:A:26:TRP:CE2	1:A:35:ASP:OD1	0.57	2.58	20	2
1:A:27:LEU:C	1:A:27:LEU:HD13	0.57	2.20	20	19
1:A:53:GLN:NE2	2:A:105:HEM:C2C	0.57	2.72	37	36
1:A:31:TYR:O	1:A:31:TYR:CG	0.57	2.58	20	1
1:A:34:TYR:CD2	1:A:79:ILE:HG12	0.57	2.35	30	22
1:A:36:LEU:CD1	1:A:50:LEU:HB3	0.57	2.21	42	21
1:A:28:ILE:CD1	1:A:33:VAL:HG12	0.57	2.30	11	1
1:A:38:LYS:O	1:A:39:PHE:CD1	0.56	2.58	22	1
1:A:53:GLN:NE2	2:A:105:HEM:HMC3	0.56	2.15	5	9
1:A:39:PHE:CE1	1:A:78:PHE:HB3	0.56	2.35	24	4
1:A:13:LEU:HD11	1:A:91:ILE:HG22	0.56	1.77	18	1
1:A:38:LYS:HB2	1:A:78:PHE:CE1	0.56	2.36	26	3
1:A:20:ASN:N	1:A:20:ASN:HD22	0.56	1.98	34	1
1:A:19:HIS:ND1	1:A:24:SER:CB	0.56	2.69	1	7
1:A:34:TYR:CE2	1:A:75:SER:HB3	0.56	2.35	35	6
1:A:11:TYR:CD1	1:A:15:GLU:HB3	0.56	2.35	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LYS:HG3	1:A:78:PHE:CE1	0.56	2.35	30	3
1:A:84:HIS:CD2	1:A:85:PRO:HD3	0.56	2.35	39	27
1:A:19:HIS:CG	1:A:26:TRP:CD1	0.56	2.94	12	1
1:A:38:LYS:CG	1:A:78:PHE:CD2	0.56	2.88	35	1
1:A:43:HIS:CE1	1:A:49:VAL:CG1	0.56	2.85	12	6
1:A:38:LYS:HG2	1:A:78:PHE:CZ	0.56	2.35	38	1
1:A:99:ILE:C	1:A:99:ILE:HD13	0.56	2.21	38	1
1:A:38:LYS:HG2	1:A:78:PHE:CD1	0.56	2.35	42	1
1:A:39:PHE:HB3	1:A:50:LEU:HD22	0.56	1.77	40	4
1:A:43:HIS:NE2	2:A:105:HEM:ND	0.56	2.53	38	2
1:A:39:PHE:HB3	1:A:78:PHE:CE2	0.56	2.35	22	1
1:A:38:LYS:CB	1:A:78:PHE:CD1	0.56	2.89	26	1
1:A:38:LYS:HG3	1:A:78:PHE:CD1	0.56	2.36	26	1
1:A:19:HIS:CD2	1:A:24:SER:HB3	0.56	2.36	12	1
1:A:30:HIS:CG	1:A:31:TYR:CZ	0.56	2.93	4	1
1:A:39:PHE:CE2	1:A:78:PHE:CA	0.56	2.89	22	1
1:A:16:ILE:HG23	1:A:26:TRP:CB	0.56	2.31	7	2
1:A:88:ARG:C	1:A:90:LYS:H	0.55	2.04	8	7
1:A:65:VAL:CG2	1:A:67:HIS:CE1	0.55	2.88	2	8
1:A:77:THR:CG2	1:A:78:PHE:CE1	0.55	2.89	9	4
1:A:84:HIS:CB	1:A:85:PRO:HD2	0.55	2.31	35	42
1:A:99:ILE:HD13	1:A:100:THR:N	0.55	2.16	10	3
1:A:53:GLN:HB2	1:A:58:ALA:HB2	0.55	1.76	42	4
1:A:65:VAL:HG23	1:A:65:VAL:O	0.55	2.01	30	7
1:A:38:LYS:HD3	1:A:78:PHE:CD1	0.55	2.36	33	1
1:A:43:HIS:CG	1:A:49:VAL:CG1	0.55	2.86	22	9
1:A:26:TRP:CZ3	1:A:35:ASP:N	0.55	2.74	37	3
1:A:39:PHE:CE1	1:A:78:PHE:HB2	0.55	2.37	40	4
1:A:31:TYR:CE2	1:A:32:LYS:HD3	0.55	2.37	35	4
1:A:29:LEU:CD1	2:A:105:HEM:CBB	0.55	2.84	32	26
1:A:11:TYR:CE2	1:A:15:GLU:HG3	0.55	2.36	38	5
1:A:39:PHE:CE2	1:A:78:PHE:HA	0.55	2.37	22	1
1:A:57:ASP:OD2	1:A:59:THR:CG2	0.55	2.54	36	6
1:A:39:PHE:CE2	1:A:74:LEU:CD2	0.55	2.87	10	2
1:A:39:PHE:HE2	1:A:74:LEU:HD21	0.55	1.58	35	3
1:A:10:TYR:HB2	1:A:84:HIS:CD2	0.55	2.37	39	12
1:A:59:THR:CG2	1:A:60:GLU:N	0.55	2.69	4	22
1:A:84:HIS:CG	1:A:85:PRO:HD3	0.55	2.36	35	33
1:A:40:LEU:HD23	1:A:47:GLU:OE2	0.55	2.02	40	1
1:A:38:LYS:HB2	1:A:78:PHE:CD1	0.55	2.36	26	1
1:A:33:VAL:HG12	1:A:82:GLU:N	0.55	2.16	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:ILE:HD13	1:A:99:ILE:C	0.55	2.21	10	1
1:A:102:ILE:HD12	1:A:103:ASP:N	0.55	2.17	12	1
1:A:30:HIS:ND1	1:A:30:HIS:N	0.55	2.54	30	1
1:A:59:THR:HG22	1:A:60:GLU:N	0.54	2.17	38	10
1:A:39:PHE:O	1:A:50:LEU:CD1	0.54	2.56	42	7
1:A:34:TYR:CZ	1:A:79:ILE:HD11	0.54	2.37	8	13
1:A:28:ILE:CG2	1:A:91:ILE:CD1	0.54	2.85	16	4
1:A:28:ILE:HD13	1:A:83:LEU:HD22	0.54	1.78	34	5
1:A:25:THR:HG22	1:A:54:ALA:HB3	0.54	1.79	5	1
1:A:61:ASN:HB3	2:A:105:HEM:HMC3	0.54	1.77	9	1
1:A:34:TYR:CE2	1:A:79:ILE:HG12	0.54	2.36	20	16
1:A:28:ILE:HA	1:A:32:LYS:O	0.54	2.01	30	14
1:A:20:ASN:ND2	1:A:20:ASN:O	0.54	2.41	14	17
1:A:26:TRP:CE2	1:A:80:ILE:HD13	0.54	2.38	36	2
1:A:30:HIS:C	1:A:31:TYR:CD2	0.54	2.80	3	1
1:A:42:GLU:O	1:A:43:HIS:CB	0.54	2.54	8	24
1:A:32:LYS:HG3	1:A:79:ILE:HD11	0.54	1.79	12	6
1:A:39:PHE:C	1:A:50:LEU:HD13	0.54	2.21	38	2
1:A:101:THR:HG23	1:A:101:THR:O	0.54	2.02	10	3
1:A:83:LEU:HD12	1:A:83:LEU:C	0.54	2.22	25	7
1:A:65:VAL:O	1:A:65:VAL:HG23	0.54	2.02	16	5
1:A:38:LYS:HB3	1:A:78:PHE:CD2	0.54	2.38	40	1
1:A:26:TRP:CH2	1:A:35:ASP:HB2	0.54	2.38	39	1
1:A:31:TYR:CZ	1:A:92:THR:OG1	0.54	2.60	16	5
1:A:38:LYS:CB	1:A:78:PHE:CD2	0.54	2.91	35	1
1:A:101:THR:O	1:A:102:ILE:C	0.54	2.45	36	1
1:A:11:TYR:CE1	1:A:15:GLU:HG2	0.54	2.38	30	7
1:A:38:LYS:CG	1:A:78:PHE:CD1	0.54	2.90	26	3
