



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 09:35 PM UTC

PDB ID : 1HKO / pdb_00001hko
BMRB ID : 5745
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

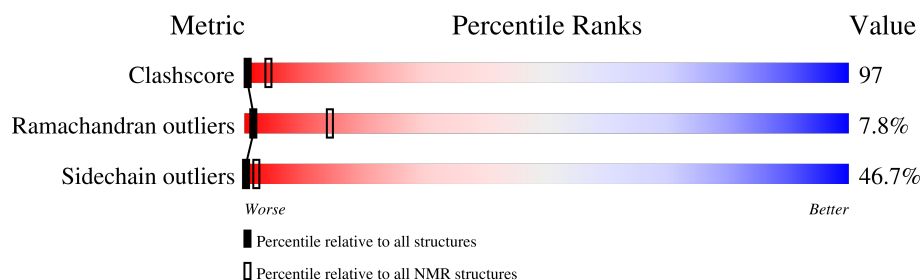
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	16% 46% 28% • 8%

2 Ensemble composition and analysis

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)	0.45	13
2	A:92-A:103 (12)	1.63	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 5 clusters and 1 single-model cluster was found.

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

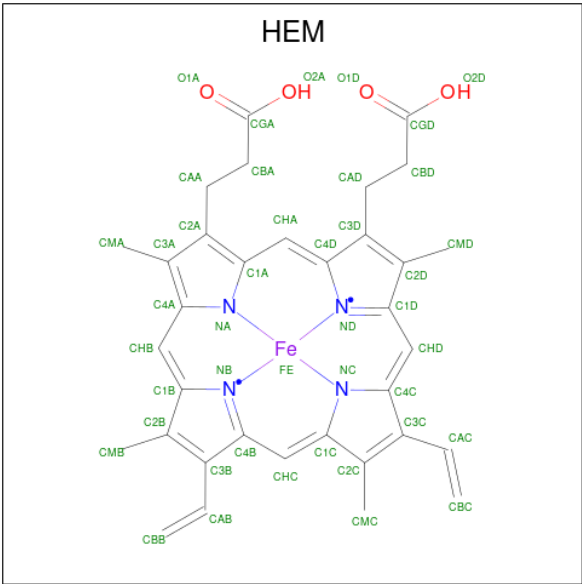
3 Entry composition [i](#)

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
1	A	104	Total	C	H	N	O	0
			1636	520	804	138	174	

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



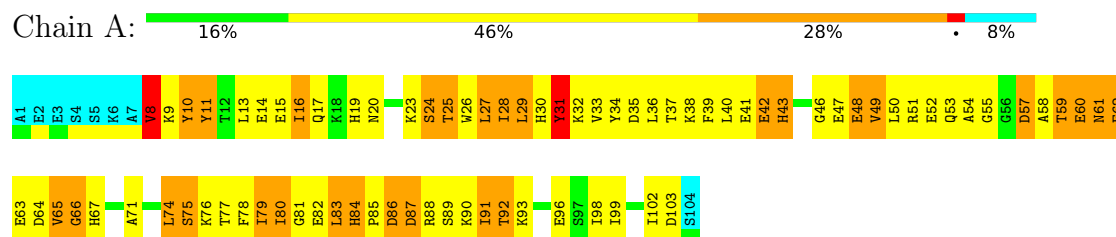
Mol	Chain	Residues	Atoms					
2	A	1	Total	C	Fe	H	N	O
			63	34	1	20	4	4

