



Full wwPDB NMR Structure Validation Report ⓘ

Mar 17, 2026 – 06:47 PM UTC

PDB ID : 2JTI / pdb_00002jti
Title : Solution structure of the yeast iso-1-cytochrome c (T12A) : yeast cytochrome c peroxidase complex
Authors : Ubbink, M.; Volkov, A.N.
Deposited on : 2007-08-01

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

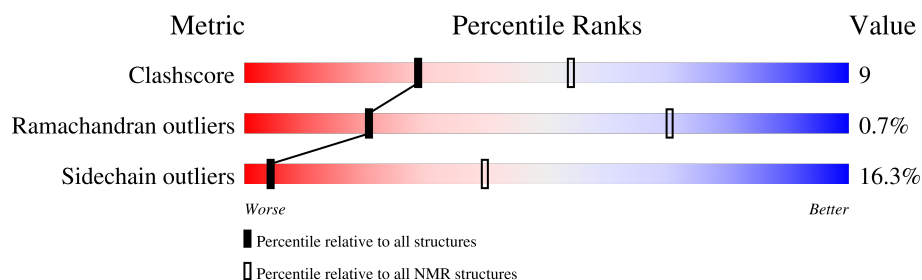
1 Overall quality at a glance

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	294	
2	B	108	

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:294, B:1-B:103 (397)	0.08	8

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 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 6, 7, 8
2	3, 5
3	4, 10
Single-model clusters	9

3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6378 atoms, of which 3117 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cytochrome c peroxidase, mitochondrial.

Mol	Chain	Residues	Atoms						Trace
1	A	294	Total	C	H	N	O	S	0
			4621	1514	2250	395	456	6	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	THR	variant	UNP P00431
A	152	GLY	ASP	variant	UNP P00431

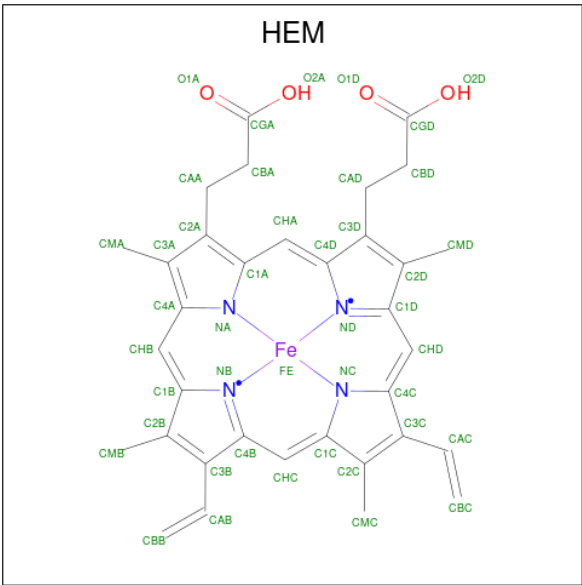
- Molecule 2 is a protein called Cytochrome c iso-1.

Mol	Chain	Residues	Atoms						Trace
2	B	103	Total	C	H	N	O	S	0
			1609	506	805	145	148	5	

There is a discrepancy between the modelled and reference sequences:

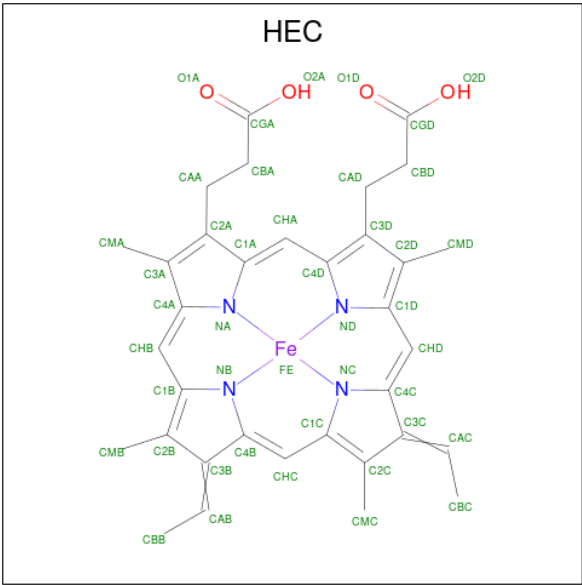
Chain	Residue	Modelled	Actual	Comment	Reference
B	12	ALA	THR	engineered mutation	UNP P00044