1:A:40:LEU:O	1:A:47:GLU:CG	0.54	2.56	26	7
1:A:73:GLU:O	1:A:76:LYS:CG	0.54	2.56	6	9
1:A:84:HIS:O	1:A:88:ARG:HB3	0.54	2.03	26	12
1:A:88:ARG:O	1:A:92:THR:CG2	0.54	2.56	35	5
1:A:28:ILE:HG23	1:A:32:LYS:O	0.54	2.03	9	6
1:A:84:HIS:O	1:A:88:ARG:CD	0.53	2.56	38	4
1:A:33:VAL:HG22	1:A:82:GLU:N	0.53	2.18	23	8
1:A:41:GLU:O	1:A:43:HIS:N	0.53	2.41	9	2
1:A:88:ARG:O	1:A:92:THR:CB	0.53	2.57	4	6
1:A:26:TRP:CE3	1:A:35:ASP:CA	0.53	2.91	41	2
1:A:48:GLU:O	1:A:50:LEU:N	0.53	2.41	9	38
1:A:28:ILE:CG2	1:A:32:LYS:O	0.53	2.56	20	13
1:A:40:LEU:HD23	1:A:47:GLU:HG2	0.53	1.79	31	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:PHE:HA	1:A:65:VAL:HG13	0.53	1.80	26	14
1:A:32:LYS:CG	1:A:34:TYR:OH	0.53	2.57	11	2
1:A:83:LEU:C	1:A:83:LEU:HD12	0.53	2.24	18	11
1:A:74:LEU:HD12	1:A:78:PHE:HE1	0.53	1.64	40	2
1:A:39:PHE:CE1	1:A:42:GLU:CB	0.53	2.92	6	1
1:A:38:LYS:HG3	1:A:78:PHE:CD2	0.53	2.38	35	1
2:A:105:HEM:C3A	2:A:105:HEM:O1A	0.53	2.62	36	4
1:A:39:PHE:CE2	1:A:75:SER:HA	0.53	2.39	30	5
1:A:27:LEU:HD22	1:A:28:ILE:C	0.53	2.24	22	35
1:A:39:PHE:CE1	1:A:42:GLU:HB2	0.53	2.38	6	2
1:A:39:PHE:HB2	1:A:78:PHE:CD2	0.53	2.38	6	14
1:A:53:GLN:NE2	2:A:105:HEM:C1C	0.53	2.77	23	12
1:A:20:ASN:OD1	1:A:54:ALA:O	0.53	2.26	34	6
1:A:30:HIS:O	1:A:31:TYR:CG	0.53	2.61	30	1
1:A:62:PHE:HA	1:A:65:VAL:CG1	0.53	2.34	20	24
1:A:59:THR:O	1:A:61:ASN:N	0.53	2.42	27	8
1:A:26:TRP:CD1	1:A:80:ILE:HD13	0.53	2.38	24	2
1:A:38:LYS:HB3	1:A:78:PHE:CD1	0.53	2.39	10	13
1:A:31:TYR:CD2	1:A:32:LYS:HG3	0.53	2.39	9	7
1:A:89:SER:HA	1:A:92:THR:CG2	0.53	2.34	24	15
1:A:43:HIS:HE1	1:A:49:VAL:HG21	0.53	1.64	19	7
1:A:39:PHE:O	1:A:42:GLU:N	0.53	2.41	20	8
1:A:11:TYR:CD1	1:A:15:GLU:HG3	0.53	2.39	31	1
1:A:10:TYR:CB	1:A:84:HIS:ND1	0.52	2.72	38	6
1:A:11:TYR:CD1	1:A:15:GLU:HG2	0.52	2.39	33	9
1:A:50:LEU:O	1:A:53:GLN:HG3	0.52	2.03	32	36
2:A:105:HEM:O2A	2:A:105:HEM:C3A	0.52	2.61	21	4
1:A:35:ASP:OD2	1:A:78:PHE:O	0.52	2.27	37	4
1:A:26:TRP:CH2	1:A:80:ILE:CG2	0.52	2.92	41	1
1:A:67:HIS:CE1	2:A:105:HEM:C1A	0.52	2.97	13	5
1:A:32:LYS:HG3	1:A:34:TYR:CZ	0.52	2.39	12	5
1:A:26:TRP:CZ2	1:A:80:ILE:CD1	0.52	2.93	40	2
1:A:39:PHE:CE1	1:A:78:PHE:CD2	0.52	2.97	40	1
1:A:29:LEU:HD11	2:A:105:HEM:CAB	0.52	2.34	26	3
1:A:19:HIS:ND1	1:A:26:TRP:CH2	0.52	2.75	6	1
1:A:50:LEU:HA	1:A:53:GLN:HG2	0.52	1.81	35	24
1:A:19:HIS:HB3	1:A:26:TRP:CD1	0.52	2.40	7	2
1:A:36:LEU:HD12	1:A:50:LEU:O	0.52	2.04	40	19
1:A:29:LEU:CD1	2:A:105:HEM:HAB	0.52	2.35	39	10
2:A:105:HEM:O1A	2:A:105:HEM:C3A	0.52	2.63	3	3
1:A:25:THR:O	1:A:36:LEU:N	0.52	2.42	24	23

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:TYR:CG	1:A:15:GLU:OE1	0.52	2.62	14	1
1:A:38:LYS:CB	1:A:78:PHE:CG	0.52	2.92	26	1
1:A:88:ARG:O	1:A:92:THR:HB	0.52	2.05	26	17
1:A:11:TYR:CE1	1:A:15:GLU:HG3	0.52	2.40	14	2
1:A:38:LYS:HB3	1:A:78:PHE:CE1	0.52	2.40	29	10
1:A:78:PHE:N	1:A:78:PHE:CD1	0.52	2.78	40	1
1:A:20:ASN:ND2	1:A:51:ARG:O	0.52	2.43	15	11
1:A:31:TYR:CE2	1:A:32:LYS:HD2	0.52	2.40	36	3
2:A:105:HEM:C3A	2:A:105:HEM:O2A	0.52	2.63	4	1
1:A:8:VAL:HB	1:A:11:TYR:CE2	0.52	2.40	18	2
1:A:16:ILE:HG21	1:A:28:ILE:HD11	0.51	1.81	3	5
1:A:29:LEU:CD2	1:A:62:PHE:CD1	0.51	2.94	14	2
1:A:61:ASN:CG	2:A:105:HEM:CBC	0.51	2.79	37	1
1:A:27:LEU:CD2	1:A:58:ALA:HB3	0.51	2.29	14	11
1:A:39:PHE:CZ	2:A:105:HEM:CMB	0.51	2.93	20	2
1:A:43:HIS:CB	1:A:50:LEU:HD11	0.51	2.34	7	1
1:A:29:LEU:C	1:A:30:HIS:CG	0.51	2.84	26	3
1:A:38:LYS:HB2	1:A:78:PHE:CG	0.51	2.41	26	1
1:A:78:PHE:O	1:A:80:ILE:HG23	0.51	2.05	14	2
1:A:39:PHE:CE1	1:A:42:GLU:HB3	0.51	2.41	8	11
1:A:49:VAL:HG22	2:A:105:HEM:C4C	0.51	2.40	18	5
1:A:11:TYR:CE2	1:A:15:GLU:HG2	0.51	2.41	11	6
1:A:19:HIS:CG	1:A:24:SER:HB2	0.51	2.41	28	6
1:A:29:LEU:HD11	1:A:62:PHE:CD2	0.51	2.40	1	2
1:A:43:HIS:HD1	1:A:50:LEU:HD21	0.51	1.65	14	4
1:A:48:GLU:O	1:A:52:GLU:CG	0.51	2.59	41	2
1:A:10:TYR:HB2	1:A:84:HIS:CE1	0.51	2.40	33	4
1:A:26:TRP:CD1	1:A:35:ASP:OD1	0.51	2.64	33	3
1:A:53:GLN:CD	2:A:105:HEM:HMC3	0.51	2.26	37	14
1:A:41:GLU:O	1:A:42:GLU:C	0.51	2.49	29	2
1:A:77:THR:HG22	1:A:78:PHE:HD1	0.51	1.66	18	2
1:A:17:GLN:O	1:A:20:ASN:ND2	0.51	2.43	23	4