4 Residue-property plots

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 B5

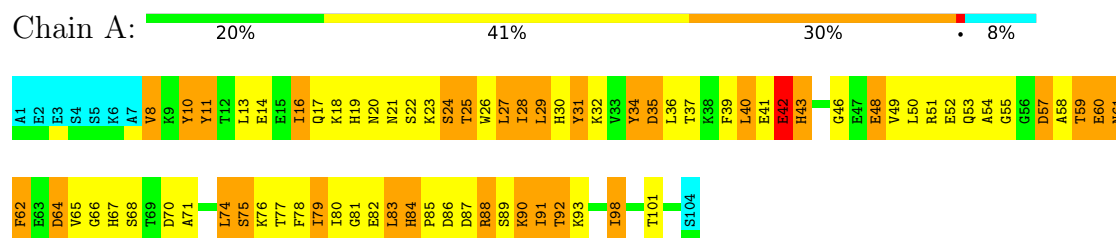


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

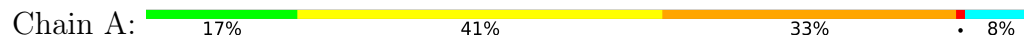
4.2.1 Score per residue for model 1

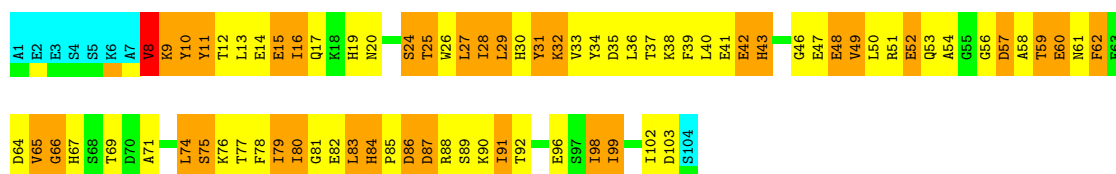
- Molecule 1: CYTOCHROME B5



4.2.2 Score per residue for model 2

- Molecule 1: CYTOCHROME B5

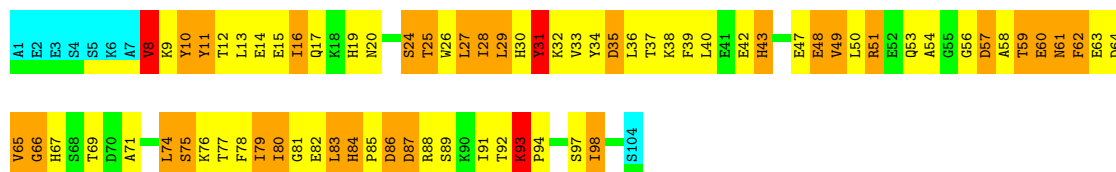




4.2.3 Score per residue for model 3

- Molecule 1: CYTOCHROME B5

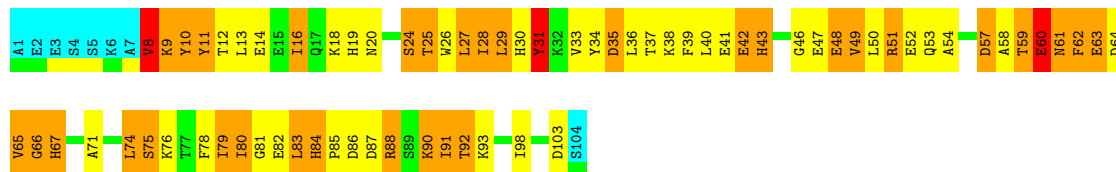
Chain A: 21% 40% 28% 8%



4.2.4 Score per residue for model 4

- Molecule 1: CYTOCHROME B5

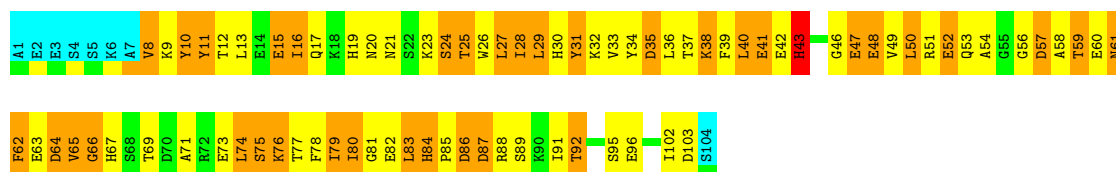
Chain A: 24% 34% 32% 8%



4.2.5 Score per residue for model 5

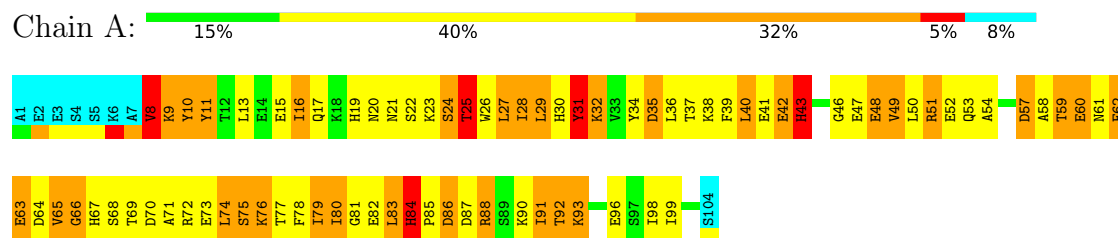
- Molecule 1: CYTOCHROME B5

Chain A: 16% 40% 35% 8%



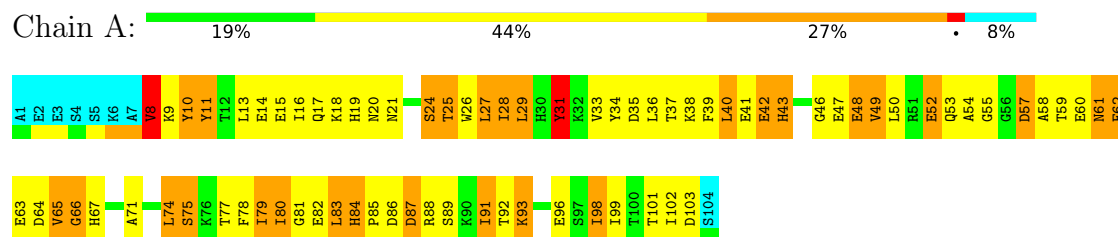
4.2.6 Score per residue for model 6

- Molecule 1: CYTOCHROME B5



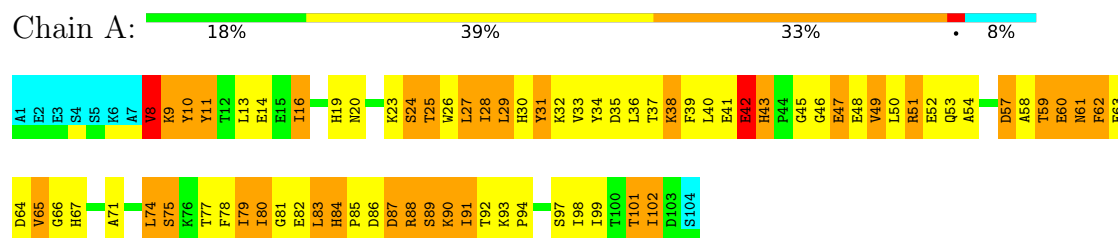
4.2.7 Score per residue for model 7

- Molecule 1: CYTOCHROME B5



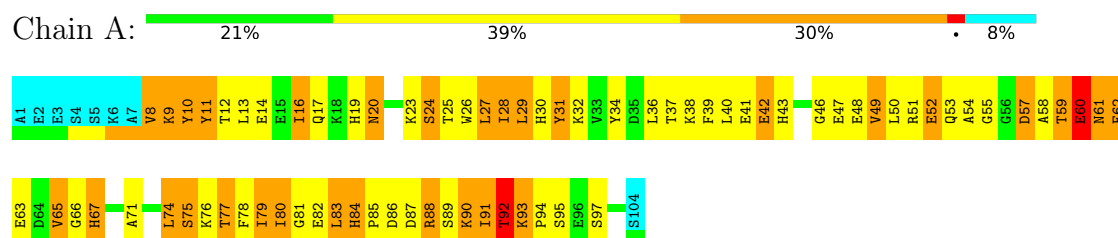
4.2.8 Score per residue for model 8

- Molecule 1: CYTOCHROME B5



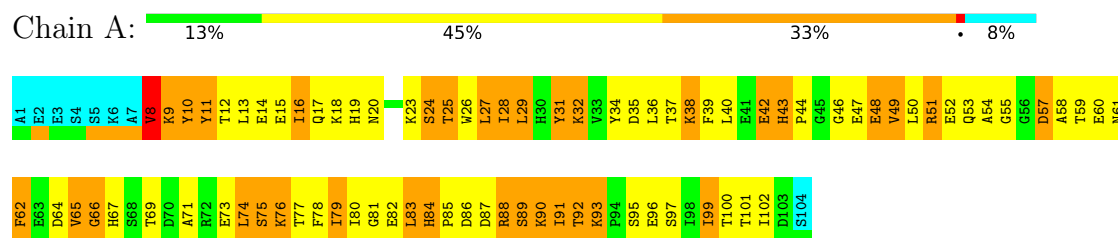
4.2.9 Score per residue for model 9

- Molecule 1: CYTOCHROME B5



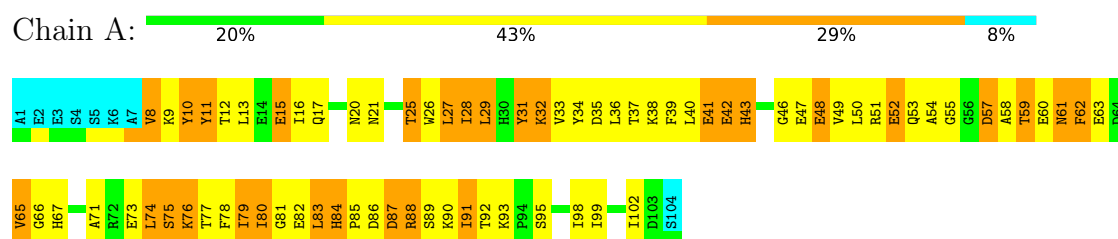
4.2.10 Score per residue for model 10

- Molecule 1: CYTOCHROME B5



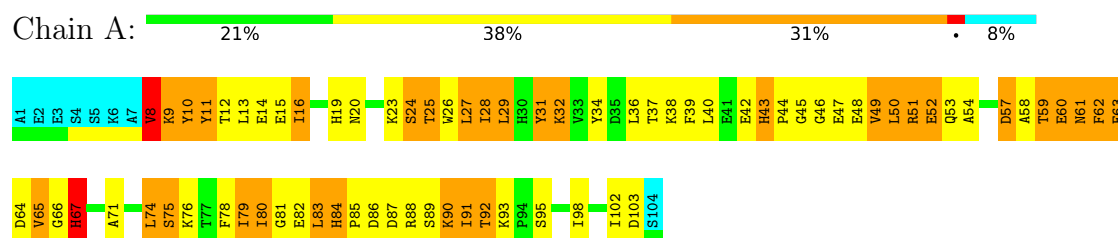
4.2.11 Score per residue for model 11

- Molecule 1: CYTOCHROME B5



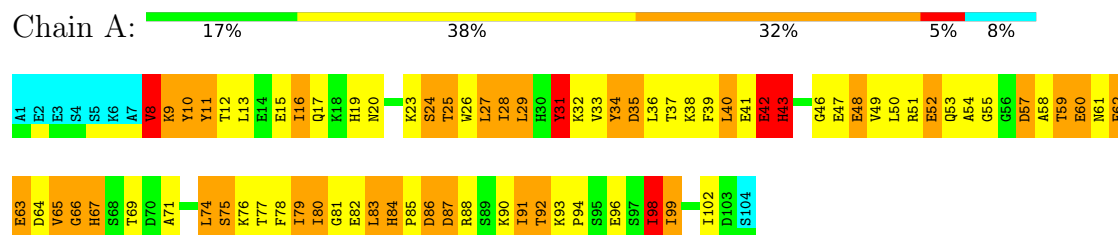
4.2.12 Score per residue for model 12

- Molecule 1: CYTOCHROME B5



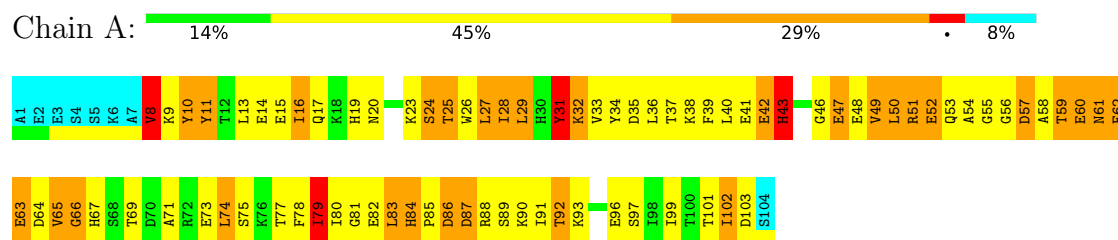
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: CYTOCHROME B5