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



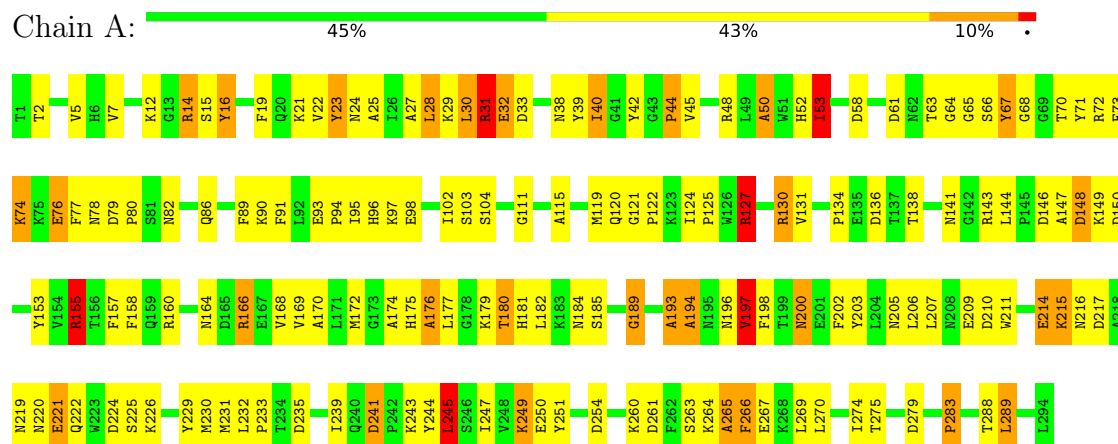
Mol	Chain	Residues	Atoms					
			Total	C	Fe	H	N	O
4	B	1	75	34	1	32	4	4

4 Residue-property plots

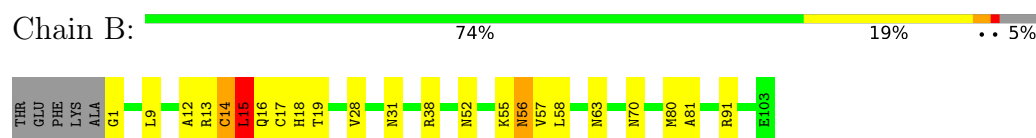
4.1 Average score per residue in the NMR ensemble

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 c peroxidase, mitochondrial



- Molecule 2: Cytochrome c iso-1



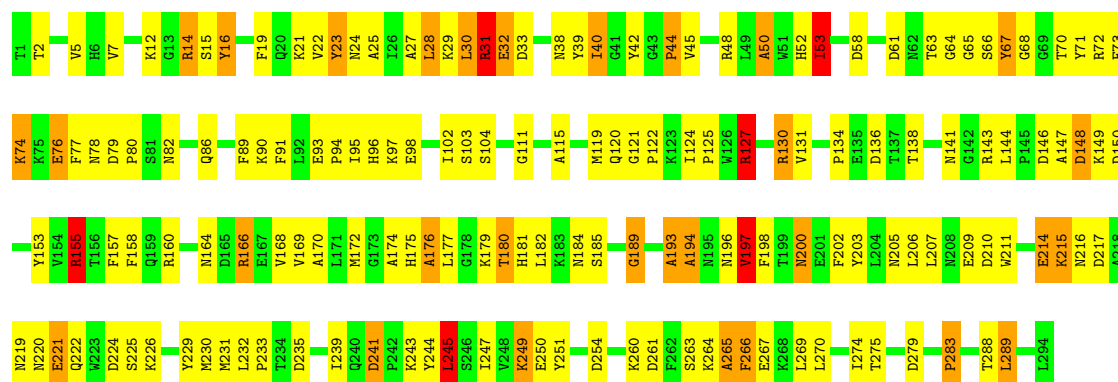
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Cytochrome c peroxidase, mitochondrial