1:A:8:VAL:HG11	1:A:80:ILE:HD13	0.51	1.81	20	1
1:A:11:TYR:CZ	1:A:15:GLU:OE2	0.51	2.64	14	1
1:A:27:LEU:C	1:A:27:LEU:HD22	0.51	2.25	7	4
1:A:31:TYR:CE1	1:A:88:ARG:NE	0.51	2.79	24	3
1:A:19:HIS:CE1	1:A:24:SER:HB3	0.51	2.41	17	3
1:A:34:TYR:CE2	1:A:79:ILE:HD11	0.51	2.41	42	6
1:A:92:THR:CG2	1:A:93:LYS:N	0.51	2.74	18	13
1:A:27:LEU:HD11	1:A:34:TYR:HB2	0.51	1.81	15	15
1:A:19:HIS:HB3	1:A:24:SER:O	0.51	2.06	21	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:THR:HG21	1:A:40:LEU:CD1	0.51	2.37	16	1
1:A:39:PHE:HE1	1:A:74:LEU:HD11	0.51	1.64	18	1
1:A:26:TRP:CD2	1:A:80:ILE:HD12	0.50	2.41	11	2
1:A:34:TYR:CE2	1:A:75:SER:CB	0.50	2.94	19	2
1:A:65:VAL:HG22	1:A:67:HIS:CE1	0.50	2.42	16	4
1:A:61:ASN:HB3	2:A:105:HEM:HMC2	0.50	1.83	37	3
1:A:39:PHE:CG	1:A:78:PHE:CG	0.50	2.99	22	1
1:A:21:ASN:O	1:A:25:THR:N	0.50	2.44	18	7
1:A:31:TYR:CD1	1:A:31:TYR:C	0.50	2.85	12	7
1:A:29:LEU:CD2	1:A:59:THR:OG1	0.50	2.60	13	5
1:A:65:VAL:HG22	1:A:67:HIS:ND1	0.50	2.20	16	8
1:A:35:ASP:C	1:A:35:ASP:OD1	0.50	2.49	40	4
1:A:39:PHE:HZ	1:A:74:LEU:HD21	0.50	1.60	10	1
1:A:29:LEU:HD13	1:A:30:HIS:CE1	0.50	2.42	30	3
1:A:98:ILE:HD13	1:A:98:ILE:H	0.50	1.66	1	2
1:A:39:PHE:CE2	2:A:105:HEM:CMB	0.50	2.94	10	7
1:A:30:HIS:HB2	1:A:31:TYR:CD1	0.50	2.42	35	3
1:A:19:HIS:NE2	1:A:26:TRP:CH2	0.50	2.80	17	1
1:A:59:THR:O	1:A:60:GLU:C	0.50	2.50	35	5
1:A:39:PHE:O	1:A:40:LEU:C	0.50	2.48	10	2
1:A:30:HIS:HB3	1:A:31:TYR:CE1	0.50	2.42	4	1
1:A:21:ASN:C	1:A:25:THR:HG23	0.50	2.26	32	2
1:A:29:LEU:HD11	2:A:105:HEM:HAB	0.50	1.84	36	2
1:A:88:ARG:CG	1:A:89:SER:N	0.50	2.74	42	11
1:A:101:THR:O	1:A:102:ILE:CG2	0.50	2.60	14	2
1:A:63:GLU:OE2	1:A:93:LYS:CG	0.50	2.60	41	1
1:A:53:GLN:CD	2:A:105:HEM:HMC2	0.50	2.27	9	6
1:A:75:SER:HA	1:A:78:PHE:CD2	0.50	2.42	7	3
1:A:74:LEU:O	1:A:77:THR:CB	0.50	2.60	42	5
1:A:39:PHE:CZ	2:A:105:HEM:HHB	0.50	2.41	33	3
1:A:39:PHE:CG	1:A:78:PHE:CZ	0.49	2.98	14	2
1:A:102:ILE:CG1	1:A:103:ASP:N	0.49	2.74	36	1
1:A:8:VAL:CG1	1:A:80:ILE:HD12	0.49	2.35	39	1
1:A:11:TYR:CD2	1:A:15:GLU:HG2	0.49	2.41	17	2
1:A:13:LEU:CA	1:A:16:ILE:HD12	0.49	2.37	2	9
1:A:57:ASP:OD1	1:A:57:ASP:C	0.49	2.50	28	8
1:A:85:PRO:HA	1:A:88:ARG:CG	0.49	2.38	39	15
1:A:29:LEU:HD23	1:A:59:THR:OG1	0.49	2.07	11	8
1:A:39:PHE:CB	1:A:78:PHE:CE2	0.49	2.94	7	6
1:A:39:PHE:HB2	1:A:78:PHE:CZ	0.49	2.42	39	3
1:A:26:TRP:CZ3	1:A:80:ILE:CG1	0.49	2.94	41	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:HIS:HD1	1:A:49:VAL:HG11	0.49	1.67	3	7
1:A:20:ASN:N	1:A:20:ASN:ND2	0.49	2.61	34	1
1:A:11:TYR:CE1	1:A:15:GLU:OE1	0.49	2.65	30	2
1:A:74:LEU:CD1	1:A:78:PHE:CE1	0.49	2.95	20	5
1:A:39:PHE:CZ	1:A:74:LEU:HD11	0.49	2.41	5	4
1:A:25:THR:HG22	1:A:54:ALA:HB1	0.49	1.81	5	1
1:A:65:VAL:O	1:A:66:GLY:C	0.49	2.51	4	27
1:A:8:VAL:HG21	1:A:11:TYR:CG	0.49	2.43	38	4
1:A:87:ASP:O	1:A:91:ILE:HG23	0.49	2.07	20	1
1:A:48:GLU:C	1:A:50:LEU:N	0.49	2.64	2	40
1:A:88:ARG:C	1:A:90:LYS:N	0.49	2.63	24	9
1:A:27:LEU:CD1	1:A:34:TYR:HB2	0.49	2.38	31	18
1:A:61:ASN:O	1:A:65:VAL:CG1	0.49	2.61	11	12
1:A:21:ASN:O	1:A:25:THR:OG1	0.49	2.30	36	5
1:A:61:ASN:ND2	2:A:105:HEM:CAC	0.49	2.75	9	1
1:A:36:LEU:O	1:A:38:LYS:N	0.49	2.45	30	5
1:A:39:PHE:CE2	2:A:105:HEM:CHB	0.49	2.96	16	4
1:A:35:ASP:OD1	1:A:38:LYS:N	0.49	2.45	39	1
1:A:8:VAL:HG11	1:A:80:ILE:CG1	0.49	2.38	37	2
1:A:26:TRP:CH2	1:A:80:ILE:HD12	0.49	2.43	3	2
1:A:46:GLY:O	1:A:49:VAL:N	0.49	2.45	17	11
1:A:33:VAL:CG2	1:A:81:GLY:C	0.49	2.80	38	3
1:A:28:ILE:HD12	1:A:33:VAL:HG22	0.49	1.84	14	2
1:A:20:ASN:OD1	1:A:55:GLY:HA3	0.49	2.08	34	1
1:A:38:LYS:HB2	1:A:78:PHE:CD2	0.49	2.43	26	3
1:A:10:TYR:HB3	1:A:84:HIS:CE1	0.49	2.42	38	2
1:A:20:ASN:HD22	1:A:54:ALA:HB3	0.49	1.67	25	8
1:A:31:TYR:CE1	1:A:88:ARG:HG2	0.49	2.43	13	1
1:A:11:TYR:CZ	1:A:15:GLU:CD	0.48	2.86	14	1
1:A:42:GLU:O	1:A:43:HIS:HB2	0.48	2.08	9	6
1:A:11:TYR:CD2	1:A:15:GLU:HB3	0.48	2.43	36	4
1:A:57:ASP:OD1	1:A:59:THR:N	0.48	2.47	33	7
1:A:84:HIS:HB3	1:A:85:PRO:HD2	0.48	1.83	8	23
1:A:99:ILE:CD1	1:A:99:ILE:C	0.48	2.82	10	1
1:A:11:TYR:CE1	1:A:15:GLU:HB3	0.48	2.44	13	2