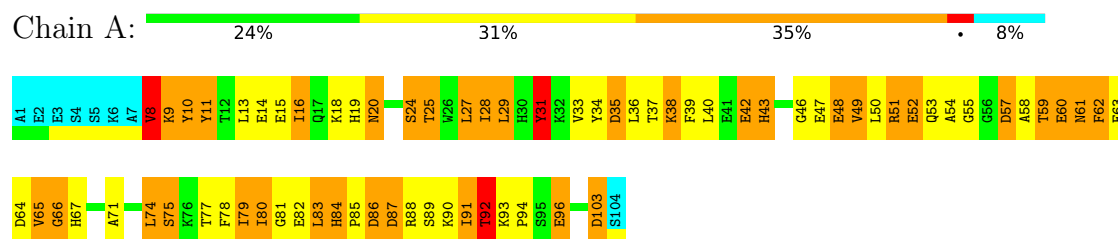
4.2.14 Score per residue for model 14

- Molecule 1: CYTOCHROME B5



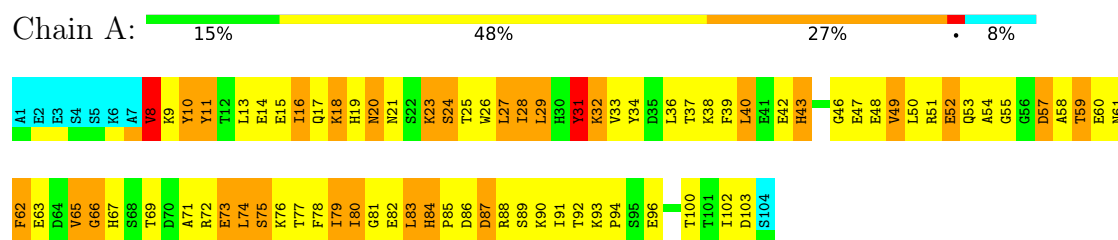
4.2.15 Score per residue for model 15

- Molecule 1: CYTOCHROME B5



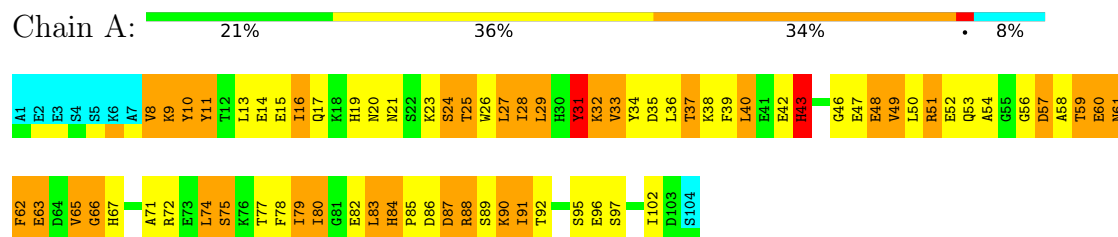
4.2.16 Score per residue for model 16

- Molecule 1: CYTOCHROME B5



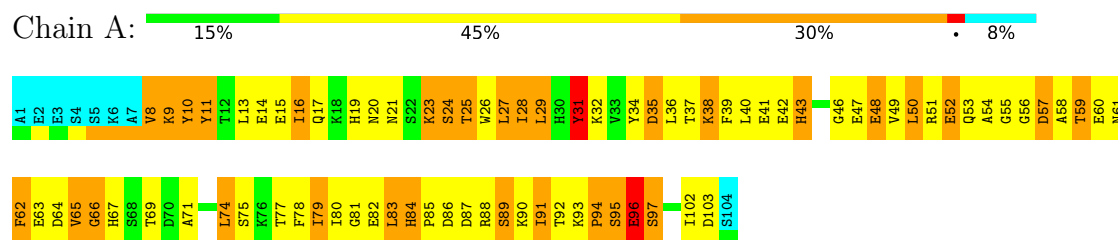
4.2.17 Score per residue for model 17

- Molecule 1: CYTOCHROME B5



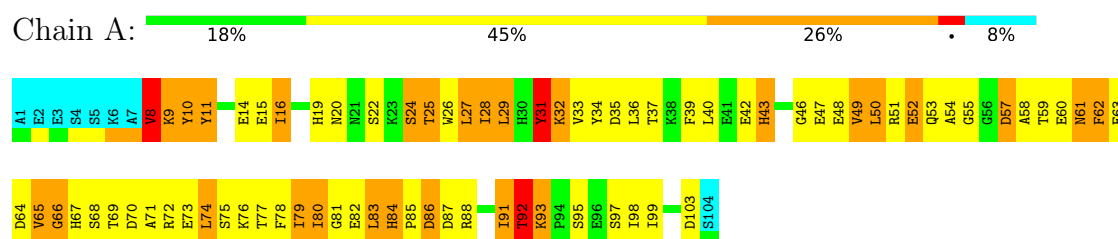
4.2.18 Score per residue for model 18

- Molecule 1: CYTOCHROME B5



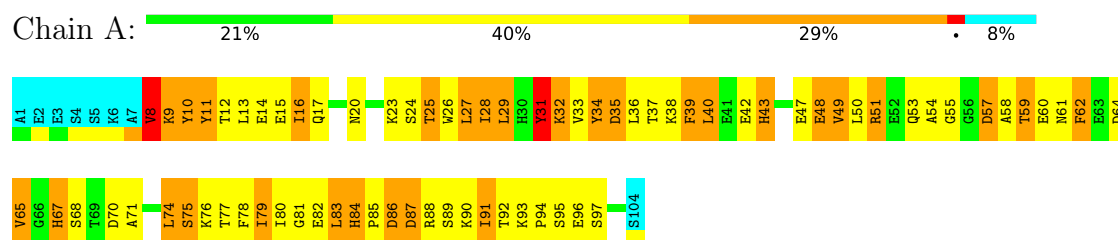
4.2.19 Score per residue for model 19

- Molecule 1: CYTOCHROME B5



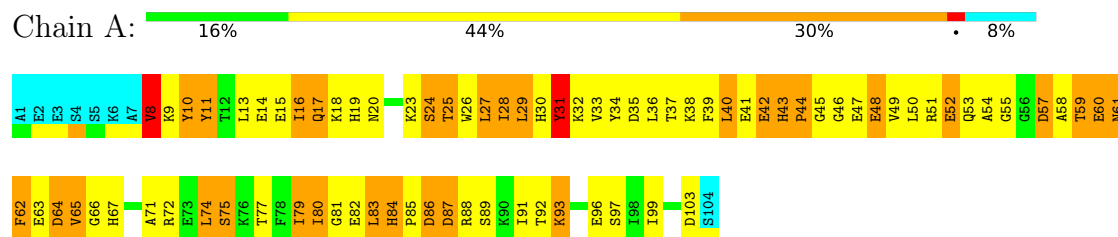
4.2.20 Score per residue for model 20

- Molecule 1: CYTOCHROME B5



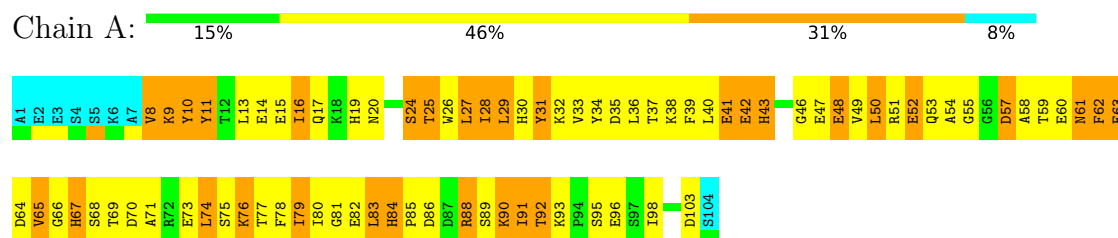
4.2.21 Score per residue for model 21

- Molecule 1: CYTOCHROME B5



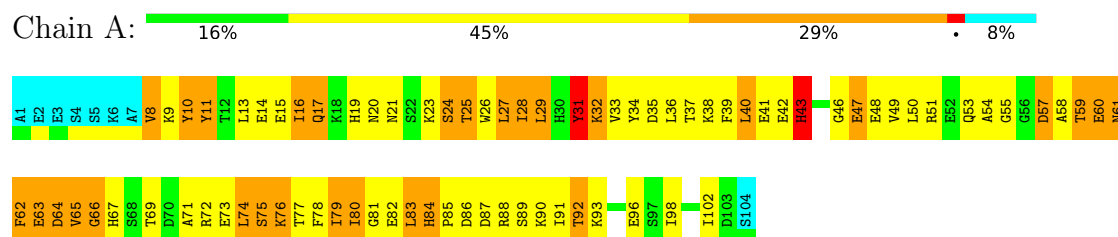
4.2.22 Score per residue for model 22

- Molecule 1: CYTOCHROME B5



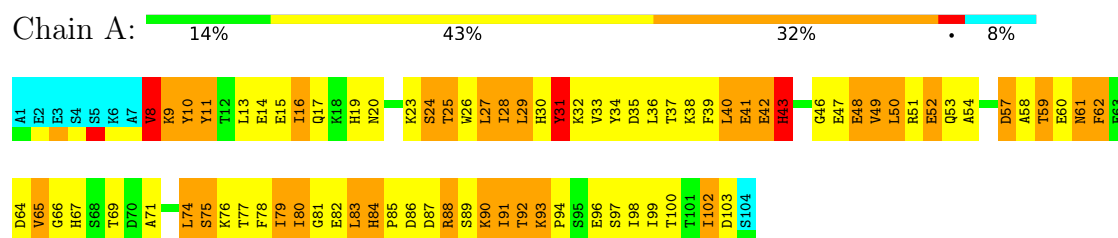
4.2.23 Score per residue for model 23

- Molecule 1: CYTOCHROME B5



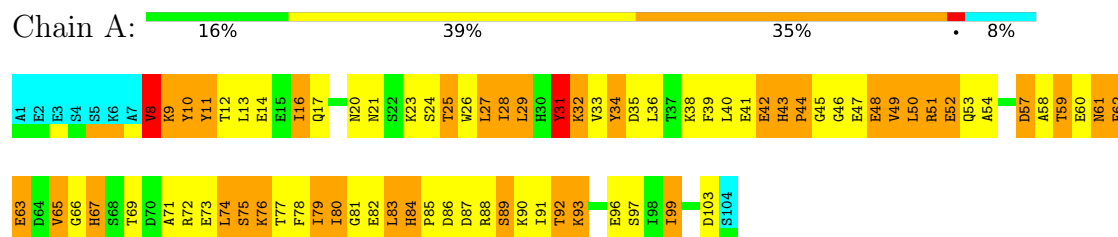
4.2.24 Score per residue for model 24

- Molecule 1: CYTOCHROME B5



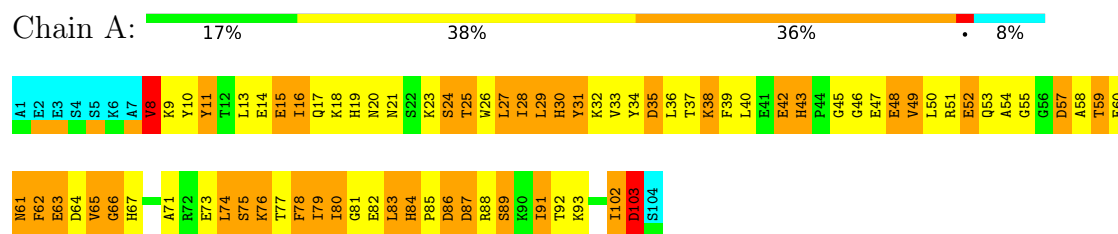
4.2.25 Score per residue for model 25

- Molecule 1: CYTOCHROME B5



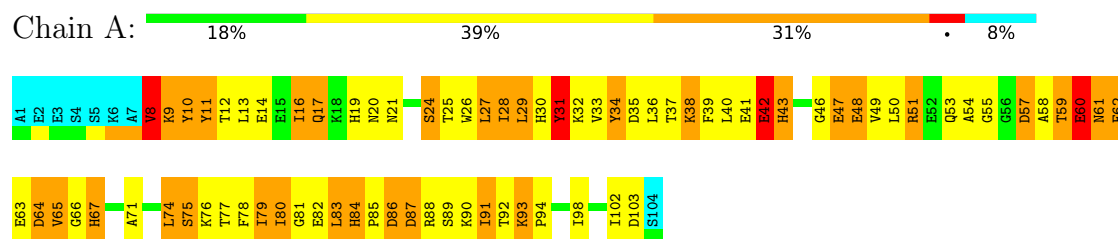
4.2.26 Score per residue for model 26

- Molecule 1: CYTOCHROME B5



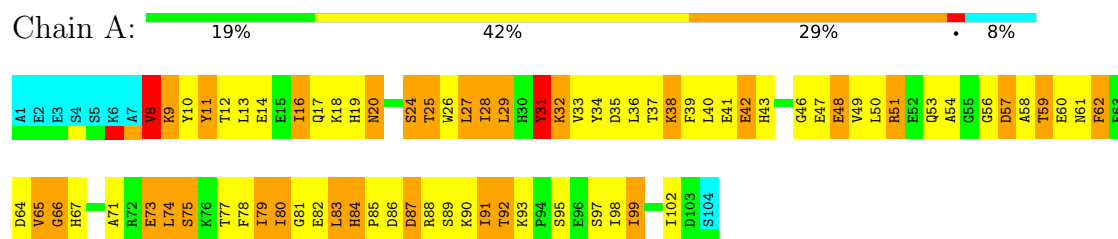
4.2.27 Score per residue for model 27

- Molecule 1: CYTOCHROME B5



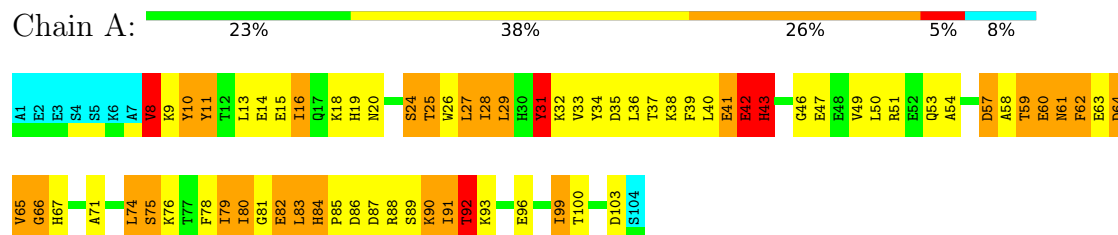
4.2.28 Score per residue for model 28

- Molecule 1: CYTOCHROME B5



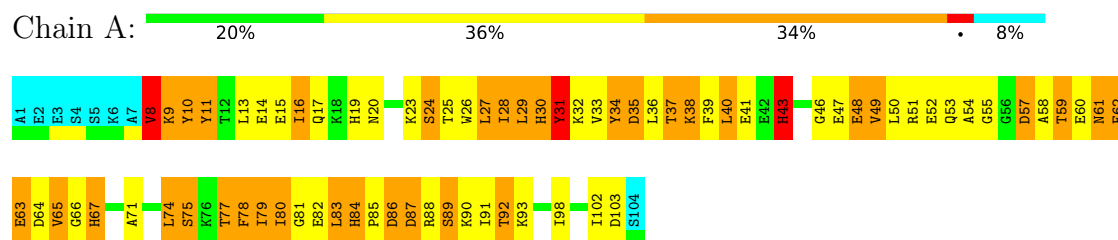
4.2.29 Score per residue for model 29

- Molecule 1: CYTOCHROME B5



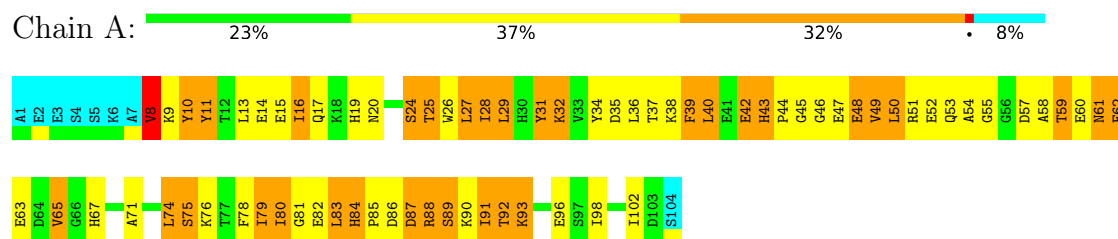
4.2.30 Score per residue for model 30

- Molecule 1: CYTOCHROME B5



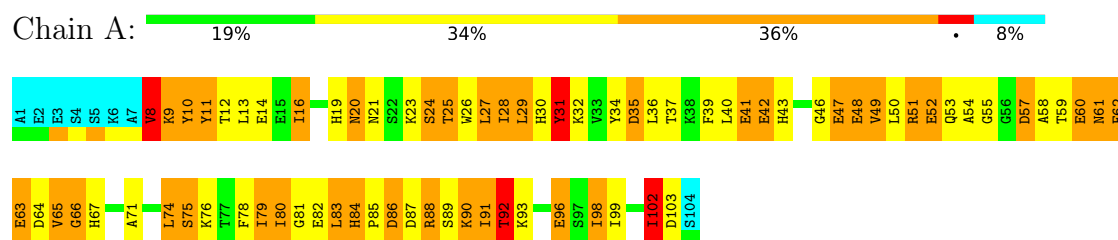
4.2.31 Score per residue for model 31

- Molecule 1: CYTOCHROME B5



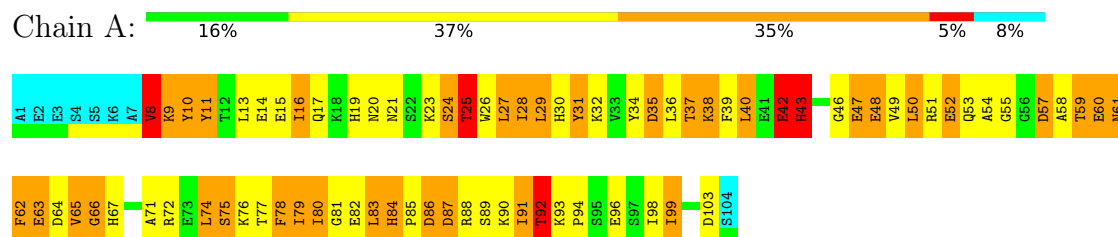
4.2.32 Score per residue for model 32

- Molecule 1: CYTOCHROME B5



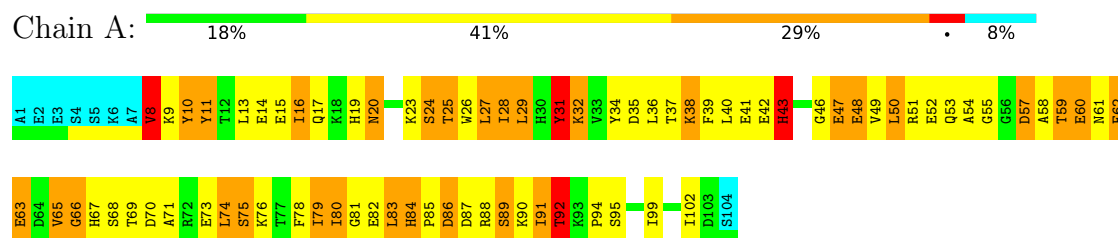
4.2.33 Score per residue for model 33

- Molecule 1: CYTOCHROME B5



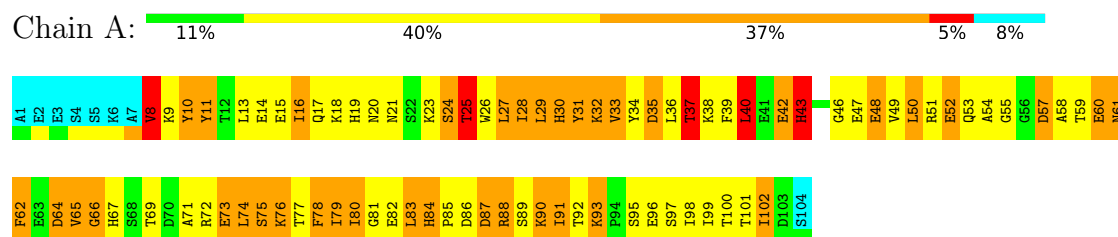
4.2.34 Score per residue for model 34

- Molecule 1: CYTOCHROME B5



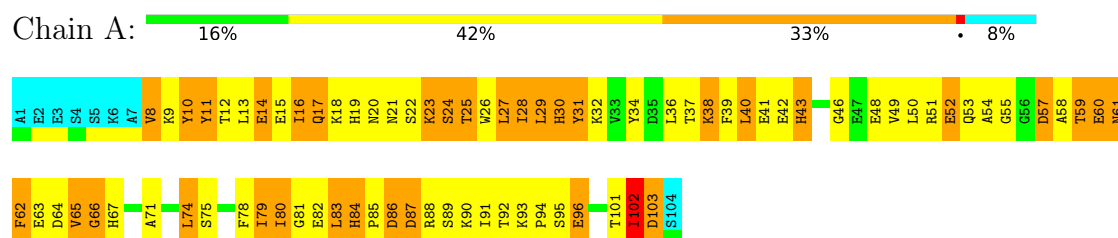
4.2.35 Score per residue for model 35

- Molecule 1: CYTOCHROME B5



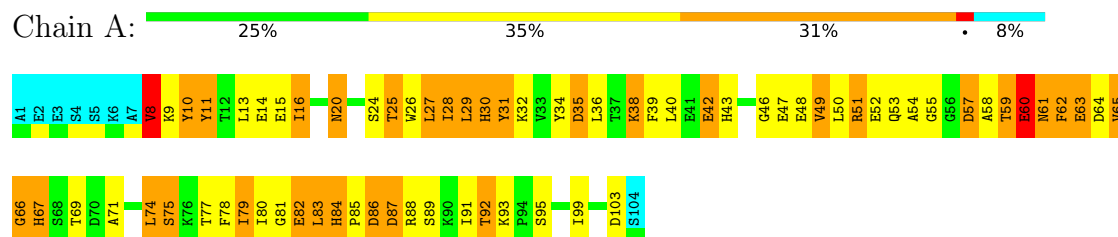
4.2.36 Score per residue for model 36

- Molecule 1: CYTOCHROME B5



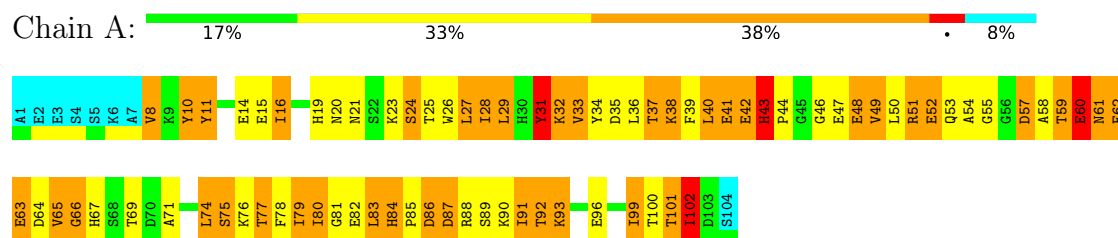
4.2.37 Score per residue for model 37

- Molecule 1: CYTOCHROME B5



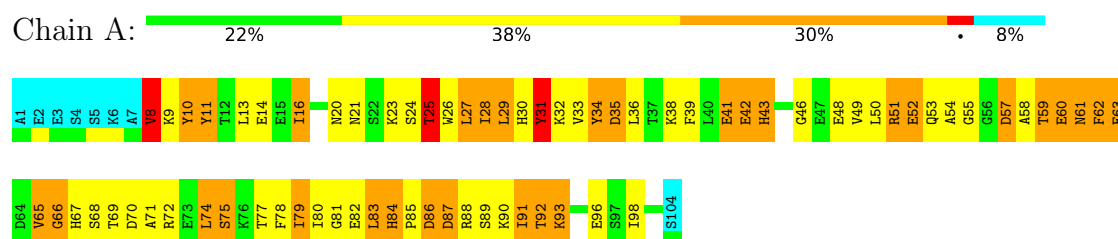
4.2.38 Score per residue for model 38

- Molecule 1: CYTOCHROME B5



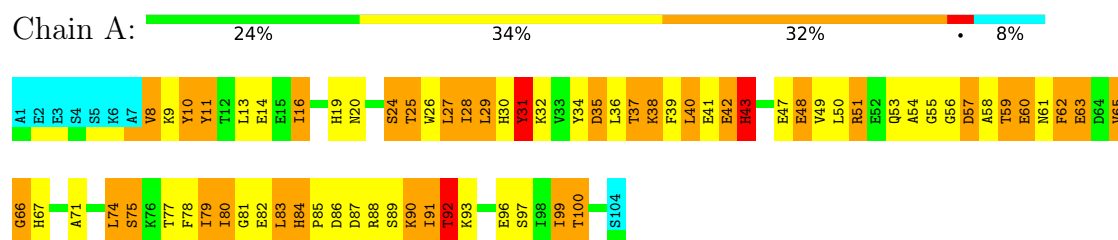
4.2.39 Score per residue for model 39

- Molecule 1: CYTOCHROME B5



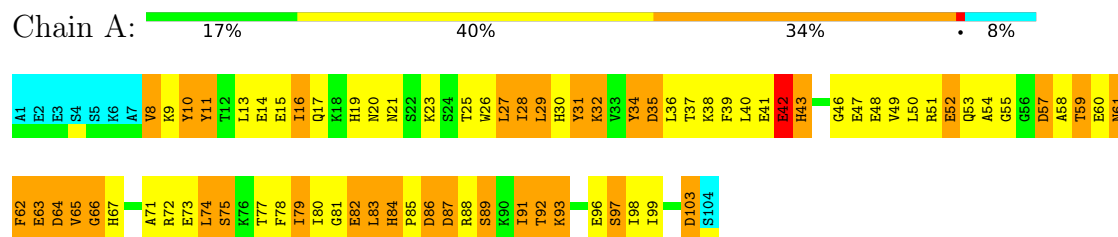
4.2.40 Score per residue for model 40

- Molecule 1: CYTOCHROME B5



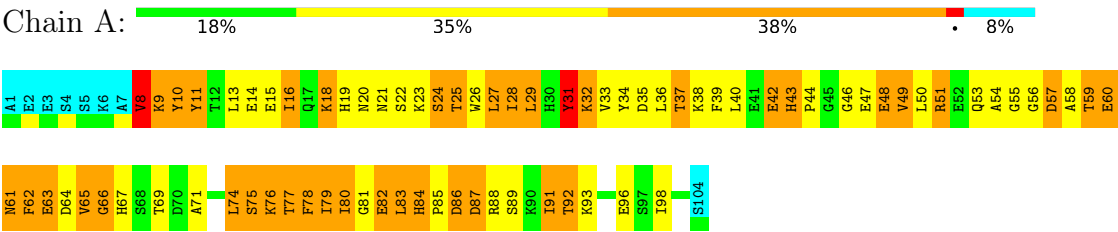
4.2.41 Score per residue for model 41

- Molecule 1: CYTOCHROME B5



4.2.42 Score per residue for model 42

● Molecule 1: CYTOCHROME B5



5 Refinement protocol and experimental data overview ⓘ

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.

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

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	0.75±0.01	0±0/794 (0.0± 0.0%)	1.13±0.01	0±0/1075 (0.0± 0.0%)
All	All	0.75	0/33348 (0.0%)	1.13	2/45150 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	31	TYR	N-CA-CB	-5.23	105.96	113.65	20	2

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	155±13
2	A	43	20	30	13±3
All	All	34440	32508	32718	6538

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 97.

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:83:LEU:HD23	1:A:91:ILE:HD13	1.11	1.21	40	28
1:A:16:ILE:HD13	1:A:28:ILE:HD11	1.11	1.15	16	35
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
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:28:ILE:HD13	1:A:83:LEU:HD23	0.93	1.41	20	8
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: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:33:VAL:HG12	1:A:81:GLY:C	0.84	1.96	39	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:33:VAL:HG22	1:A:81:GLY:C	0.82	2.00	25	8
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
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:13:LEU:HD12	1:A:87:ASP:CG	0.79	2.03	35	19
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: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:35:ASP:CG	1:A:35:ASP:O	0.75	2.29	15	2
1:A:39:PHE:CD2	1:A:78:PHE:CD2	0.75	2.75	34	5
1:A:20:ASN:CG	1:A:20:ASN:O	0.75	2.30	9	33
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ASP:OD1	1:A:80:ILE:HG21	0.74	1.82	13	3
1:A:39:PHE:CE2	1:A:78:PHE:CB	0.74	2.70	22	1
1:A:58:ALA:HB1	2:A:105:HEM:HMC2	0.74	1.59	23	15
1:A:39:PHE:CE1	1:A:78:PHE:CB	0.74	2.71	40	5
1:A:8:VAL:HG21	1:A:11:TYR:CD2	0.74	2.18	37	16
1:A:29:LEU:HD21	1:A:62:PHE:CD2	0.74	2.17	1	12
1:A:43:HIS:HD1	1:A:50:LEU:HD11	0.74	1.42	42	13
1:A:39:PHE:CE2	1:A:78:PHE:CD2	0.73	2.76	34	2
1:A:34:TYR:CE2	1:A:79:ILE:CG1	0.73	2.71	30	40
1:A:29:LEU:CB	1:A:34:TYR:CE1	0.73	2.72	22	27
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
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:65:VAL:HG11	1:A:67:HIS:CE1	0.72	2.18	1	1
1:A:19:HIS:CD2	1:A:26:TRP:CD1	0.72	2.77	12	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:39:PHE:CZ	2:A:105:HEM:HMB3	0.72	2.19	20	3
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:62:PHE:CD1	1:A:62:PHE:C	0.71	2.68	1	29
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:30:HIS:C	1:A:31:TYR:CG	0.70	2.68	30	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:29:LEU:HD21	1:A:62:PHE:CD1	0.70	2.22	14	21
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: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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:27:LEU:C	1:A:27:LEU:HD13	0.69	2.13	34	37
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:8:VAL:CG2	1:A:11:TYR:CD2	0.68	2.76	37	10
1:A:39:PHE:CZ	1:A:78:PHE:CG	0.68	2.81	40	2
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:CD1	1:A:31:TYR:O	0.68	2.47	14	20
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:36:LEU:HD22	1:A:50:LEU:CD2	0.67	2.19	37	28
1:A:50:LEU:O	1:A:53:GLN:CG	0.67	2.42	34	42
1:A:31:TYR:CD1	1:A:31:TYR:N	0.67	2.60	30	2
1:A:83:LEU:HD23	1:A:91:ILE:HD11	0.67	1.64	11	4
1:A:13:LEU:HD11	1:A:91:ILE:CG2	0.67	2.19	18	13
1:A:26:TRP:CH2	1:A:35:ASP:CG	0.67	2.72	21	10
1:A:58:ALA:HB1	2:A:105:HEM:HMC3	0.67	1.64	24	10
1:A:30:HIS:ND1	1:A:31:TYR:CE2	0.67	2.62	4	1
1:A:43:HIS:CE1	1:A:49:VAL:CG2	0.67	2.77	8	14
1:A:35:ASP:O	1:A:39:PHE:CD2	0.67	2.48	22	1
2:A:105:HEM:O1A	2:A:105:HEM:C2A	0.67	2.48	23	14
1:A:25:THR:HG21	1:A:40:LEU:HD21	0.67	1.64	22	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:PHE:CD2	1:A:50:LEU:HD21	0.67	2.25	12	11
1:A:11:TYR:CE1	1:A:15:GLU:CD	0.67	2.73	16	4
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:26:TRP:CZ3	1:A:80:ILE:HD12	0.66	2.24	4	5
1:A:57:ASP:CB	1:A:91:ILE:HD12	0.66	2.20	32	7
1:A:26:TRP:CZ2	1:A:35:ASP:CG	0.66	2.74	20	10
1:A:26:TRP:CE3	1:A:80:ILE:CD1	0.66	2.78	4	3
1:A:24:SER:O	1:A:26:TRP:CD1	0.66	2.48	36	9
1:A:39:PHE:CG	1:A:78:PHE:CD2	0.66	2.83	22	1
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
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:38:LYS:CB	1:A:78:PHE:CE2	0.66	2.79	38	2
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: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: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:39:PHE:CD1	1:A:78:PHE:CE2	0.64	2.86	19	7
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:19:HIS:ND1	1:A:26:TRP:CE2	0.64	2.66	1	8
1:A:39:PHE:CZ	1:A:78:PHE:CB	0.64	2.81	24	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:TYR:CD1	1:A:88:ARG:NH1	0.64	2.66	40	1
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	8	4
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
1:A:65:VAL:CG1	1:A:67:HIS:CE1	0.63	2.81	1	1
2:A:105:HEM:C2A	2:A:105:HEM:O2A	0.63	2.52	21	5
1:A:26:TRP:CZ2	1:A:35:ASP:OD1	0.63	2.51	20	1
1:A:25:THR:CG2	1:A:54:ALA:HB2	0.63	2.24	16	8
1:A:61:ASN:O	1:A:65:VAL:HG12	0.63	1.94	15	27
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: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:19:HIS:ND1	1:A:26:TRP:CD2	0.62	2.67	42	7
1:A:91:ILE:O	1:A:92:THR:C	0.62	2.43	19	41
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	2:A:105:HEM:HMB3	0.62	2.30	10	12
1:A:39:PHE:CE2	1:A:78:PHE:HB3	0.62	2.30	22	1
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: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:26:TRP:CE2	1:A:80:ILE:CD1	0.61	2.83	36	3
1:A:19:HIS:CG	1:A:26:TRP:CZ3	0.61	2.87	6	2
1:A:16:ILE:CD1	1:A:28:ILE:CD1	0.61	2.78	12	13
1:A:29:LEU:HB3	1:A:34:TYR:CE1	0.61	2.30	11	23
1:A:13:LEU:HD21	1:A:91:ILE:CD1	0.61	2.26	24	3
1:A:39:PHE:CZ	1:A:78:PHE:HA	0.61	2.30	22	1
1:A:34:TYR:N	1:A:34:TYR:CD1	0.61	2.69	27	41
1:A:27:LEU:HD13	1:A:27:LEU:O	0.61	1.94	34	32