• Molecule 2: Cytochrome c iso-1

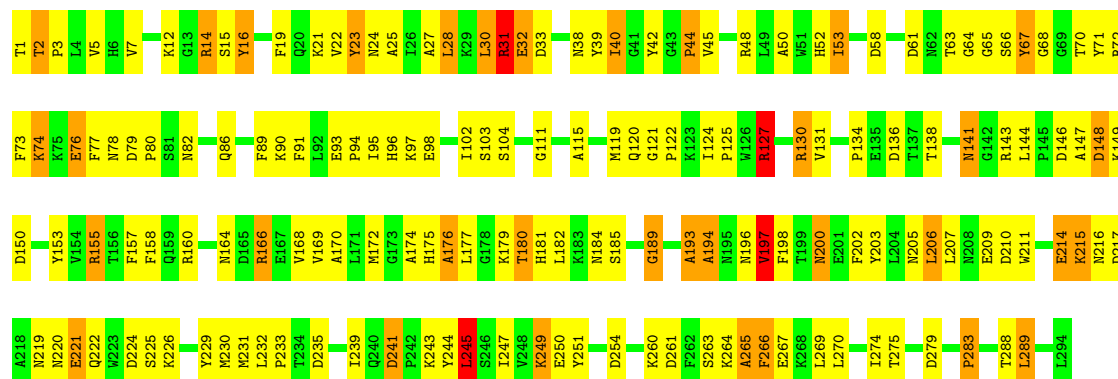
Chain B: 74% 19% 5%



4.2.2 Score per residue for model 2

• Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A: 45% 43% 12%



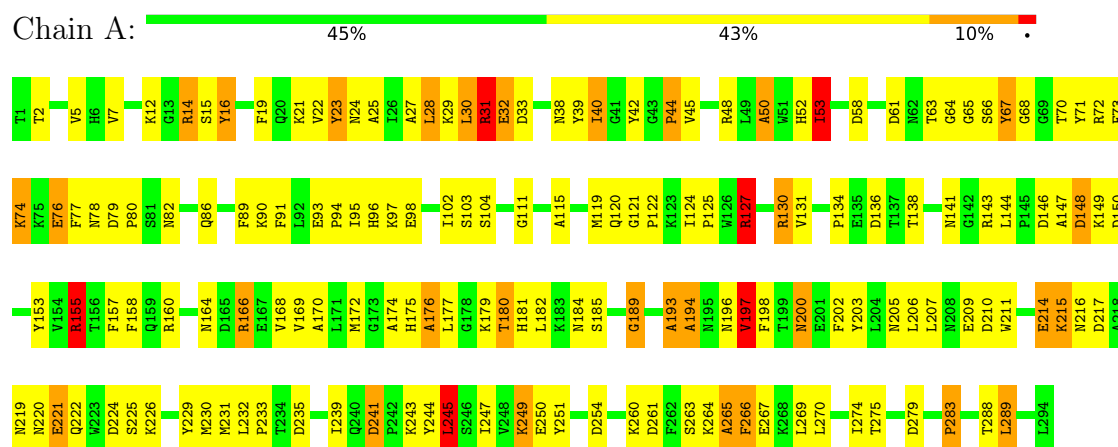
• Molecule 2: Cytochrome c iso-1

Chain B: 72% 20% 5%

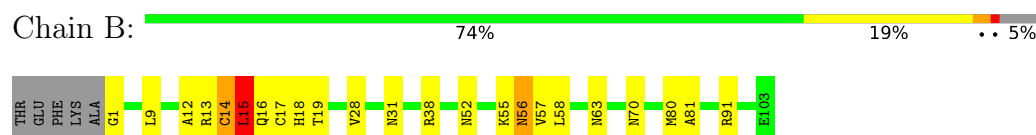


4.2.3 Score per residue for model 3