1:A:16:ILE:HG12	1:A:33:VAL:HG11	0.48	1.84	24	1
1:A:19:HIS:CA	1:A:24:SER:O	0.48	2.61	21	3
1:A:62:PHE:CD2	1:A:67:HIS:HB2	0.48	2.42	30	3
1:A:21:ASN:C	1:A:23:LYS:H	0.48	2.12	42	2
1:A:22:SER:HA	1:A:40:LEU:HD11	0.48	1.85	42	1
1:A:20:ASN:OD1	1:A:55:GLY:CA	0.48	2.61	34	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:PHE:N	1:A:39:PHE:CD1	0.48	2.79	30	2
1:A:63:GLU:OE1	1:A:93:LYS:CE	0.48	2.61	25	1
1:A:62:PHE:CE2	1:A:67:HIS:HB2	0.48	2.43	16	6
1:A:29:LEU:O	1:A:31:TYR:N	0.48	2.43	36	15
1:A:74:LEU:HD11	1:A:78:PHE:HE2	0.48	1.67	19	1
1:A:39:PHE:CD1	1:A:78:PHE:CD2	0.48	3.01	40	1
1:A:19:HIS:C	1:A:24:SER:O	0.48	2.52	22	20
1:A:48:GLU:O	1:A:49:VAL:C	0.48	2.51	8	26
1:A:11:TYR:CE2	1:A:15:GLU:OE2	0.48	2.66	31	2
1:A:83:LEU:HG	1:A:87:ASP:O	0.48	2.08	28	18
1:A:29:LEU:HB2	1:A:34:TYR:CD1	0.48	2.43	8	3
1:A:19:HIS:CB	1:A:26:TRP:HB2	0.48	2.39	23	8
1:A:15:GLU:O	1:A:18:LYS:HG2	0.48	2.09	16	1
1:A:38:LYS:CG	1:A:78:PHE:CE2	0.48	2.96	38	1
1:A:29:LEU:CD2	1:A:59:THR:HA	0.48	2.38	30	7
1:A:27:LEU:CD2	1:A:28:ILE:O	0.48	2.62	16	4
1:A:20:ASN:ND2	1:A:55:GLY:HA3	0.48	2.24	32	2
1:A:9:LYS:HB3	1:A:10:TYR:CE1	0.48	2.43	23	1
1:A:9:LYS:O	1:A:82:GLU:N	0.48	2.46	33	25
1:A:39:PHE:CE2	2:A:105:HEM:HMB1	0.48	2.43	3	4
1:A:28:ILE:CD1	1:A:83:LEU:CD2	0.48	2.85	21	4
1:A:71:ALA:CB	2:A:105:HEM:HMA2	0.48	2.39	33	11
1:A:38:LYS:CG	1:A:78:PHE:CE1	0.48	2.97	33	2
1:A:33:VAL:C	1:A:34:TYR:CD1	0.48	2.87	20	1
1:A:11:TYR:CD2	1:A:15:GLU:CD	0.48	2.87	31	1
1:A:8:VAL:HB	1:A:11:TYR:CE1	0.48	2.44	10	4
1:A:41:GLU:O	1:A:42:GLU:O	0.48	2.32	13	9
1:A:83:LEU:HD12	1:A:84:HIS:O	0.48	2.09	42	9
1:A:84:HIS:O	1:A:88:ARG:HG2	0.48	2.09	40	14
1:A:91:ILE:O	1:A:93:LYS:O	0.48	2.31	7	1
1:A:19:HIS:CD2	1:A:26:TRP:CD2	0.48	3.02	32	1
1:A:33:VAL:HG23	1:A:82:GLU:C	0.48	2.29	3	2
1:A:30:HIS:C	1:A:31:TYR:CD1	0.48	2.87	30	1
1:A:39:PHE:CZ	1:A:78:PHE:HB3	0.48	2.43	24	1
1:A:19:HIS:CB	1:A:26:TRP:CG	0.48	2.97	12	1
1:A:59:THR:CG2	1:A:94:PRO:HA	0.47	2.39	24	1
1:A:101:THR:O	1:A:102:ILE:CG1	0.47	2.62	35	1
1:A:53:GLN:NE2	2:A:105:HEM:HMC2	0.47	2.23	35	4
1:A:83:LEU:CD2	1:A:87:ASP:O	0.47	2.62	33	3
1:A:91:ILE:O	1:A:93:LYS:N	0.47	2.46	30	10
1:A:8:VAL:CG2	1:A:9:LYS:N	0.47	2.76	26	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:TYR:CZ	1:A:92:THR:CB	0.47	2.97	13	4
1:A:19:HIS:CB	1:A:26:TRP:CD1	0.47	2.97	7	2
1:A:65:VAL:HG21	2:A:105:HEM:C1D	0.47	2.44	1	3
1:A:32:LYS:HB2	1:A:34:TYR:CE1	0.47	2.45	30	2
1:A:74:LEU:HD12	1:A:78:PHE:CZ	0.47	2.44	39	2
1:A:39:PHE:CE2	1:A:75:SER:OG	0.47	2.68	28	1
1:A:71:ALA:O	1:A:75:SER:OG	0.47	2.33	31	7
1:A:13:LEU:HD12	1:A:87:ASP:OD2	0.47	2.10	12	1
1:A:8:VAL:CG2	1:A:11:TYR:CG	0.47	2.98	17	1
1:A:26:TRP:NE1	1:A:35:ASP:OD1	0.47	2.47	1	8
1:A:38:LYS:HB3	1:A:78:PHE:CE2	0.47	2.44	40	3
1:A:100:THR:OG1	1:A:102:ILE:CD1	0.47	2.62	10	1
1:A:10:TYR:CD1	1:A:10:TYR:N	0.47	2.83	35	1
1:A:25:THR:HG21	1:A:51:ARG:HG2	0.47	1.87	25	2
1:A:102:ILE:HG23	1:A:103:ASP:H	0.47	1.70	36	1
1:A:9:LYS:HB3	1:A:10:TYR:CE2	0.47	2.45	10	11
1:A:31:TYR:CZ	1:A:32:LYS:HD2	0.47	2.44	1	3
1:A:50:LEU:C	1:A:53:GLN:HG2	0.47	2.30	25	41
1:A:40:LEU:O	1:A:50:LEU:CD1	0.47	2.63	22	1
1:A:19:HIS:HB3	1:A:26:TRP:CG	0.47	2.45	12	1
1:A:57:ASP:CG	1:A:59:THR:HG22	0.47	2.31	19	1
1:A:85:PRO:HA	1:A:88:ARG:HG2	0.47	1.87	6	6
1:A:8:VAL:O	1:A:9:LYS:CB	0.47	2.63	26	6
1:A:91:ILE:CG1	1:A:92:THR:N	0.46	2.78	4	4
1:A:59:THR:C	1:A:61:ASN:N	0.46	2.68	9	9
1:A:29:LEU:C	1:A:31:TYR:H	0.46	2.13	41	8
1:A:35:ASP:OD2	1:A:38:LYS:CG	0.46	2.63	39	1
1:A:39:PHE:CD2	1:A:78:PHE:HB3	0.46	2.45	22	1
1:A:50:LEU:CA	1:A:53:GLN:HG2	0.46	2.39	33	20
1:A:20:ASN:CG	1:A:54:ALA:O	0.46	2.53	7	5
1:A:28:ILE:O	1:A:58:ALA:N	0.46	2.46	21	4
1:A:58:ALA:O	1:A:61:ASN:CB	0.46	2.64	9	1
1:A:16:ILE:HD13	1:A:28:ILE:CG1	0.46	2.40	15	2
1:A:88:ARG:O	1:A:90:LYS:N	0.46	2.49	24	4
1:A:49:VAL:CG1	1:A:50:LEU:HD12	0.46	2.41	7	2
1:A:11:TYR:CE2	1:A:15:GLU:CD	0.46	2.89	14	1
1:A:98:ILE:HD13	1:A:98:ILE:C	0.46	2.30	13	1
1:A:39:PHE:CZ	2:A:105:HEM:HMB2	0.46	2.46	20	2
1:A:10:TYR:CB	1:A:84:HIS:NE2	0.46	2.78	39	5
1:A:49:VAL:HG22	2:A:105:HEM:CHD	0.46	2.40	25	2