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:GLN:OE1	1:A:58:ALA:CB	0.61	2.48	5	21
2:A:105:HEM:O2A	2:A:105:HEM:C2A	0.61	2.54	4	2
1:A:30:HIS:O	1:A:31:TYR:CD2	0.61	2.54	3	1
1:A:40:LEU:HD22	1:A:47:GLU:CB	0.61	2.26	10	6
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: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:99:ILE:C	1:A:99:ILE:HD13	0.60	2.21	38	2
1:A:11:TYR:CE1	1:A:15:GLU:OE2	0.60	2.54	33	1
1:A:13:LEU:HD23	1:A:28:ILE:CD1	0.60	2.26	36	2
1:A:20:ASN:O	1:A:20:ASN:ND2	0.60	2.33	39	28
1:A:26:TRP:CZ3	1:A:80:ILE:HG12	0.60	2.31	37	3
1:A:10:TYR:HB3	1:A:84:HIS:CD2	0.60	2.32	39	27
1:A:36:LEU:HD13	1:A:50:LEU:CA	0.60	2.26	39	37
1:A:88:ARG:C	1:A:90:LYS:H	0.60	2.04	8	9
1:A:8:VAL:HG21	1:A:11:TYR:CD1	0.60	2.31	38	1
1:A:31:TYR:O	1:A:31:TYR:CG	0.60	2.55	38	4
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:39:PHE:CB	1:A:50:LEU:HD22	0.60	2.27	40	4
1:A:11:TYR:CD2	1:A:15:GLU:OE1	0.60	2.55	14	2
1:A:38:LYS:HB2	1:A:78:PHE:CE2	0.60	2.31	38	7
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:38:LYS:HG2	1:A:78:PHE:CE1	0.59	2.33	38	2
1:A:39:PHE:N	1:A:39:PHE:CD1	0.59	2.68	38	3
1:A:39:PHE:HB2	1:A:78:PHE:CE2	0.59	2.33	7	15
1:A:13:LEU:CD2	1:A:83:LEU:HD21	0.59	2.27	14	5
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	4
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:30:HIS:C	1:A:31:TYR:CD2	0.59	2.80	3	1
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:49:VAL:HG13	1:A:50:LEU:HG	0.59	1.74	24	11
1:A:39:PHE:CD1	1:A:78:PHE:CD1	0.59	2.90	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:PHE:C	1:A:50:LEU:HD13	0.59	2.21	38	4
1:A:36:LEU:CD1	1:A:50:LEU:O	0.59	2.51	40	29
1:A:83:LEU:HD12	1:A:83:LEU:C	0.59	2.22	25	20
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:11:TYR:CD2	1:A:26:TRP:CZ3	0.58	2.91	11	5
1:A:20:ASN:ND2	1:A:55:GLY:CA	0.58	2.66	16	1
1:A:101:THR:O	1:A:102:ILE:C	0.58	2.45	36	1
1:A:16:ILE:O	1:A:55:GLY:HA2	0.58	1.98	36	29
1:A:11:TYR:CE2	1:A:15:GLU:CG	0.58	2.85	41	5
1:A:25:THR:CG2	1:A:54:ALA:CB	0.58	2.81	41	14
1:A:29:LEU:HB2	1:A:34:TYR:CE1	0.58	2.32	22	15
1:A:38:LYS:NZ	1:A:74:LEU:CD1	0.58	2.66	35	1
1:A:26:TRP:CE3	1:A:80:ILE:HD12	0.58	2.33	32	4
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: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:27:LEU:HD22	1:A:28:ILE:C	0.58	2.24	22	41
1:A:67:HIS:CE1	2:A:105:HEM:C1C	0.58	2.92	31	28
1:A:65:VAL:CG2	1:A:65:VAL:O	0.58	2.52	18	19
1:A:43:HIS:NE2	2:A:105:HEM:NA	0.57	2.52	30	6
1:A:28:ILE:HB	1:A:57:ASP:HA	0.57	1.74	36	19
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: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:48:GLU:O	1:A:51:ARG:N	0.57	2.38	8	18
1:A:36:LEU:HA	1:A:39:PHE:CD1	0.57	2.35	28	6
1:A:19:HIS:NE2	1:A:26:TRP:CZ3	0.57	2.71	16	1
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:53:GLN:NE2	2:A:105:HEM:C2C	0.57	2.72	37	36
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:53:GLN:NE2	2:A:105:HEM:HMC3	0.56	2.15	5	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:PHE:CE1	1:A:78:PHE:HB3	0.56	2.35	24	4
1:A:38:LYS:O	1:A:39:PHE:CD1	0.56	2.58	22	1
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:HD22	1:A:20:ASN:N	0.56	1.98	34	2
1:A:61:ASN:CG	2:A:105:HEM:CBC	0.56	2.79	37	1
1:A:19:HIS:ND1	1:A:24:SER:CB	0.56	2.69	1	7
1:A:11:TYR:CD1	1:A:15:GLU:HB3	0.56	2.35	13	4
1:A:27:LEU:HD13	1:A:27:LEU:C	0.56	2.26	19	3
1:A:34:TYR:CE2	1:A:75:SER:HB3	0.56	2.35	35	6
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:39:PHE:HB3	1:A:50:LEU:HD22	0.56	1.77	40	4
1:A:38:LYS:HG2	1:A:78:PHE:CZ	0.56	2.35	38	1
1:A:38:LYS:HG2	1:A:78:PHE:CD1	0.56	2.35	42	1
1:A:30:HIS:CG	1:A:31:TYR:CZ	0.56	2.93	4	1
1:A:19:HIS:CD2	1:A:24:SER:HB3	0.56	2.36	12	1
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:43:HIS:NE2	2:A:105:HEM:ND	0.56	2.53	38	2
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:65:VAL:O	1:A:65:VAL:CG2	0.56	2.54	37	13
1:A:41:GLU:O	1:A:42:GLU:C	0.55	2.49	29	3
1:A:77:THR:CG2	1:A:78:PHE:CE1	0.55	2.89	9	4
1:A:65:VAL:CG2	1:A:67:HIS:CE1	0.55	2.88	2	8
1:A:27:LEU:HD22	1:A:27:LEU:C	0.55	2.25	7	16
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:65:VAL:HG23	1:A:65:VAL:O	0.55	2.01	30	3
1:A:53:GLN:HB2	1:A:58:ALA:HB2	0.55	1.76	42	4
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:31:TYR:C	1:A:31:TYR:CD1	0.55	2.85	12	4
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LEU:C	1:A:30:HIS:CG	0.55	2.84	26	4
1:A:29:LEU:CD1	2:A:105:HEM:CBB	0.55	2.84	32	26
1:A:39:PHE:CE2	1:A:74:LEU:CD2	0.55	2.87	10	2
1:A:11:TYR:CE2	1:A:15:GLU:HG3	0.55	2.36	38	5
1:A:39:PHE:HE2	1:A:74:LEU:HD21	0.55	1.58	35	3
1:A:57:ASP:OD2	1:A:59:THR:CG2	0.55	2.54	36	6
1:A:39:PHE:CE2	1:A:78:PHE:HA	0.55	2.37	22	1
1:A:35:ASP:OD1	1:A:35:ASP:C	0.55	2.49	40	4
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:65:VAL:O	1:A:65:VAL:HG23	0.55	2.02	37	9
1:A:33:VAL:HG12	1:A:82:GLU:N	0.55	2.16	4	2
1:A:38:LYS:HB2	1:A:78:PHE:CD1	0.55	2.36	26	1
1:A:40:LEU:HD23	1:A:47:GLU:OE2	0.55	2.02	40	1
1:A:59:THR:O	1:A:60:GLU:C	0.55	2.50	35	15
1:A:53:GLN:CD	2:A:105:HEM:HMC3	0.55	2.26	37	20
1:A:39:PHE:O	1:A:40:LEU:C	0.55	2.48	10	2
1:A:102:ILE:HD12	1:A:103:ASP:N	0.55	2.17	12	1
1:A:30:HIS:N	1:A:30:HIS:ND1	0.55	2.54	30	1
1:A:21:ASN:C	1:A:25:THR:HG23	0.55	2.26	32	3
1:A:34:TYR:CZ	1:A:79:ILE:HD11	0.54	2.37	8	13
1:A:59:THR:HG22	1:A:60:GLU:N	0.54	2.17	38	10
1:A:25:THR:HG22	1:A:54:ALA:HB3	0.54	1.79	5	1
1:A:39:PHE:O	1:A:50:LEU:CD1	0.54	2.56	42	7
1:A:61:ASN:HB3	2:A:105:HEM:HMC3	0.54	1.77	9	1
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:34:TYR:CE2	1:A:79:ILE:HG12	0.54	2.36	20	16
1:A:53:GLN:CD	2:A:105:HEM:HMC2	0.54	2.27	9	10
1:A:28:ILE:HA	1:A:32:LYS:O	0.54	2.01	30	14
1:A:57:ASP:C	1:A:57:ASP:OD1	0.54	2.50	28	10
1:A:26:TRP:CE2	1:A:80:ILE:HD13	0.54	2.38	36	2
1:A:42:GLU:O	1:A:43:HIS:CB	0.54	2.54	8	24
1:A:101:THR:HG23	1:A:101:THR:O	0.54	2.02	10	2
1:A:32:LYS:HG3	1:A:79:ILE:HD11	0.54	1.79	12	6
1:A:26:TRP:CH2	1:A:35:ASP:HB2	0.54	2.38	39	1
1:A:38:LYS:HB3	1:A:78:PHE:CD2	0.54	2.38	40	1
1:A:65:VAL:O	1:A:66:GLY:C	0.54	2.51	4	31
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LEU:O	1:A:47:GLU:CG	0.54	2.56	26	7
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:73:GLU:O	1:A:76:LYS:CG	0.54	2.56	6	9
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: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:88:ARG:C	1:A:90:LYS:N	0.54	2.63	24	15
1:A:33:VAL:CG2	1:A:81:GLY:C	0.54	2.80	38	4
1:A:88:ARG:O	1:A:92:THR:CB	0.53	2.57	4	6
1:A:41:GLU:O	1:A:43:HIS:N	0.53	2.41	9	2
1:A:33:VAL:HG22	1:A:82:GLU:N	0.53	2.18	23	8
1:A:84:HIS:O	1:A:88:ARG:CD	0.53	2.56	38	4
1:A:26:TRP:CE3	1:A:35:ASP:CA	0.53	2.91	41	2
1:A:28:ILE:CG2	1:A:32:LYS:O	0.53	2.56	20	13
1:A:48:GLU:O	1:A:50:LEU:N	0.53	2.41	9	38
1:A:19:HIS:C	1:A:24:SER:O	0.53	2.52	22	25
1:A:62:PHE:HA	1:A:65:VAL:HG13	0.53	1.80	26	14
1:A:21:ASN:C	1:A:23:LYS:H	0.53	2.12	42	6
1:A:39:PHE:CE1	1:A:42:GLU:CB	0.53	2.92	6	1
1:A:74:LEU:HD12	1:A:78:PHE:HE1	0.53	1.64	40	2
1:A:32:LYS:CG	1:A:34:TYR:OH	0.53	2.57	11	2
1:A:40:LEU:HD23	1:A:47:GLU:HG2	0.53	1.79	31	2
1:A:38:LYS:HG3	1:A:78:PHE:CD2	0.53	2.38	35	1
2:A:105:HEM:O1A	2:A:105:HEM:C3A	0.53	2.62	36	7
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:39:PHE:CE2	1:A:75:SER:HA	0.53	2.39	30	5
1:A:39:PHE:CE1	1:A:42:GLU:HB2	0.53	2.38	6	2
1:A:20:ASN:OD1	1:A:54:ALA:O	0.53	2.27	21	6
1:A:11:TYR:CZ	1:A:15:GLU:CD	0.53	2.86	14	1
1:A:48:GLU:O	1:A:49:VAL:C	0.53	2.51	8	38
1:A:99:ILE:C	1:A:99:ILE:CD1	0.53	2.82	10	1
1:A:30:HIS:O	1:A:31:TYR:CG	0.53	2.61	30	1
1:A:59:THR:O	1:A:61:ASN:N	0.53	2.42	27	8
1:A:62:PHE:HA	1:A:65:VAL:CG1	0.53	2.34	20	24
1:A:38:LYS:HB3	1:A:78:PHE:CD1	0.53	2.39	10	13
1:A:33:VAL:C	1:A:34:TYR:CD1	0.53	2.87	20	1
1:A:26:TRP:CD1	1:A:80:ILE:HD13	0.53	2.38	24	2
1:A:39:PHE:O	1:A:42:GLU:N	0.53	2.41	20	8
1:A:43:HIS:HE1	1:A:49:VAL:HG21	0.53	1.64	19	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:SER:HA	1:A:92:THR:CG2	0.53	2.34	24	15
1:A:31:TYR:CD2	1:A:32:LYS:HG3	0.53	2.39	9	7
1:A:11:TYR:CD2	1:A:15:GLU:CD	0.53	2.87	31	1
1:A:11:TYR:CD1	1:A:15:GLU:HG3	0.53	2.39	31	1
1:A:50:LEU:O	1:A:53:GLN:HG3	0.52	2.03	32	36
1:A:33:VAL:HG23	1:A:82:GLU:C	0.52	2.29	3	7
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:30:HIS:C	1:A:31:TYR:CD1	0.52	2.87	30	1
1:A:67:HIS:CE1	2:A:105:HEM:C1A	0.52	2.97	13	5
2:A:105:HEM:O2A	2:A:105:HEM:C3A	0.52	2.61	21	5
1:A:35:ASP:OD2	1:A:78:PHE:O	0.52	2.27	37	4
1:A:21:ASN:C	1:A:25:THR:HG1	0.52	2.11	16	1
1:A:26:TRP:CH2	1:A:80:ILE:CG2	0.52	2.92	41	1
1:A:19:HIS:ND1	1:A:26:TRP:CH2	0.52	2.75	6	1
1:A:32:LYS:HG3	1:A:34:TYR:CZ	0.52	2.39	12	5
1:A:29:LEU:HD11	2:A:105:HEM:CAB	0.52	2.34	26	3
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: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
1:A:25:THR:O	1:A:36:LEU:N	0.52	2.42	24	23
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:38:LYS:HB3	1:A:78:PHE:CE1	0.52	2.40	29	10
1:A:11:TYR:CE1	1:A:15:GLU:HG3	0.52	2.40	14	2
1:A:78:PHE:CD1	1:A:78:PHE:N	0.52	2.78	40	1
1:A:20:ASN:ND2	1:A:51:ARG:O	0.52	2.43	15	11
1:A:29:LEU:C	1:A:31:TYR:H	0.52	2.13	41	13
1:A:31:TYR:CE2	1:A:32:LYS:HD2	0.52	2.40	36	3
1:A:48:GLU:C	1:A:50:LEU:N	0.52	2.67	15	40
1:A:8:VAL:HB	1:A:11:TYR:CE2	0.52	2.40	18	2
1:A:29:LEU:CD2	1:A:62:PHE:CD1	0.51	2.94	14	2
1:A:16:ILE:HG21	1:A:28:ILE:HD11	0.51	1.81	3	5
1:A:27:LEU:CD2	1:A:58:ALA:HB3	0.51	2.29	14	11
1:A:43:HIS:CB	1:A:50:LEU:HD11	0.51	2.34	7	1
1:A:50:LEU:C	1:A:53:GLN:HG2	0.51	2.30	25	42
1:A:57:ASP:CG	1:A:59:THR:HG22	0.51	2.31	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LYS:HB2	1:A:78:PHE:CG	0.51	2.41	26	1
1:A:39:PHE:CE1	1:A:42:GLU:HB3	0.51	2.41	7	11
1:A:59:THR:C	1:A:61:ASN:N	0.51	2.68	9	16
1:A:49:VAL:HG22	2:A:105:HEM:C4C	0.51	2.40	18	5
1:A:78:PHE:O	1:A:80:ILE:HG23	0.51	2.05	14	2
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:20:ASN:CG	1:A:54:ALA:O	0.51	2.53	7	6
1:A:11:TYR:CE2	1:A:15:GLU:HG2	0.51	2.41	11	6