• Molecule 1: Cytochrome c peroxidase, mitochondrial

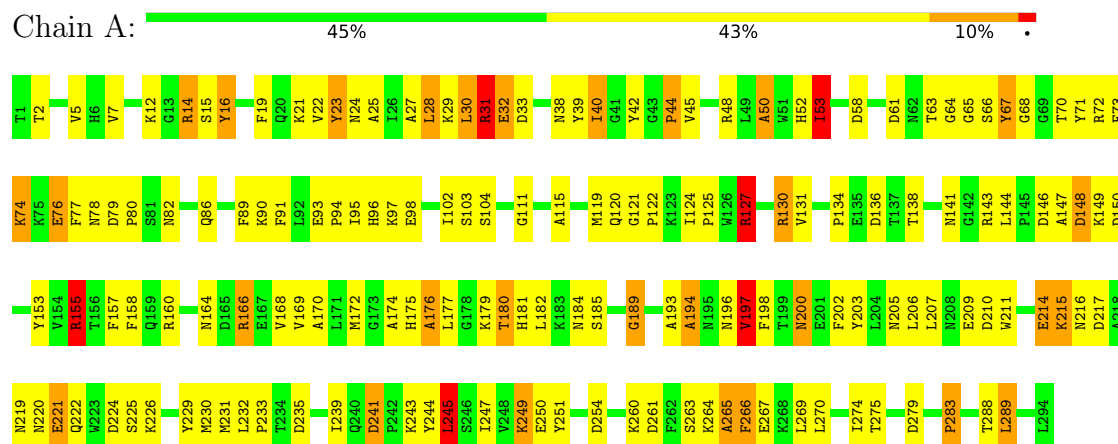


• Molecule 2: Cytochrome c iso-1

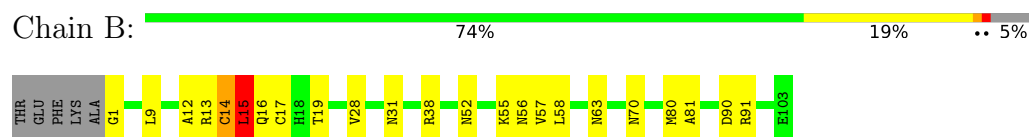


4.2.4 Score per residue for model 4

• Molecule 1: Cytochrome c peroxidase, mitochondrial

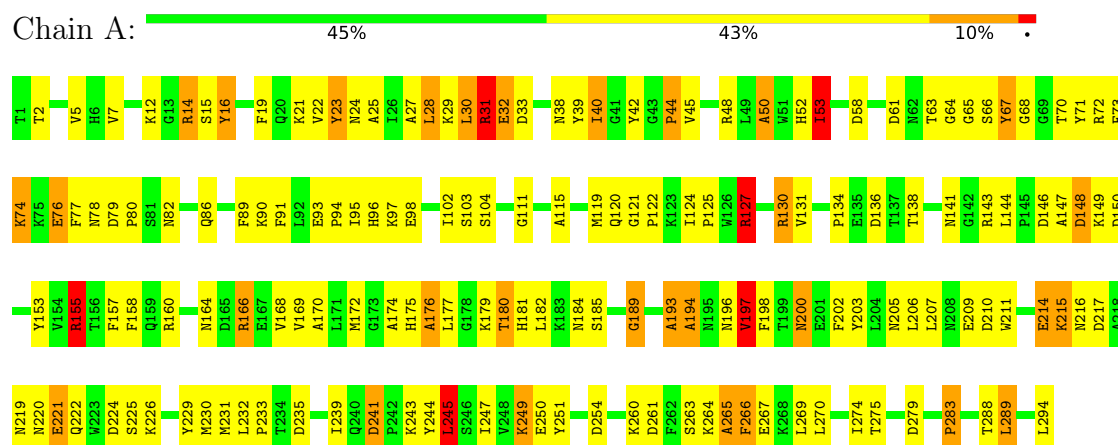


• Molecule 2: Cytochrome c iso-1

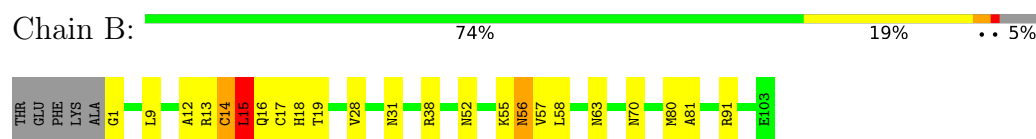