1:A:27:LEU:HD21	2:A:105:HEM:CBB	0.46	2.37	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LEU:HG	1:A:47:GLU:CB	0.46	2.41	24	6
1:A:36:LEU:C	1:A:38:LYS:N	0.46	2.69	33	6
1:A:29:LEU:HB3	1:A:34:TYR:CZ	0.46	2.46	22	8
1:A:53:GLN:NE2	2:A:105:HEM:CMC	0.46	2.79	25	8
1:A:41:GLU:CG	1:A:42:GLU:N	0.46	2.79	23	1
1:A:10:TYR:HB3	1:A:84:HIS:ND1	0.46	2.26	38	11
1:A:11:TYR:CZ	1:A:15:GLU:HG2	0.46	2.46	38	5
1:A:9:LYS:HD2	1:A:10:TYR:CE2	0.46	2.46	19	3
1:A:16:ILE:HD13	1:A:28:ILE:HG12	0.46	1.88	37	3
1:A:19:HIS:CG	1:A:24:SER:HB3	0.46	2.46	34	6
1:A:39:PHE:CE1	2:A:105:HEM:HMB2	0.46	2.45	20	2
1:A:40:LEU:HD23	1:A:47:GLU:CG	0.46	2.41	6	1
1:A:88:ARG:HG3	1:A:89:SER:N	0.46	2.26	14	9
1:A:24:SER:O	1:A:26:TRP:N	0.46	2.49	36	1
1:A:8:VAL:O	1:A:9:LYS:HB2	0.46	2.12	41	3
1:A:16:ILE:CD1	1:A:83:LEU:HD22	0.46	2.41	2	3
1:A:26:TRP:NE1	1:A:35:ASP:OD2	0.46	2.49	26	1
1:A:19:HIS:ND1	1:A:24:SER:OG	0.46	2.48	35	6
1:A:20:ASN:ND2	1:A:54:ALA:HB3	0.46	2.25	25	2
1:A:46:GLY:O	1:A:47:GLU:C	0.45	2.53	15	10
1:A:28:ILE:CG1	1:A:57:ASP:HA	0.45	2.40	35	12
1:A:92:THR:HG23	1:A:93:LYS:N	0.45	2.26	42	2
1:A:14:GLU:O	1:A:17:GLN:N	0.45	2.49	34	2
1:A:29:LEU:O	1:A:30:HIS:ND1	0.45	2.49	26	1
1:A:29:LEU:N	1:A:32:LYS:O	0.45	2.49	20	1
1:A:32:LYS:HB2	1:A:34:TYR:CZ	0.45	2.46	30	1
1:A:38:LYS:HD2	1:A:78:PHE:CD1	0.45	2.45	30	1
1:A:43:HIS:ND1	1:A:49:VAL:HG21	0.45	2.26	8	1
1:A:32:LYS:HG3	1:A:79:ILE:CD1	0.45	2.40	12	2
1:A:11:TYR:CZ	1:A:26:TRP:CZ3	0.45	3.04	35	1
1:A:62:PHE:CE1	1:A:63:GLU:HG2	0.45	2.46	33	3
1:A:9:LYS:HD3	1:A:10:TYR:CE2	0.45	2.47	22	2
1:A:83:LEU:CD1	1:A:84:HIS:N	0.45	2.79	39	10
1:A:35:ASP:HB2	1:A:80:ILE:HD11	0.45	1.88	40	1
1:A:11:TYR:CE1	1:A:15:GLU:CG	0.45	2.99	26	2
1:A:8:VAL:CG1	1:A:80:ILE:O	0.45	2.58	20	1
1:A:99:ILE:CG2	1:A:99:ILE:O	0.45	2.64	28	1
1:A:31:TYR:CD1	1:A:92:THR:HA	0.45	2.46	30	1
1:A:40:LEU:HG	1:A:47:GLU:CG	0.45	2.42	17	3
1:A:27:LEU:O	1:A:33:VAL:HA	0.45	2.11	23	6
1:A:50:LEU:O	1:A:54:ALA:N	0.45	2.48	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ILE:HD12	1:A:102:ILE:C	0.45	2.32	34	1
1:A:32:LYS:CG	1:A:34:TYR:CE1	0.45	2.99	17	1
1:A:81:GLY:C	1:A:82:GLU:CG	0.45	2.85	33	31
1:A:19:HIS:CE1	1:A:26:TRP:CE2	0.45	3.04	1	2
1:A:83:LEU:HD12	1:A:84:HIS:H	0.45	1.65	38	1
1:A:8:VAL:HB	1:A:11:TYR:CZ	0.45	2.46	31	2
1:A:38:LYS:HZ2	1:A:74:LEU:CD1	0.45	2.25	35	1
1:A:20:ASN:HD22	1:A:20:ASN:N	0.45	2.10	36	1
1:A:36:LEU:CD2	1:A:50:LEU:HD22	0.45	2.34	3	1
1:A:36:LEU:O	1:A:39:PHE:N	0.45	2.50	33	10
1:A:35:ASP:OD2	1:A:38:LYS:CD	0.45	2.65	40	1
1:A:26:TRP:CE3	1:A:80:ILE:HD11	0.45	2.46	4	1
1:A:43:HIS:HE1	2:A:105:HEM:NB	0.45	2.10	38	2
1:A:19:HIS:ND1	1:A:24:SER:HB3	0.45	2.26	42	1
1:A:28:ILE:CB	1:A:57:ASP:HA	0.45	2.42	40	10
1:A:35:ASP:OD2	1:A:80:ILE:HG21	0.45	2.11	5	2
1:A:26:TRP:NE1	1:A:35:ASP:CG	0.45	2.71	26	1
1:A:72:ARG:CB	1:A:72:ARG:CZ	0.45	2.95	16	4
1:A:91:ILE:C	1:A:93:LYS:N	0.45	2.71	40	3
1:A:43:HIS:HB2	1:A:50:LEU:HD11	0.45	1.89	26	2
1:A:31:TYR:CE1	1:A:88:ARG:NH1	0.45	2.85	40	1
1:A:20:ASN:ND2	1:A:55:GLY:HA2	0.45	2.27	16	1
1:A:27:LEU:HD22	1:A:27:LEU:C	0.44	2.32	38	2
1:A:15:GLU:O	1:A:19:HIS:CD2	0.44	2.71	41	1
1:A:9:LYS:CD	1:A:10:TYR:CE2	0.44	3.00	12	1
1:A:59:THR:O	1:A:62:PHE:N	0.44	2.50	27	3
1:A:31:TYR:CD2	1:A:32:LYS:HE2	0.44	2.47	10	1
1:A:47:GLU:OE1	1:A:47:GLU:N	0.44	2.50	10	1
1:A:49:VAL:CG2	2:A:105:HEM:C1D	0.44	3.00	34	1
1:A:9:LYS:HB3	1:A:10:TYR:CD2	0.44	2.46	42	3
1:A:57:ASP:C	1:A:57:ASP:OD1	0.44	2.56	6	5
1:A:59:THR:O	1:A:63:GLU:N	0.44	2.51	40	2
1:A:33:VAL:HG23	1:A:82:GLU:HA	0.44	1.88	26	1
1:A:98:ILE:O	1:A:99:ILE:CG1	0.44	2.65	33	1
1:A:34:TYR:CE2	1:A:79:ILE:CD1	0.44	3.00	38	2
1:A:73:GLU:O	1:A:77:THR:HG23	0.44	2.12	28	2
1:A:99:ILE:HG23	1:A:99:ILE:O	0.44	2.12	28	1
1:A:29:LEU:HD12	2:A:105:HEM:CAB	0.44	2.41	19	3
1:A:35:ASP:HB2	1:A:80:ILE:CD1	0.44	2.42	40	1
1:A:19:HIS:C	1:A:20:ASN:ND2	0.44	2.71	34	2
1:A:31:TYR:C	1:A:31:TYR:CD1	0.44	2.90	34	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:LEU:HG	1:A:75:SER:N	0.44	2.27	9	4
1:A:31:TYR:CD1	1:A:88:ARG:CZ	0.44	3.00	7	2
1:A:67:HIS:ND1	2:A:105:HEM:O2A	0.44	2.50	25	1