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:26:TRP:CD1	1:A:35:ASP:OD1	0.51	2.64	33	3
1:A:10:TYR:HB2	1:A:84:HIS:CE1	0.51	2.40	33	4
1:A:98:ILE:HD13	1:A:98:ILE:C	0.51	2.30	13	2
1:A:77:THR:HG22	1:A:78:PHE:HD1	0.51	1.66	18	2
1:A:11:TYR:CE2	1:A:15:GLU:CD	0.51	2.89	14	2
1:A:8:VAL:HG11	1:A:80:ILE:HD13	0.51	1.81	20	1
1:A:17:GLN:O	1:A:20:ASN:ND2	0.51	2.43	23	4
1:A:31:TYR:CE1	1:A:88:ARG:NE	0.51	2.79	24	3
1:A:11:TYR:CZ	1:A:15:GLU:OE2	0.51	2.64	14	1
1:A:19:HIS:CE1	1:A:24:SER:HB3	0.51	2.41	17	3
1:A:27:LEU:HD11	1:A:34:TYR:HB2	0.51	1.81	15	15
1:A:92:THR:CG2	1:A:93:LYS:N	0.51	2.74	18	13
1:A:34:TYR:CE2	1:A:79:ILE:HD11	0.51	2.41	42	6
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:19:HIS:HB3	1:A:24:SER:O	0.51	2.06	21	7
1:A:26:TRP:CD2	1:A:80:ILE:HD12	0.50	2.41	11	2
1:A:65:VAL:HG22	1:A:67:HIS:CE1	0.50	2.42	16	4
1:A:34:TYR:CE2	1:A:75:SER:CB	0.50	2.94	19	2
1:A:35:ASP:O	1:A:35:ASP:CG	0.50	2.54	40	1
1:A:21:ASN:O	1:A:25:THR:N	0.50	2.44	18	7
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:98:ILE:H	1:A:98:ILE:HD13	0.50	1.66	1	2
1:A:65:VAL:HG22	1:A:67:HIS:ND1	0.50	2.20	16	8
1:A:29:LEU:CD2	1:A:59:THR:OG1	0.50	2.60	13	5
1:A:46:GLY:O	1:A:47:GLU:C	0.50	2.53	15	18
1:A:29:LEU:HD13	1:A:30:HIS:CE1	0.50	2.42	30	3
1:A:39:PHE:HZ	1:A:74:LEU:HD21	0.50	1.60	10	1
1:A:39:PHE:CE2	2:A:105:HEM:CMB	0.50	2.94	10	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:HIS:HB2	1:A:31:TYR:CD1	0.50	2.42	35	3
1:A:30:HIS:HB3	1:A:31:TYR:CE1	0.50	2.42	4	1
1:A:19:HIS:NE2	1:A:26:TRP:CH2	0.50	2.80	17	1
1:A:102:ILE:C	1:A:102:ILE:HD12	0.50	2.32	34	1
1:A:31:TYR:CD1	1:A:31:TYR:C	0.50	2.89	14	6
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:36:LEU:C	1:A:38:LYS:N	0.50	2.68	30	14
1:A:75:SER:HA	1:A:78:PHE:CD2	0.50	2.42	7	3
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:39:PHE:CZ	2:A:105:HEM:HBB	0.50	2.41	33	3
1:A:74:LEU:O	1:A:77:THR:CB	0.50	2.60	42	5
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:39:PHE:CB	1:A:78:PHE:CE2	0.49	2.94	7	6
1:A:13:LEU:CA	1:A:16:ILE:HD12	0.49	2.37	2	9
1:A:29:LEU:HD23	1:A:59:THR:OG1	0.49	2.07	11	8
1:A:43:HIS:HD1	1:A:49:VAL:HG11	0.49	1.67	3	7
1:A:39:PHE:HB2	1:A:78:PHE:CZ	0.49	2.42	39	3
1:A:85:PRO:HA	1:A:88:ARG:CG	0.49	2.38	39	15
1:A:11:TYR:CD2	1:A:15:GLU:HG2	0.49	2.41	17	2
1:A:15:GLU:CD	1:A:15:GLU:C	0.49	2.80	31	1
1:A:26:TRP:CZ3	1:A:80:ILE:CG1	0.49	2.94	41	3
1:A:26:TRP:NE1	1:A:35:ASP:CG	0.49	2.71	26	2
1:A:20:ASN:N	1:A:20:ASN:ND2	0.49	2.61	34	1
1:A:25:THR:HG22	1:A:54:ALA:HB1	0.49	1.81	5	1
1:A:39:PHE:CZ	1:A:74:LEU:HD11	0.49	2.41	5	4
1:A:74:LEU:CD1	1:A:78:PHE:CE1	0.49	2.95	20	5
1:A:91:ILE:C	1:A:93:LYS:N	0.49	2.71	40	7
1:A:11:TYR:CE1	1:A:15:GLU:OE1	0.49	2.65	30	2
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:21:ASN:O	1:A:25:THR:OG1	0.49	2.30	36	6
1:A:27:LEU:CD1	1:A:34:TYR:HB2	0.49	2.38	31	18
1:A:57:ASP:OD1	1:A:57:ASP:C	0.49	2.56	17	9
1:A:61:ASN:O	1:A:65:VAL:CG1	0.49	2.61	11	12
1:A:61:ASN:ND2	2:A:105:HEM:CAC	0.49	2.75	9	1
1:A:81:GLY:C	1:A:82:GLU:CG	0.49	2.85	33	41
1:A:39:PHE:CE2	2:A:105:HEM:CHB	0.49	2.96	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:O	1:A:38:LYS:N	0.49	2.45	30	5
1:A:35:ASP:OD1	1:A:38:LYS:N	0.49	2.45	39	1
1:A:26:TRP:CH2	1:A:80:ILE:HD12	0.49	2.43	3	2
1:A:8:VAL:HG11	1:A:80:ILE:CG1	0.49	2.38	37	2
1:A:28:ILE:HD12	1:A:33:VAL:HG22	0.49	1.84	14	2
1:A:46:GLY:O	1:A:49:VAL:N	0.49	2.45	17	11
1:A:19:HIS:C	1:A:20:ASN:ND2	0.49	2.71	34	2
1:A:38:LYS:HB2	1:A:78:PHE:CD2	0.49	2.43	26	3
1:A:20:ASN:OD1	1:A:55:GLY:HA3	0.49	2.08	34	1
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:10:TYR:HB3	1:A:84:HIS:CE1	0.49	2.42	38	2
1:A:11:TYR:CD2	1:A:15:GLU:HB3	0.48	2.43	36	4
1:A:42:GLU:O	1:A:43:HIS:HB2	0.48	2.08	9	6
1:A:84:HIS:HB3	1:A:85:PRO:HD2	0.48	1.83	8	23
1:A:57:ASP:OD1	1:A:59:THR:N	0.48	2.47	33	7
1:A:19:HIS:CA	1:A:24:SER:O	0.48	2.61	21	3
1:A:39:PHE:CZ	2:A:105:HEM:CMB	0.48	2.93	20	2
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:92:THR:O	1:A:93:LYS:C	0.48	2.57	10	6
1:A:39:PHE:CE1	2:A:105:HEM:HMB3	0.48	2.41	20	1
1:A:63:GLU:OE1	1:A:93:LYS:CE	0.48	2.61	25	1
1:A:62:PHE:CD2	1:A:67:HIS:HB2	0.48	2.42	30	3
1:A:20:ASN:OD1	1:A:55:GLY:CA	0.48	2.61	34	1
1:A:22:SER:HA	1:A:40:LEU:HD11	0.48	1.85	42	1
1:A:29:LEU:O	1:A:31:TYR:N	0.48	2.43	36	15
1:A:62:PHE:CE2	1:A:67:HIS:HB2	0.48	2.43	16	6
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: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:16:ILE:CG2	1:A:26:TRP:C	0.48	2.87	7	1
1:A:27:LEU:CD2	1:A:28:ILE:O	0.48	2.62	16	4
1:A:29:LEU:CD2	1:A:59:THR:HA	0.48	2.38	30	7
1:A:9:LYS:HB3	1:A:10:TYR:CE1	0.48	2.43	23	1
1:A:20:ASN:ND2	1:A:55:GLY:HA3	0.48	2.24	32	2
1:A:38:LYS:CG	1:A:78:PHE:CE2	0.48	2.96	38	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LEU:O	1:A:41:GLU:C	0.48	2.57	1	9
1:A:71:ALA:CB	2:A:105:HEM:HMA2	0.48	2.39	33	11
1:A:9:LYS:O	1:A:82:GLU:N	0.48	2.46	33	25
1:A:86:ASP:O	1:A:87:ASP:CG	0.48	2.57	37	16
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:38:LYS:CG	1:A:78:PHE:CE1	0.48	2.97	33	2
1:A:41:GLU:O	1:A:42:GLU:O	0.48	2.32	13	9
1:A:64:ASP:C	1:A:66:GLY:N	0.48	2.72	21	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	2.08	12	14
1:A:91:ILE:O	1:A:93:LYS:O	0.48	2.31	7	1
1:A:8:VAL:HB	1:A:11:TYR:CE1	0.48	2.44	10	4
1:A:19:HIS:CD2	1:A:26:TRP:CD2	0.48	3.02	32	1
1:A:19:HIS:CB	1:A:26:TRP:CG	0.48	2.97	12	1
1:A:39:PHE:CZ	1:A:78:PHE:HB3	0.48	2.43	24	1
1:A:28:ILE:HG12	1:A:56:GLY:C	0.47	2.33	40	9
1:A:53:GLN:NE2	2:A:105:HEM:HMC2	0.47	2.23	35	4
1:A:38:LYS:C	1:A:39:PHE:CD1	0.47	2.92	22	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:8:VAL:CG2	1:A:9:LYS:N	0.47	2.76	26	5
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:101:THR:O	1:A:101:THR:HG23	0.47	2.09	35	1
1:A:19:HIS:CB	1:A:26:TRP:CD1	0.47	2.97	7	2
1:A:31:TYR:CZ	1:A:92:THR:CB	0.47	2.97	13	4
1:A:39:PHE:CE2	1:A:75:SER:OG	0.47	2.68	28	1
1:A:65:VAL:HG21	2:A:105:HEM:C1D	0.47	2.44	1	3
1:A:58:ALA:O	1:A:59:THR:C	0.47	2.58	35	4
1:A:32:LYS:HB2	1:A:34:TYR:CE1	0.47	2.45	30	2
1:A:19:HIS:C	1:A:20:ASN:HD22	0.47	2.18	34	1
1:A:74:LEU:HD12	1:A:78:PHE:CZ	0.47	2.44	39	2
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:39:PHE:C	1:A:41:GLU:N	0.47	2.70	24	5
1:A:26:TRP:NE1	1:A:35:ASP:OD1	0.47	2.47	1	8
1:A:100:THR:OG1	1:A:102:ILE:CD1	0.47	2.62	10	1
1:A:8:VAL:CG2	1:A:11:TYR:CG	0.47	2.98	17	1
1:A:25:THR:HG21	1:A:51:ARG:HG2	0.47	1.87	25	2
1:A:38:LYS:HB3	1:A:78:PHE:CE2	0.47	2.45	34	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:TYR:CD1	1:A:10:TYR:N	0.47	2.83	35	1
1:A:102:ILE:HG23	1:A:103:ASP:H	0.47	1.70	36	1
1:A:31:TYR:CZ	1:A:32:LYS:HD2	0.47	2.44	1	3
1:A:61:ASN:C	1:A:63:GLU:N	0.47	2.72	36	27
1:A:9:LYS:HB3	1:A:10:TYR:CE2	0.47	2.45	10	11
1:A:19:HIS:ND1	1:A:24:SER:OG	0.47	2.48	35	6
1:A:27:LEU:C	1:A:28:ILE:HD13	0.47	2.35	27	3
1:A:24:SER:O	1:A:25:THR:C	0.47	2.57	18	7
1:A:19:HIS:HB3	1:A:26:TRP:CG	0.47	2.45	12	1
1:A:40:LEU:O	1:A:50:LEU:CD1	0.47	2.63	22	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:35:ASP:OD2	1:A:38:LYS:CG	0.46	2.63	39	1
1:A:8:VAL:HG13	1:A:80:ILE:C	0.46	2.35	37	6
1:A:50:LEU:CA	1:A:53:GLN:HG2	0.46	2.39	33	20
1:A:36:LEU:O	1:A:37:THR:C	0.46	2.58	38	7
1:A:58:ALA:O	1:A:61:ASN:CB	0.46	2.64	9	1
1:A:28:ILE:O	1:A:58:ALA:N	0.46	2.46	21	4
1:A:39:PHE:CD2	1:A:78:PHE:HB3	0.46	2.45	22	1
1:A:33:VAL:C	1:A:80:ILE:CD1	0.46	2.88	24	2
1:A:44:PRO:O	1:A:45:GLY:C	0.46	2.59	31	4
1:A:16:ILE:HD13	1:A:28:ILE:CG1	0.46	2.40	15	2
1:A:49:VAL:CG1	1:A:50:LEU:HD12	0.46	2.41	7	2
1:A:88:ARG:O	1:A:90:LYS:N	0.46	2.49	24	4
1:A:68:SER:C	1:A:70:ASP:N	0.46	2.73	20	7
1:A:27:LEU:HD21	2:A:105:HEM:CBB	0.46	2.37	15	1
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:53:GLN:NE2	2:A:105:HEM:CMC	0.46	2.79	25	8
1:A:29:LEU:HB3	1:A:34:TYR:CZ	0.46	2.46	22	8
1:A:40:LEU:HG	1:A:47:GLU:CB	0.46	2.41	24	6
1:A:41:GLU:CG	1:A:42:GLU:N	0.46	2.79	23	1
1:A:9:LYS:HD2	1:A:10:TYR:CE2	0.46	2.46	19	3
1:A:10:TYR:HB3	1:A:84:HIS:ND1	0.46	2.26	38	11
1:A:40:LEU:HD23	1:A:47:GLU:CG	0.46	2.41	6	1
1:A:19:HIS:CG	1:A:24:SER:HB3	0.46	2.46	34	6
1:A:11:TYR:CZ	1:A:15:GLU:HG2	0.46	2.46	38	5
1:A:16:ILE:HD13	1:A:28:ILE:HG12	0.46	1.88	37	3
1:A:88:ARG:HG3	1:A:89:SER:N	0.46	2.26	14	9
1:A:57:ASP:OD1	1:A:60:GLU:CD	0.46	2.59	25	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:SER:O	1:A:26:TRP:N	0.46	2.49	36	1
1:A:16:ILE:CD1	1:A:83:LEU:HD22	0.46	2.41	2	3
1:A:20:ASN:ND2	1:A:54:ALA:HB3	0.46	2.25	25	2
1:A:8:VAL:O	1:A:9:LYS:HB2	0.46	2.12	41	3
1:A:26:TRP:NE1	1:A:35:ASP:OD2	0.46	2.49	26	1
1:A:92:THR:HG23	1:A:93:LYS:N	0.45	2.26	42	2
1:A:28:ILE:CG1	1:A:57:ASP:HA	0.45	2.40	35	12
1:A:29:LEU:N	1:A:32:LYS:O	0.45	2.49	20	1
1:A:29:LEU:O	1:A:30:HIS:ND1	0.45	2.49	26	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:14:GLU:O	1:A:17:GLN:N	0.45	2.49	34	2
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:62:PHE:CE1	1:A:63:GLU:HG2	0.45	2.46	33	3
1:A:11:TYR:CZ	1:A:26:TRP:CZ3	0.45	3.04	35	1
1:A:83:LEU:CD1	1:A:84:HIS:N	0.45	2.79	39	10
1:A:39:PHE:CZ	2:A:105:HEM:HMB2	0.45	2.46	5	1
1:A:9:LYS:HD3	1:A:10:TYR:CE2	0.45	2.47	22	2
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:O	1:A:99:ILE:CG2	0.45	2.64	28	1
1:A:31:TYR:CD1	1:A:92:THR:HA	0.45	2.46	30	1
1:A:35:ASP:HB2	1:A:80:ILE:HD11	0.45	1.88	40	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
1:A:32:LYS:CG	1:A:34:TYR:CE1	0.45	2.99	17	1
1:A:86:ASP:CG	1:A:87:ASP:OD2	0.45	2.60	37	1
1:A:19:HIS:CE1	1:A:26:TRP:CE2	0.45	3.04	1	2
1:A:36:LEU:CD2	1:A:50:LEU:HD22	0.45	2.34	3	1
1:A:21:ASN:C	1:A:23:LYS:N	0.45	2.73	41	7
1:A:8:VAL:HB	1:A:11:TYR:CZ	0.45	2.46	31	2
1:A:83:LEU:HD12	1:A:84:HIS:H	0.45	1.65	38	1
1:A:36:LEU:O	1:A:39:PHE:N	0.45	2.50	33	10
1:A:26:TRP:CE3	1:A:80:ILE:HD11	0.45	2.46	4	1
1:A:83:LEU:C	1:A:83:LEU:CD1	0.45	2.89	18	13
1:A:39:PHE:CE1	2:A:105:HEM:HMB2	0.45	2.46	5	1
1:A:39:PHE:C	1:A:41:GLU:H	0.45	2.18	5	1
1:A:35:ASP:OD2	1:A:38:LYS:CD	0.45	2.65	40	1