4.2.5 Score per residue for model 5

- Molecule 1: Cytochrome c peroxidase, mitochondrial

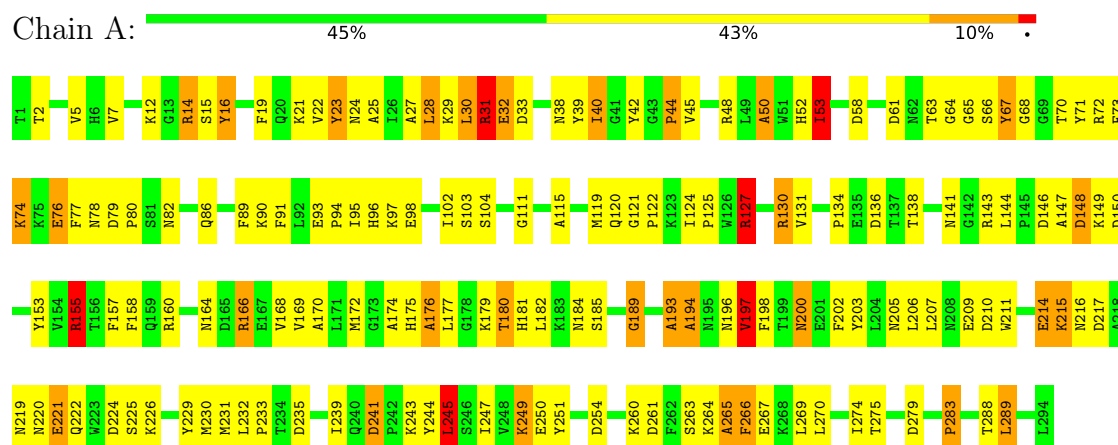


- Molecule 2: Cytochrome c iso-1

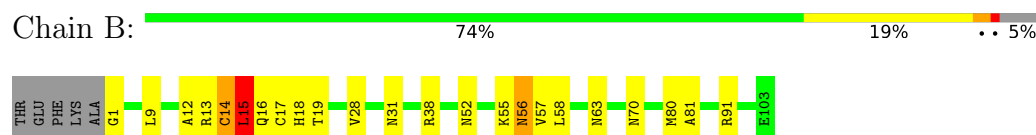


4.2.6 Score per residue for model 6

- Molecule 1: Cytochrome c peroxidase, mitochondrial

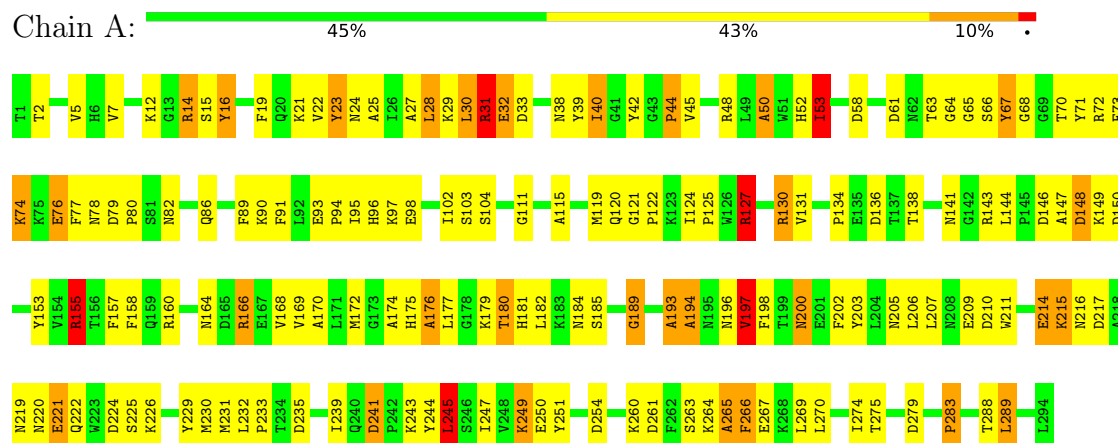


- Molecule 2: Cytochrome c iso-1