1:A:43:HIS:CD2	2:A:105:HEM:CHB	0.44	3.01	20	1
1:A:19:HIS:CB	1:A:26:TRP:CE3	0.44	3.00	17	2
1:A:32:LYS:HG2	1:A:34:TYR:CE1	0.44	2.48	14	1
1:A:31:TYR:CE2	1:A:32:LYS:HG3	0.44	2.48	29	4
1:A:40:LEU:CD2	1:A:47:GLU:HB3	0.44	2.42	16	2
1:A:96:GLU:O	1:A:97:SER:CB	0.44	2.65	18	1
1:A:26:TRP:CE3	1:A:35:ASP:OD1	0.44	2.71	25	1
1:A:77:THR:HG23	1:A:78:PHE:HD1	0.44	1.73	25	1
1:A:35:ASP:O	1:A:35:ASP:OD1	0.44	2.35	7	2
1:A:77:THR:HG23	1:A:78:PHE:CE1	0.44	2.47	1	2
1:A:30:HIS:HB3	1:A:31:TYR:CD1	0.44	2.48	4	1
1:A:27:LEU:CD2	1:A:28:ILE:N	0.44	2.72	39	1
1:A:32:LYS:CG	1:A:34:TYR:CZ	0.44	3.01	17	1
1:A:43:HIS:CE1	2:A:105:HEM:NB	0.44	2.86	38	2
1:A:50:LEU:HA	1:A:53:GLN:NE2	0.44	2.28	27	8
1:A:57:ASP:O	1:A:57:ASP:OD1	0.44	2.36	9	4
1:A:71:ALA:CA	1:A:74:LEU:HD23	0.44	2.39	37	3
1:A:28:ILE:HG12	1:A:33:VAL:HG12	0.44	1.89	19	2
1:A:92:THR:O	1:A:93:LYS:C	0.44	2.57	10	4
1:A:29:LEU:HD11	1:A:62:PHE:CE2	0.44	2.47	20	2
1:A:92:THR:O	1:A:94:PRO:N	0.43	2.51	13	1
1:A:67:HIS:ND1	2:A:105:HEM:O1A	0.43	2.50	37	1
1:A:43:HIS:ND1	1:A:49:VAL:CG1	0.43	2.72	7	1
1:A:35:ASP:OD2	1:A:80:ILE:HG23	0.43	2.13	7	1
1:A:25:THR:HG21	1:A:40:LEU:HD11	0.43	1.90	36	1
1:A:35:ASP:OD2	1:A:38:LYS:N	0.43	2.50	15	1
1:A:29:LEU:HG	2:A:105:HEM:HAB	0.43	1.90	33	3
1:A:43:HIS:ND1	1:A:44:PRO:HD2	0.43	2.28	21	3
1:A:18:LYS:HG2	1:A:19:HIS:CD2	0.43	2.48	16	1
1:A:12:THR:O	1:A:15:GLU:N	0.43	2.51	5	4
1:A:36:LEU:HD11	1:A:53:GLN:HG3	0.43	1.89	28	1
1:A:74:LEU:O	1:A:77:THR:HB	0.43	2.13	35	4
1:A:86:ASP:O	1:A:87:ASP:CG	0.43	2.57	37	10
1:A:39:PHE:O	1:A:39:PHE:CG	0.43	2.70	16	4
1:A:98:ILE:HD12	1:A:99:ILE:O	0.43	2.12	24	1
1:A:33:VAL:O	1:A:80:ILE:CD1	0.43	2.65	23	1
2:A:105:HEM:C1A	2:A:105:HEM:O1A	0.43	2.71	7	1
1:A:102:ILE:HG12	1:A:103:ASP:N	0.43	2.27	32	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:GLN:OE1	2:A:105:HEM:HMC2	0.43	2.13	29	1
1:A:28:ILE:HG12	1:A:56:GLY:C	0.43	2.33	40	1
1:A:83:LEU:O	1:A:88:ARG:CD	0.43	2.66	34	4
2:A:105:HEM:O1A	2:A:105:HEM:C1A	0.43	2.71	37	2
1:A:16:ILE:CG2	1:A:26:TRP:C	0.43	2.87	7	1
1:A:40:LEU:O	1:A:41:GLU:C	0.43	2.57	1	5
1:A:26:TRP:CD1	1:A:80:ILE:HG12	0.43	2.49	14	1
1:A:35:ASP:O	1:A:39:PHE:CD1	0.43	2.71	24	1
1:A:13:LEU:CD2	1:A:28:ILE:CD1	0.43	2.96	37	1
1:A:99:ILE:H	1:A:99:ILE:HD13	0.43	1.73	25	1
1:A:19:HIS:ND1	1:A:24:SER:HB2	0.43	2.28	42	2
1:A:31:TYR:CB	1:A:92:THR:OG1	0.43	2.67	35	2
1:A:64:ASP:C	1:A:66:GLY:N	0.43	2.72	21	6
1:A:39:PHE:C	1:A:41:GLU:N	0.43	2.70	28	5
1:A:24:SER:O	1:A:26:TRP:CG	0.43	2.71	6	1
1:A:43:HIS:CD2	2:A:105:HEM:NA	0.43	2.87	12	1
1:A:83:LEU:HD23	1:A:91:ILE:CG1	0.43	2.42	15	1
1:A:61:ASN:C	1:A:63:GLU:N	0.43	2.72	36	7
1:A:43:HIS:CD2	1:A:44:PRO:HD2	0.43	2.48	42	2
1:A:58:ALA:O	1:A:61:ASN:N	0.43	2.52	20	4
1:A:57:ASP:OD1	1:A:57:ASP:O	0.43	2.37	20	2
1:A:29:LEU:HD21	1:A:62:PHE:HB3	0.43	1.90	23	2
1:A:38:LYS:HB3	1:A:78:PHE:CZ	0.43	2.48	25	1
1:A:19:HIS:HB2	1:A:26:TRP:CE3	0.43	2.48	17	1
1:A:38:LYS:C	1:A:39:PHE:CD1	0.43	2.92	22	1
1:A:34:TYR:CE2	1:A:75:SER:OG	0.43	2.72	14	1
1:A:32:LYS:CG	1:A:82:GLU:OE1	0.43	2.67	41	1
1:A:39:PHE:HB3	1:A:50:LEU:CD2	0.43	2.43	25	2
1:A:61:ASN:CB	2:A:105:HEM:HMC2	0.43	2.43	37	1
1:A:83:LEU:HD21	1:A:87:ASP:O	0.43	2.14	33	3
1:A:72:ARG:O	1:A:75:SER:OG	0.43	2.36	25	3
1:A:86:ASP:OD2	1:A:87:ASP:OD2	0.43	2.37	13	2
1:A:92:THR:O	1:A:92:THR:CG2	0.43	2.67	7	1
1:A:29:LEU:HD23	1:A:29:LEU:HA	0.43	1.72	30	1
1:A:39:PHE:HE1	1:A:74:LEU:HD21	0.43	1.73	34	1
1:A:85:PRO:HA	1:A:88:ARG:CD	0.43	2.44	3	2
1:A:42:GLU:O	1:A:43:HIS:HB3	0.43	2.14	12	3
1:A:31:TYR:CZ	1:A:32:LYS:HD3	0.43	2.49	35	2
1:A:62:PHE:HA	1:A:67:HIS:CE1	0.43	2.48	30	3
1:A:91:ILE:O	1:A:92:THR:O	0.42	2.38	41	6
1:A:19:HIS:C	1:A:20:ASN:HD22	0.42	2.18	34	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:PHE:CE2	2:A:105:HEM:HHB	0.42	2.49	35	2
1:A:22:SER:HA	1:A:25:THR:OG1	0.42	2.14	36	1
1:A:43:HIS:NE2	2:A:105:HEM:C4A	0.42	2.87	20	2
1:A:57:ASP:CB	1:A:91:ILE:HB	0.42	2.44	28	1
1:A:62:PHE:HA	1:A:65:VAL:HG12	0.42	1.91	1	1
1:A:16:ILE:HG21	1:A:28:ILE:HD13	0.42	1.89	30	1
1:A:29:LEU:HA	1:A:29:LEU:HD23	0.42	1.76	26	2