1:A:35:ASP:OD2	1:A:80:ILE:HG21	0.45	2.11	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ILE:CB	1:A:57:ASP:HA	0.45	2.42	40	10
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:101:THR:C	1:A:102:ILE:CG2	0.45	2.89	8	1
1:A:31:TYR:OH	1:A:82:GLU:CD	0.45	2.60	38	2
1:A:43:HIS:HB2	1:A:50:LEU:HD11	0.45	1.89	26	2
1:A:20:ASN:ND2	1:A:55:GLY:HA2	0.45	2.27	16	1
1:A:72:ARG:CZ	1:A:72:ARG:CB	0.45	2.95	16	5
1:A:31:TYR:CE1	1:A:88:ARG:NH1	0.45	2.85	40	1
1:A:27:LEU:C	1:A:27:LEU:CD1	0.44	2.89	24	6
1:A:59:THR:O	1:A:62:PHE:N	0.44	2.50	27	3
1:A:9:LYS:CD	1:A:10:TYR:CE2	0.44	3.00	12	1
1:A:15:GLU:O	1:A:19:HIS:CD2	0.44	2.71	41	1
1:A:57:ASP:OD2	1:A:60:GLU:CD	0.44	2.60	2	1
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:33:VAL:HG23	1:A:82:GLU:HA	0.44	1.88	26	1
1:A:9:LYS:HB3	1:A:10:TYR:CD2	0.44	2.46	42	3
1:A:98:ILE:O	1:A:99:ILE:CG1	0.44	2.65	33	1
1:A:59:THR:O	1:A:63:GLU:N	0.44	2.51	40	2
1:A:99:ILE:O	1:A:99:ILE:HG23	0.44	2.12	28	2
1:A:73:GLU:O	1:A:77:THR:HG23	0.44	2.12	28	2
1:A:72:ARG:O	1:A:75:SER:OG	0.44	2.32	19	3
1:A:34:TYR:CE2	1:A:79:ILE:CD1	0.44	3.00	38	2
1:A:31:TYR:CD1	1:A:88:ARG:CZ	0.44	3.00	7	2
1:A:74:LEU:HG	1:A:75:SER:N	0.44	2.27	9	4
1:A:29:LEU:HD12	2:A:105:HEM:CAB	0.44	2.41	19	3
1:A:43:HIS:CD2	2:A:105:HEM:CHB	0.44	3.01	20	1
1:A:67:HIS:ND1	2:A:105:HEM:O2A	0.44	2.50	25	1
1:A:35:ASP:HB2	1:A:80:ILE:CD1	0.44	2.42	40	1
1:A:19:HIS:CB	1:A:26:TRP:CE3	0.44	3.00	17	2
1:A:40:LEU:CD2	1:A:47:GLU:HB3	0.44	2.42	16	2
1:A:31:TYR:CE2	1:A:32:LYS:HG3	0.44	2.48	29	4
1:A:32:LYS:HG2	1:A:34:TYR:CE1	0.44	2.48	14	1
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: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:35:ASP:O	1:A:35:ASP:OD1	0.44	2.35	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:TRP:CD1	1:A:35:ASP:CG	0.44	2.95	26	1
1:A:27:LEU:CD2	1:A:28:ILE:N	0.44	2.72	39	1
1:A:12:THR:O	1:A:13:LEU:C	0.44	2.61	2	10
1:A:50:LEU:HA	1:A:53:GLN:NE2	0.44	2.28	27	8
1:A:57:ASP:OD1	1:A:57:ASP:O	0.44	2.36	9	5
1:A:32:LYS:CG	1:A:34:TYR:CZ	0.44	3.01	17	1
1:A:71:ALA:CA	1:A:74:LEU:HD23	0.44	2.39	37	3
1:A:43:HIS:CE1	2:A:105:HEM:NB	0.44	2.86	38	2
1:A:26:TRP:CE3	1:A:34:TYR:C	0.44	2.95	41	1
1:A:29:LEU:HD11	1:A:62:PHE:CE2	0.44	2.47	20	2
1:A:28:ILE:HG12	1:A:33:VAL:HG12	0.44	1.89	19	2
1:A:35:ASP:OD2	1:A:80:ILE:HG23	0.43	2.13	7	1
1:A:43:HIS:ND1	1:A:49:VAL:CG1	0.43	2.72	7	1
1:A:90:LYS:C	1:A:91:ILE:CG2	0.43	2.91	9	1
1:A:92:THR:O	1:A:94:PRO:N	0.43	2.51	13	1
1:A:35:ASP:OD2	1:A:38:LYS:N	0.43	2.50	15	1
1:A:25:THR:HG21	1:A:40:LEU:HD11	0.43	1.90	36	1
1:A:67:HIS:ND1	2:A:105:HEM:O1A	0.43	2.50	37	1
1:A:12:THR:O	1:A:15:GLU:N	0.43	2.51	5	4
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:29:LEU:HG	2:A:105:HEM:HAB	0.43	1.90	33	3
1:A:33:VAL:HG23	1:A:81:GLY:C	0.43	2.38	24	1
1:A:36:LEU:HD11	1:A:53:GLN:HG3	0.43	1.89	28	1
1:A:34:TYR:C	1:A:80:ILE:HD11	0.43	2.37	33	1
2:A:105:HEM:O1A	2:A:105:HEM:C1A	0.43	2.71	7	3
1:A:33:VAL:O	1:A:80:ILE:CD1	0.43	2.65	23	1
1:A:98:ILE:HD12	1:A:99:ILE:O	0.43	2.12	24	1
1:A:74:LEU:O	1:A:77:THR:HB	0.43	2.13	35	4
1:A:102:ILE:HG12	1:A:103:ASP:N	0.43	2.27	32	1
1:A:83:LEU:O	1:A:88:ARG:CD	0.43	2.66	34	4
1:A:53:GLN:OE1	2:A:105:HEM:HMC2	0.43	2.13	29	1
1:A:57:ASP:O	1:A:57:ASP:OD1	0.43	2.36	36	1
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:99:ILE:H	1:A:99:ILE:HD13	0.43	1.73	25	1
1:A:13:LEU:CD2	1:A:28:ILE:CD1	0.43	2.96	37	1
1:A:19:HIS:ND1	1:A:24:SER:HB2	0.43	2.28	42	2
1:A:24:SER:O	1:A:26:TRP:CG	0.43	2.71	6	1
1:A:31:TYR:CB	1:A:92:THR:OG1	0.43	2.67	35	2
1:A:43:HIS:CD2	2:A:105:HEM:NA	0.43	2.87	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:LEU:HD23	1:A:91:ILE:CG1	0.43	2.42	15	1
1:A:29:LEU:C	1:A:31:TYR:N	0.43	2.76	39	2
1:A:58:ALA:O	1:A:61:ASN:N	0.43	2.52	20	4
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:43:HIS:CD2	1:A:44:PRO:HD2	0.43	2.48	42	2
1:A:34:TYR:CE2	1:A:75:SER:OG	0.43	2.72	14	1
1:A:19:HIS:HB2	1:A:26:TRP:CE3	0.43	2.48	17	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:32:LYS:CG	1:A:82:GLU:OE1	0.43	2.67	41	1
1:A:92:THR:CG2	1:A:92:THR:O	0.43	2.67	7	1
1:A:75:SER:C	1:A:77:THR:N	0.43	2.77	39	9
1:A:86:ASP:OD2	1:A:87:ASP:OD2	0.43	2.37	13	2
1:A:83:LEU:HD21	1:A:87:ASP:O	0.43	2.14	33	3
1:A:36:LEU:O	1:A:39:PHE:C	0.43	2.61	22	1
1:A:29:LEU:HD23	1:A:29:LEU:HA	0.43	1.72	30	3
1:A:85:PRO:HA	1:A:88:ARG:CD	0.43	2.44	3	2
1:A:31:TYR:CZ	1:A:32:LYS:HD3	0.43	2.48	11	2
1:A:42:GLU:O	1:A:43:HIS:HB3	0.43	2.14	12	3
1:A:39:PHE:CG	1:A:39:PHE:O	0.43	2.70	16	1
1:A:62:PHE:HA	1:A:67:HIS:CE1	0.43	2.48	30	3
1:A:39:PHE:HE1	1:A:74:LEU:HD21	0.43	1.73	34	1
1:A:62:PHE:HA	1:A:65:VAL:HG12	0.42	1.91	1	1
1:A:43:HIS:NE2	2:A:105:HEM:C4A	0.42	2.87	20	2
1:A:33:VAL:CG1	1:A:81:GLY:C	0.42	2.91	4	2
1:A:91:ILE:O	1:A:92:THR:O	0.42	2.38	41	6
1:A:88:ARG:C	1:A:92:THR:HB	0.42	2.39	24	1
1:A:57:ASP:CB	1:A:91:ILE:HB	0.42	2.44	28	1
1:A:16:ILE:HG21	1:A:28:ILE:HD13	0.42	1.89	30	1
1:A:39:PHE:CE2	2:A:105:HEM:HMB	0.42	2.49	35	2
1:A:22:SER:HA	1:A:25:THR:OG1	0.42	2.14	36	1
1:A:84:HIS:C	1:A:88:ARG:HD3	0.42	2.40	19	1
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:57:ASP:HB2	1:A:91:ILE:CD1	0.42	2.43	9	2
1:A:16:ILE:C	1:A:18:LYS:N	0.42	2.76	16	1
1:A:39:PHE:CD1	1:A:39:PHE:N	0.42	2.87	17	3
1:A:39:PHE:HB3	1:A:50:LEU:HD13	0.42	1.91	35	1
1:A:62:PHE:HB2	2:A:105:HEM:CHC	0.42	2.45	2	1
1:A:98:ILE:C	1:A:98:ILE:CD1	0.42	2.92	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:VAL:HG13	1:A:82:GLU:CA	0.42	2.44	17	1
1:A:35:ASP:C	1:A:37:THR:N	0.42	2.75	17	1
1:A:19:HIS:CB	1:A:24:SER:O	0.42	2.68	21	1
1:A:19:HIS:HB2	1:A:26:TRP:HB2	0.42	1.90	21	3
1:A:40:LEU:HA	1:A:50:LEU:HD13	0.42	1.90	21	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:40:LEU:CD1	1:A:47:GLU:HB3	0.42	2.44	12	2
1:A:35:ASP:OD1	1:A:78:PHE:HB3	0.42	2.14	41	1
1:A:39:PHE:O	1:A:39:PHE:CG	0.42	2.73	2	3
1:A:35:ASP:CG	1:A:80:ILE:HD13	0.42	2.39	3	1
1:A:30:HIS:H	1:A:59:THR:HG23	0.42	1.75	27	1
1:A:102:ILE:N	1:A:102:ILE:HD13	0.42	2.29	32	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:13:LEU:CD2	1:A:83:LEU:CD2	0.42	2.98	17	3
1:A:30:HIS:CG	1:A:72:ARG:NH2	0.42	2.88	33	1
1:A:32:LYS:HE3	1:A:79:ILE:CD1	0.42	2.44	35	1
1:A:26:TRP:CZ3	1:A:35:ASP:OD2	0.42	2.73	41	1
1:A:40:LEU:O	1:A:42:GLU:O	0.42	2.38	7	1
1:A:101:THR:C	1:A:102:ILE:HG23	0.42	2.40	7	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:65:VAL:O	1:A:66:GLY:O	0.42	2.38	19	1
1:A:28:ILE:HB	1:A:57:ASP:CA	0.42	2.45	36	1
1:A:30:HIS:NE2	1:A:62:PHE:CE2	0.42	2.88	27	1
1:A:36:LEU:O	1:A:40:LEU:HD23	0.42	2.15	33	1
1:A:35:ASP:OD1	1:A:37:THR:HB	0.42	2.15	40	1
1:A:76:LYS:HA	1:A:79:ILE:HD12	0.42	1.92	42	1
1:A:76:LYS:CE	1:A:76:LYS:O	0.41	2.68	6	1
1:A:29:LEU:HD23	1:A:59:THR:CA	0.41	2.45	30	1
1:A:26:TRP:CZ2	1:A:80:ILE:HD12	0.41	2.50	40	1
1:A:36:LEU:HA	1:A:39:PHE:HD1	0.41	1.73	40	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:39:PHE:CD1	1:A:78:PHE:HE2	0.41	2.30	19	1
1:A:74:LEU:O	1:A:77:THR:OG1	0.41	2.33	27	1
1:A:101:THR:O	1:A:102:ILE:O	0.41	2.38	38	1
1:A:72:ARG:HB3	1:A:72:ARG:CZ	0.41	2.45	41	1
1:A:84:HIS:HB3	1:A:85:PRO:CD	0.41	2.45	8	1
1:A:31:TYR:CE2	1:A:82:GLU:OE2	0.41	2.73	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:TRP:HE1	1:A:80:ILE:HD12	0.41	1.71	34	1
1:A:49:VAL:HG21	2:A:105:HEM:C1D	0.41	2.50	34	1
1:A:11:TYR:CE2	1:A:15:GLU:HB3	0.41	2.50	36	1
1:A:39:PHE:CD2	2:A:105:HEM:HMB3	0.41	2.51	15	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:40:LEU:HD23	1:A:40:LEU:HA	0.41	1.81	8	1
1:A:17:GLN:O	1:A:20:ASN:OD1	0.41	2.37	16	1
1:A:61:ASN:HB3	2:A:105:HEM:CBC	0.41	2.46	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:19:HIS:ND1	1:A:26:TRP:CE3	0.41	2.88	18	2
1:A:20:ASN:O	1:A:51:ARG:NE	0.41	2.54	34	1
1:A:32:LYS:CB	1:A:34:TYR:CE1	0.41	3.04	20	1
1:A:29:LEU:HD21	1:A:62:PHE:CB	0.41	2.45	23	2
1:A:86:ASP:O	1:A:87:ASP:OD1	0.41	2.38	33	2
1:A:98:ILE:HD13	1:A:98:ILE:N	0.41	2.30	1	1
1:A:40:LEU:C	1:A:47:GLU:HG2	0.41	2.41	16	1
1:A:8:VAL:CG2	1:A:11:TYR:CE2	0.41	3.03	21	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:28:ILE:CD1	1:A:33:VAL:HG22	0.41	2.46	5	1
1:A:84:HIS:C	1:A:86:ASP:H	0.41	2.23	6	2
1:A:92:THR:C	1:A:93:LYS:O	0.41	2.64	7	1
1:A:30:HIS:O	1:A:92:THR:O	0.41	2.39	35	2
1:A:39:PHE:CD1	1:A:42:GLU:HB2	0.41	2.51	19	1
1:A:38:LYS:HZ3	1:A:74:LEU:CD1	0.41	2.26	35	1
1:A:12:THR:O	1:A:16:ILE:CD1	0.41	2.67	36	1
1:A:38:LYS:HD3	1:A:78:PHE:CE1	0.41	2.51	38	1
1:A:53:GLN:HB2	1:A:58:ALA:CB	0.41	2.45	42	2
1:A:13:LEU:HA	1:A:13:LEU:HD23	0.41	1.83	41	1
1:A:25:THR:CG2	1:A:36:LEU:HB2	0.41	2.46	42	1
1:A:41:GLU:C	1:A:42:GLU:O	0.41	2.64	21	3
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:88:ARG:CZ	1:A:88:ARG:HB3	0.41	2.46	40	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:13:LEU:CD1	1:A:87:ASP:HB3	0.40	2.44	3	1
1:A:100:THR:O	1:A:100:THR:CG2	0.40	2.69	24	1
1:A:29:LEU:HB3	1:A:30:HIS:CE1	0.40	2.51	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:TYR:HB2	1:A:84:HIS:ND1	0.40	2.32	33	1
1:A:11:TYR:CZ	1:A:15:GLU:CG	0.40	3.05	38	1
1:A:93:LYS:CG	1:A:94:PRO:HD2	0.40	2.47	8	1
1:A:86:ASP:O	1:A:87:ASP:OD2	0.40	2.39	15	1
1:A:33:VAL:HG13	1:A:82:GLU:C	0.40	2.42	17	1
1:A:83:LEU:CD2	1:A:91:ILE:CD1	0.40	2.99	24	1
1:A:34:TYR:O	1:A:80:ILE:HD11	0.40	2.16	33	1
1:A:83:LEU:O	1:A:88:ARG:HG3	0.40	2.17	37	1
1:A:18:LYS:CG	1:A:19:HIS:N	0.40	2.84	42	1
1:A:27:LEU:CD1	1:A:36:LEU:HG	0.40	2.46	4	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: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:26:TRP:CH2	1:A:80:ILE:CG1	0.40	3.05	37	1
1:A:99:ILE:HG23	1:A:100:THR:N	0.40	2.31	40	1
1:A:36:LEU:CD1	1:A:53:GLN:HG3	0.40	2.47	41	1
1:A:34:TYR:HB3	1:A:39:PHE:CE1	0.40	2.51	3	1
1:A:13:LEU:HG	1:A:87:ASP:CB	0.40	2.47	11	1
1:A:74:LEU:HD12	1:A:78:PHE:CE2	0.40	2.50	16	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/104 (92%)	71±3 (74±3%)	17±3 (18±3%)	7±2 (8±2%)	1	14
All	All	4032/4368 (92%)	2985 (74%)	734 (18%)	313 (8%)	1	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