1:A:58:ALA:O	1:A:59:THR:C	0.42	2.58	35	3
1:A:11:TYR:CD2	1:A:15:GLU:CG	0.42	3.02	22	3
1:A:39:PHE:CD2	1:A:78:PHE:CB	0.42	3.02	22	1
1:A:39:PHE:HB3	1:A:50:LEU:HD13	0.42	1.91	35	1
1:A:57:ASP:HB2	1:A:91:ILE:CD1	0.42	2.43	9	2
1:A:33:VAL:HG13	1:A:82:GLU:CA	0.42	2.44	17	1
1:A:19:HIS:HB2	1:A:26:TRP:HB2	0.42	1.90	21	3
1:A:19:HIS:CB	1:A:24:SER:O	0.42	2.68	21	1
1:A:40:LEU:HA	1:A:50:LEU:HD13	0.42	1.90	21	1
1:A:62:PHE:HB2	2:A:105:HEM:CHC	0.42	2.45	2	1
1:A:49:VAL:HG13	1:A:50:LEU:HD12	0.42	1.92	30	1
1:A:30:HIS:H	1:A:59:THR:CB	0.42	2.28	37	4
1:A:35:ASP:OD1	1:A:78:PHE:HB3	0.42	2.14	41	1
1:A:40:LEU:CD1	1:A:47:GLU:HB3	0.42	2.44	12	2
1:A:24:SER:O	1:A:25:THR:C	0.42	2.57	18	2
1:A:102:ILE:HD13	1:A:102:ILE:N	0.42	2.29	32	1
1:A:27:LEU:C	1:A:28:ILE:HD13	0.42	2.35	27	1
1:A:30:HIS:H	1:A:59:THR:HG23	0.42	1.75	27	1
1:A:13:LEU:CD2	1:A:83:LEU:CD2	0.42	2.98	17	3
1:A:26:TRP:CZ3	1:A:35:ASP:OD2	0.42	2.73	41	1
1:A:33:VAL:C	1:A:80:ILE:CD1	0.42	2.88	24	1
1:A:32:LYS:HE3	1:A:79:ILE:CD1	0.42	2.44	35	1
1:A:30:HIS:CG	1:A:72:ARG:NH2	0.42	2.88	33	1
1:A:31:TYR:CE2	1:A:88:ARG:NH2	0.42	2.88	7	1
1:A:92:THR:O	1:A:93:LYS:O	0.42	2.37	7	2
1:A:65:VAL:O	1:A:66:GLY:O	0.42	2.38	19	1
1:A:39:PHE:CE2	1:A:74:LEU:CG	0.42	3.03	10	1
1:A:50:LEU:HA	1:A:53:GLN:CG	0.42	2.45	12	3
1:A:40:LEU:O	1:A:42:GLU:O	0.42	2.38	7	1
1:A:28:ILE:HB	1:A:57:ASP:CA	0.42	2.45	36	1
1:A:36:LEU:O	1:A:37:THR:C	0.42	2.58	38	2
1:A:76:LYS:HA	1:A:79:ILE:HD12	0.42	1.92	42	1
1:A:8:VAL:HG13	1:A:80:ILE:C	0.42	2.35	37	2
1:A:35:ASP:OD1	1:A:37:THR:HB	0.42	2.15	40	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:O	1:A:40:LEU:HD23	0.42	2.15	33	1
1:A:30:HIS:NE2	1:A:62:PHE:CE2	0.42	2.88	27	1
1:A:21:ASN:C	1:A:23:LYS:N	0.41	2.73	16	2
1:A:36:LEU:HA	1:A:39:PHE:HD1	0.41	1.73	40	1
1:A:26:TRP:CZ2	1:A:80:ILE:HD12	0.41	2.50	40	1
1:A:76:LYS:CE	1:A:76:LYS:O	0.41	2.68	6	1
1:A:44:PRO:O	1:A:45:GLY:C	0.41	2.59	31	3
1:A:29:LEU:HD23	1:A:59:THR:CA	0.41	2.45	30	1
1:A:101:THR:O	1:A:102:ILE:O	0.41	2.38	38	1
1:A:39:PHE:CD1	1:A:78:PHE:HE2	0.41	2.30	19	1
1:A:72:ARG:HB3	1:A:72:ARG:CZ	0.41	2.45	41	1
1:A:99:ILE:O	1:A:99:ILE:HG23	0.41	2.15	10	1
1:A:12:THR:OG1	1:A:15:GLU:CG	0.41	2.67	20	2
1:A:94:PRO:O	1:A:95:SER:CB	0.41	2.68	18	1
1:A:74:LEU:O	1:A:77:THR:OG1	0.41	2.37	32	2
1:A:31:TYR:CE2	1:A:82:GLU:OE2	0.41	2.73	17	2
1:A:84:HIS:HB3	1:A:85:PRO:CD	0.41	2.45	8	1
1:A:49:VAL:HG21	2:A:105:HEM:C1D	0.41	2.50	34	1
1:A:26:TRP:HE1	1:A:80:ILE:HD12	0.41	1.71	34	1
1:A:11:TYR:CE2	1:A:15:GLU:HB3	0.41	2.50	36	1
1:A:68:SER:C	1:A:70:ASP:N	0.41	2.73	20	1
1:A:43:HIS:CE1	2:A:105:HEM:C1D	0.41	3.08	16	1
1:A:27:LEU:HD22	1:A:28:ILE:CA	0.41	2.45	39	1
1:A:72:ARG:CZ	1:A:72:ARG:CB	0.41	2.98	39	1
1:A:39:PHE:CD2	2:A:105:HEM:HMB3	0.41	2.51	15	1
1:A:40:LEU:HD23	1:A:40:LEU:HA	0.41	1.81	8	1
1:A:27:LEU:C	1:A:27:LEU:CD1	0.41	2.89	24	1
1:A:61:ASN:HB3	2:A:105:HEM:CBC	0.41	2.46	16	1
1:A:17:GLN:O	1:A:20:ASN:OD1	0.41	2.37	16	1
1:A:9:LYS:HB3	1:A:10:TYR:CD1	0.41	2.50	23	1
1:A:39:PHE:HE2	2:A:105:HEM:CHB	0.41	2.29	36	3
1:A:20:ASN:O	1:A:51:ARG:NE	0.41	2.54	34	1
1:A:19:HIS:ND1	1:A:26:TRP:CE3	0.41	2.88	18	2
1:A:27:LEU:CD1	1:A:27:LEU:C	0.41	2.89	9	1
1:A:86:ASP:O	1:A:87:ASP:OD1	0.41	2.39	34	2
1:A:29:LEU:HD21	1:A:62:PHE:CB	0.41	2.45	23	2
1:A:32:LYS:CB	1:A:34:TYR:CE1	0.41	3.04	20	1
1:A:8:VAL:CG2	1:A:11:TYR:CE2	0.41	3.03	21	1
1:A:57:ASP:OD1	1:A:60:GLU:CD	0.41	2.59	25	1
1:A:98:ILE:HD13	1:A:98:ILE:N	0.41	2.30	1	1
1:A:38:LYS:HD3	1:A:78:PHE:CE1	0.41	2.51	38	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:GLN:HB2	1:A:58:ALA:CB	0.41	2.45	42	2
1:A:25:THR:CG2	1:A:36:LEU:HB2	0.41	2.46	42	1
1:A:39:PHE:CD1	1:A:42:GLU:HB2	0.41	2.51	19	1
1:A:30:HIS:O	1:A:92:THR:O	0.41	2.39	35	2
1:A:13:LEU:HD23	1:A:13:LEU:HA	0.41	1.83	41	1
1:A:28:ILE:CD1	1:A:33:VAL:HG22	0.41	2.46	5	1
1:A:65:VAL:HG21	1:A:67:HIS:CE1	0.41	2.51	2	3
1:A:30:HIS:ND1	1:A:31:TYR:CD2	0.41	2.89	4	1
1:A:98:ILE:C	1:A:98:ILE:HD13	0.41	2.36	2	1
1:A:12:THR:O	1:A:16:ILE:CD1	0.41	2.67	36	1
1:A:88:ARG:CZ	1:A:88:ARG:HB3	0.41	2.46	40	1
1:A:91:ILE:HG12	1:A:92:THR:N	0.41	2.31	9	1
1:A:66:GLY:O	1:A:67:HIS:O	0.41	2.39	30	1
1:A:30:HIS:NE2	1:A:72:ARG:NE	0.40	2.61	6	1
1:A:43:HIS:HD1	1:A:45:GLY:N	0.40	2.13	21	1
1:A:11:TYR:CZ	1:A:15:GLU:CG	0.40	3.05	38	1
1:A:29:LEU:HB3	1:A:30:HIS:CE1	0.40	2.51	26	1
1:A:100:THR:CG2	1:A:100:THR:O	0.40	2.69	24	1
1:A:10:TYR:HB2	1:A:84:HIS:ND1	0.40	2.32	33	1
1:A:13:LEU:CD1	1:A:87:ASP:HB3	0.40	2.44	3	1
1:A:18:LYS:CG	1:A:19:HIS:N	0.40	2.84	42	1
1:A:93:LYS:CG	1:A:94:PRO:HD2	0.40	2.47	8	1
1:A:83:LEU:CD2	1:A:91:ILE:CD1	0.40	2.99	24	1
1:A:83:LEU:O	1:A:88:ARG:HG3	0.40	2.17	37	1
1:A:34:TYR:O	1:A:80:ILE:HD11	0.40	2.16	33	1
1:A:86:ASP:O	1:A:87:ASP:OD2	0.40	2.39	15	1
1:A:36:LEU:CD1	1:A:53:GLN:HG3	0.40	2.47	41	1
1:A:99:ILE:HG23	1:A:100:THR:N	0.40	2.31	40	1
1:A:39:PHE:C	1:A:41:GLU:H	0.40	2.18	5	1
1:A:61:ASN:O	1:A:64:ASP:N	0.40	2.55	5	1
1:A:39:PHE:CE2	1:A:50:LEU:HD21	0.40	2.51	12	1
1:A:83:LEU:CD1	1:A:83:LEU:C	0.40	2.89	18	1
1:A:26:TRP:CH2	1:A:80:ILE:CG1	0.40	3.05	37	1
1:A:86:ASP:CG	1:A:87:ASP:OD2	0.40	2.60	37	1
1:A:27:LEU:CD1	1:A:36:LEU:HG	0.40	2.46	4	1
1:A:39:PHE:CZ	1:A:74:LEU:CD1	0.40	3.03	20	1
1:A:32:LYS:CG	1:A:79:ILE:HD11	0.40	2.46	31	1
1:A:74:LEU:HD12	1:A:78:PHE:CE2	0.40	2.50	16	1
1:A:13:LEU:HG	1:A:87:ASP:CB	0.40	2.47	11	1
1:A:34:TYR:HB3	1:A:39:PHE:CE1	0.40	2.51	3	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	96/104 (92%)	71±3 (74±3%)	17±3 (18±3%)	7±2 (8±2%)	2 14
All	All	4032/4368 (92%)	2985 (74%)	734 (18%)	313 (8%)	2 14

All 33 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	31	TYR	40
1	A	43	HIS	32
1	A	8	VAL	30
1	A	66	GLY	29
1	A	49	VAL	24
1	A	92	THR	22
1	A	42	GLU	20
1	A	87	ASP	18
1	A	94	PRO	10
1	A	103	ASP	8
1	A	93	LYS	8
1	A	25	THR	7
1	A	102	ILE	7
1	A	99	ILE	6
1	A	67	HIS	6
1	A	60	GLU	6
1	A	96	GLU	5
1	A	37	THR	5
1	A	89	SER	4
1	A	88	ARG	3
1	A	100	THR	3
1	A	98	ILE	3
1	A	41	GLU	2
1	A	40	LEU	2
1	A	59	THR	2
1	A	44	PRO	2
1	A	95	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	45	GLY	2
1	A	79	ILE	1
1	A	24	SER	1
1	A	101	THR	1
1	A	97	SER	1
1	A	84	HIS	1

6.3.2 Protein sidechains [\(1\)](#)

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	87/93 (94%)	50±4 (57±4%)	37±4 (43±4%)	0 3
All	All	3654/3906 (94%)	2094 (57%)	1560 (43%)	0 3

All 69 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	8	VAL	42
1	A	11	TYR	42
1	A	10	TYR	42
1	A	62	PHE	42
1	A	84	HIS	42
1	A	74	LEU	42
1	A	83	LEU	42
1	A	28	ILE	42
1	A	86	ASP	42
1	A	29	LEU	42
1	A	27	LEU	42
1	A	61	ASN	41
1	A	57	ASP	41
1	A	24	SER	38
1	A	65	VAL	38
1	A	60	GLU	38
1	A	59	THR	37
1	A	75	SER	37
1	A	14	GLU	36

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Mol	Chain	Res	Type	Models (Total)
1	A	51	ARG	35
1	A	79	ILE	34
1	A	64	ASP	34
1	A	25	THR	32
1	A	31	TYR	30
1	A	17	GLN	27
1	A	37	THR	27
1	A	76	LYS	27
1	A	91	ILE	27
1	A	96	GLU	25
1	A	9	LYS	24
1	A	63	GLU	24
1	A	35	ASP	23
1	A	52	GLU	23
1	A	90	LYS	22
1	A	32	LYS	21
1	A	38	LYS	20
1	A	43	HIS	20
1	A	48	GLU	20
1	A	93	LYS	18
1	A	42	GLU	18
1	A	97	SER	17
1	A	80	ILE	16
1	A	40	LEU	16
1	A	98	ILE	15
1	A	23	LYS	15
1	A	102	ILE	14
1	A	50	LEU	14
1	A	103	ASP	14
1	A	95	SER	14
1	A	92	THR	12
1	A	18	LYS	11
1	A	41	GLU	10
1	A	99	ILE	10
1	A	87	ASP	10
1	A	89	SER	9
1	A	39	PHE	8
1	A	47	GLU	8
1	A	20	ASN	7
1	A	34	TYR	6
1	A	78	PHE	6
1	A	88	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	73	GLU	5
1	A	30	HIS	5
1	A	22	SER	4
1	A	15	GLU	4
1	A	82	GLU	2
1	A	33	VAL	2
1	A	67	HIS	1
1	A	77	THR	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 carbohydrates in this entry.

6.6 Ligand geometry [\(i\)](#)

1 ligand is 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	HEM	A	105	1	27,50,50	1.61±0.00	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
2	HEM	A	105	1	17,82,82	1.48±0.01	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
2	HEM	A	105	1	-	0±0,6,54,54	-

There are no bond-length outliers.

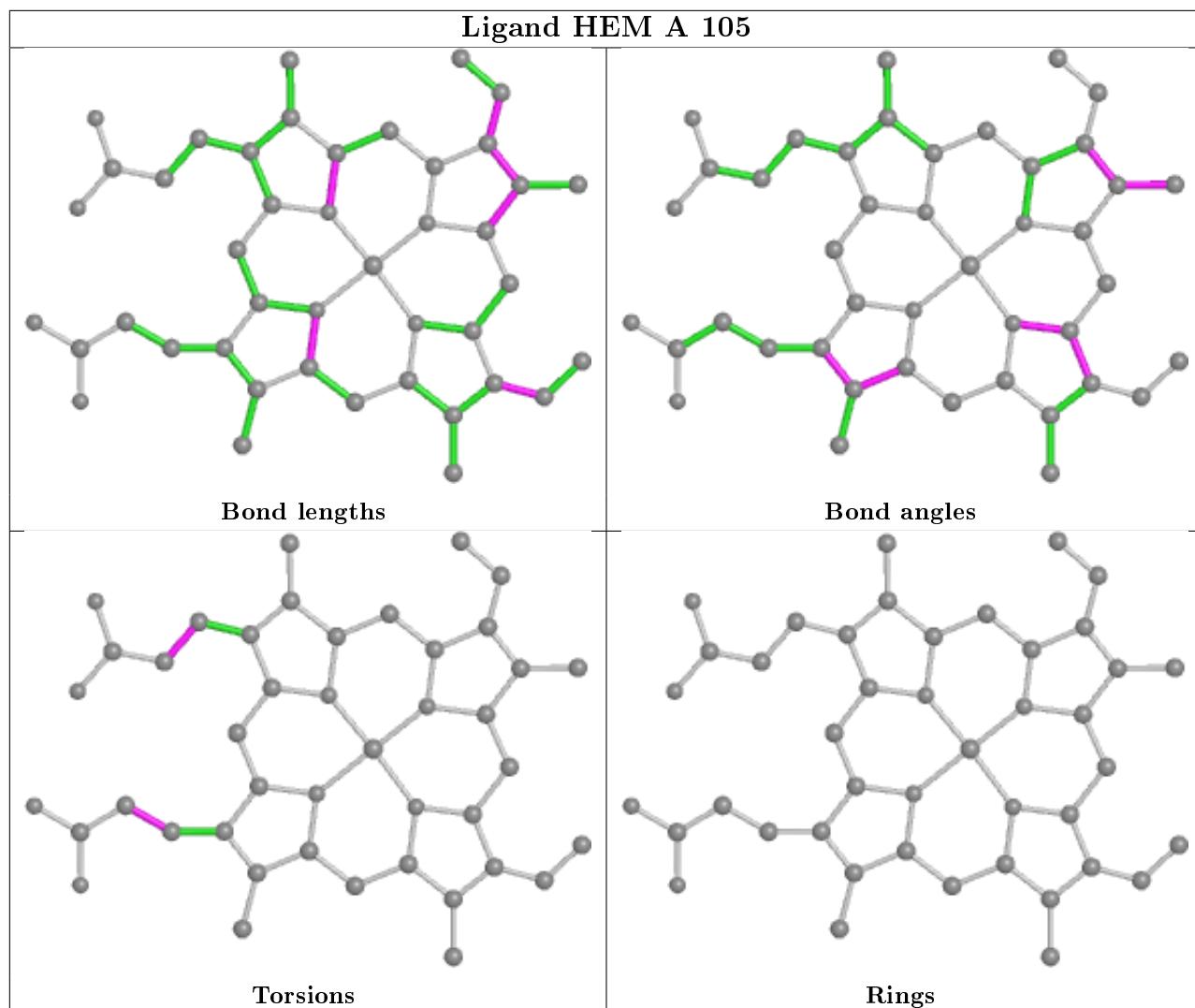
There are no bond-angle outliers.

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

No chemical shift data were provided