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Mol	Chain	Res	Type	Models (Total)
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	93	LYS	8
1	A	103	ASP	8
1	A	25	THR	7
1	A	102	ILE	7
1	A	60	GLU	6
1	A	99	ILE	6
1	A	67	HIS	6
1	A	96	GLU	5
1	A	37	THR	5
1	A	89	SER	4
1	A	88	ARG	3
1	A	98	ILE	3
1	A	100	THR	3
1	A	45	GLY	2
1	A	59	THR	2
1	A	95	SER	2
1	A	44	PRO	2
1	A	41	GLU	2
1	A	40	LEU	2
1	A	84	HIS	1
1	A	24	SER	1
1	A	79	ILE	1
1	A	101	THR	1
1	A	97	SER	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	87/93 (94%)	46±3 (53±4%)	41±3 (47±4%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3654/3906 (94%)	1946 (53%)	1708 (47%)	0 2

All 72 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	10	TYR	42
1	A	11	TYR	42
1	A	27	LEU	42
1	A	28	ILE	42
1	A	29	LEU	42
1	A	62	PHE	42
1	A	74	LEU	42
1	A	79	ILE	42
1	A	83	LEU	42
1	A	84	HIS	42
1	A	86	ASP	42
1	A	57	ASP	41
1	A	65	VAL	41
1	A	16	ILE	40
1	A	60	GLU	40
1	A	24	SER	38
1	A	14	GLU	37
1	A	59	THR	37
1	A	75	SER	37
1	A	51	ARG	34
1	A	80	ILE	34
1	A	25	THR	33
1	A	37	THR	33
1	A	61	ASN	33
1	A	91	ILE	32
1	A	64	ASP	31
1	A	48	GLU	30
1	A	90	LYS	29
1	A	17	GLN	28
1	A	76	LYS	28
1	A	52	GLU	27
1	A	63	GLU	27
1	A	96	GLU	26
1	A	31	TYR	26
1	A	32	LYS	24

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Mol	Chain	Res	Type	Models (Total)
1	A	9	LYS	23
1	A	38	LYS	22
1	A	23	LYS	21
1	A	42	GLU	20
1	A	98	ILE	20
1	A	43	HIS	20
1	A	35	ASP	19
1	A	69	THR	19
1	A	40	LEU	18
1	A	93	LYS	18
1	A	102	ILE	16
1	A	97	SER	16
1	A	99	ILE	14
1	A	92	THR	14
1	A	18	LYS	13
1	A	95	SER	13
1	A	103	ASP	12
1	A	50	LEU	12
1	A	47	GLU	11
1	A	88	ARG	10
1	A	41	GLU	10
1	A	89	SER	9
1	A	34	TYR	8
1	A	87	ASP	8
1	A	20	ASN	7
1	A	73	GLU	7
1	A	15	GLU	6
1	A	67	HIS	5
1	A	30	HIS	5
1	A	78	PHE	5
1	A	77	THR	4
1	A	82	GLU	4
1	A	22	SER	3
1	A	33	VAL	3
1	A	39	PHE	2
1	A	101	THR	1

6.3.3 RNA ⓘ

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 oligosaccharides 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	50,50,50	1.11±0.00	4±1 (7±1%)

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	67,82,82	0.98±0.01	2±0 (2±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±0,14,54,54	-

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
2	A	105	HEM	CAC-C3C	2.59	1.40	1.47	11	42
2	A	105	HEM	CMC-C2C	2.31	1.55	1.50	14	42
2	A	105	HEM	CAB-C3B	2.12	1.41	1.47	17	41
2	A	105	HEM	C4A-NA	2.08	1.43	1.39	30	24

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

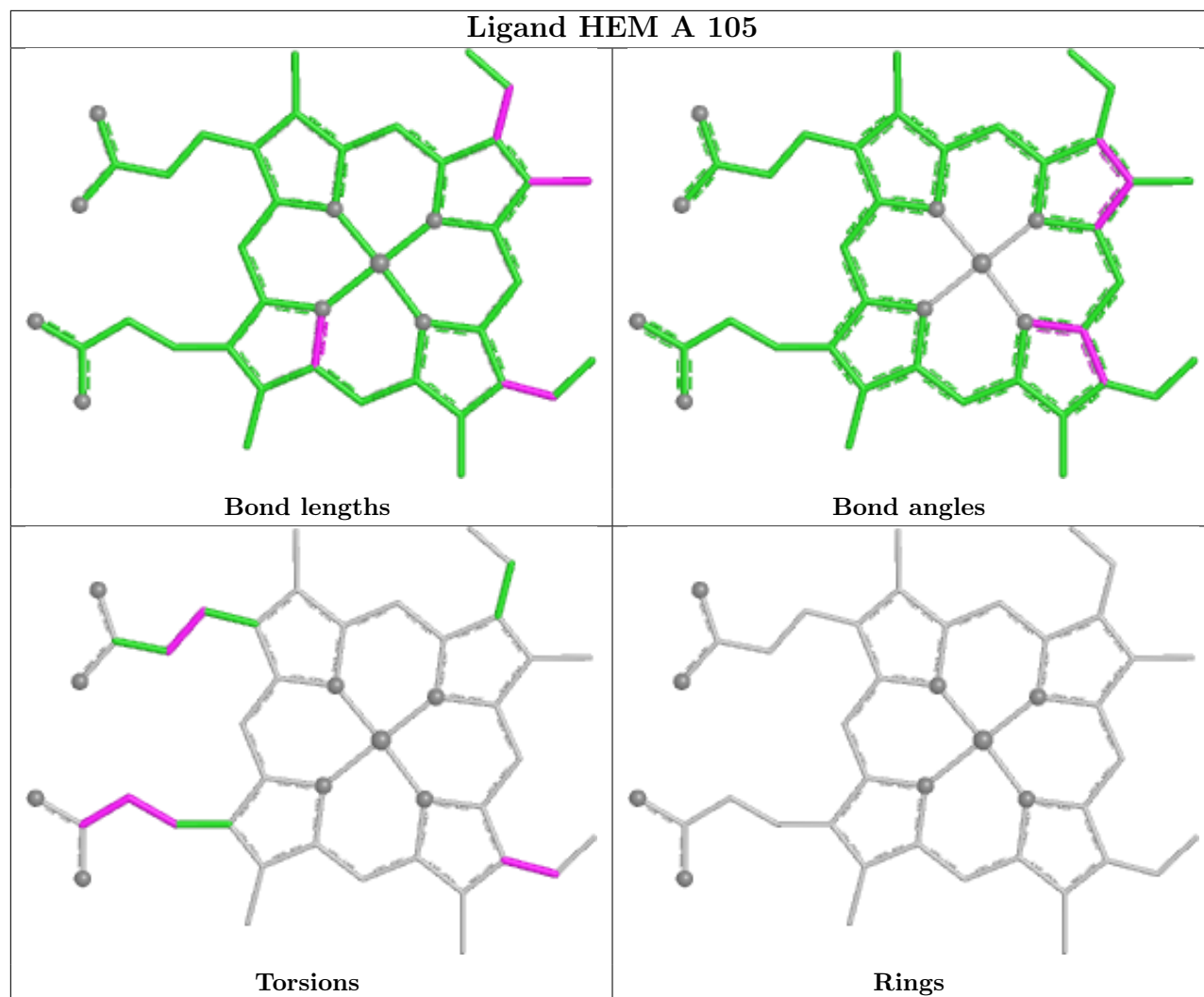
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	105	HEM	C3B-C4B-NB	3.85	112.23	109.47	23	42
2	A	105	HEM	C3C-C2C-C1C	2.34	104.83	107.05	4	42

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

No chemical shift data were provided