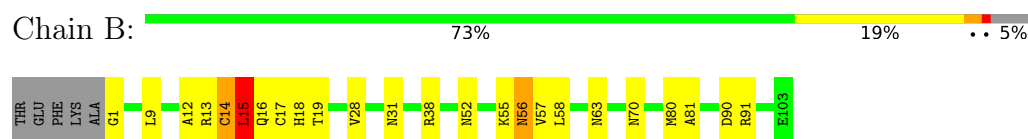


4.2.7 Score per residue for model 7

- Molecule 1: Cytochrome c peroxidase, mitochondrial

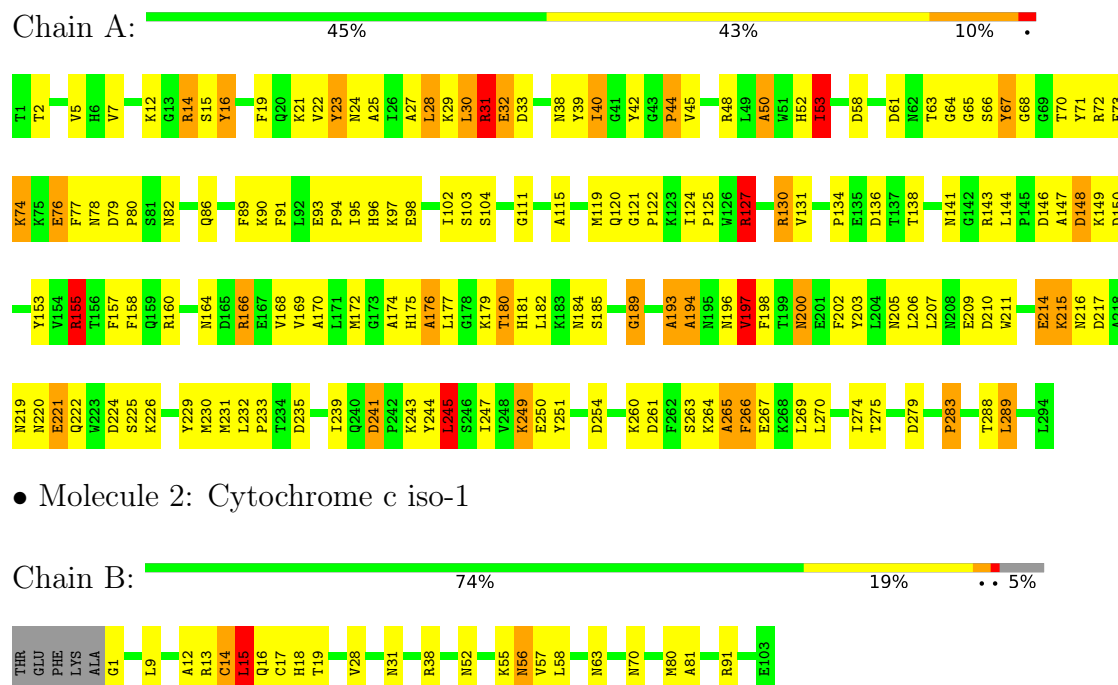


- Molecule 2: Cytochrome c iso-1



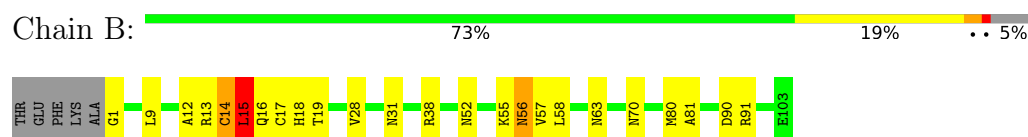
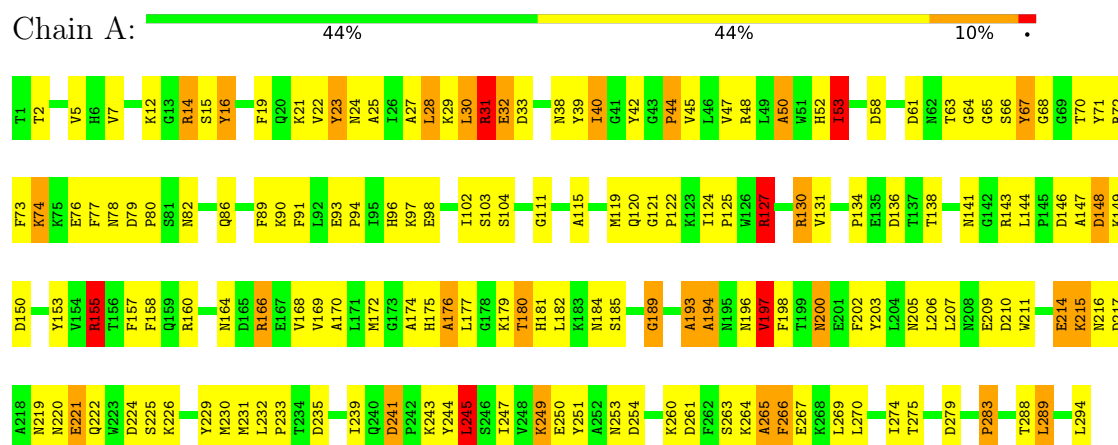
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Cytochrome c peroxidase, mitochondrial

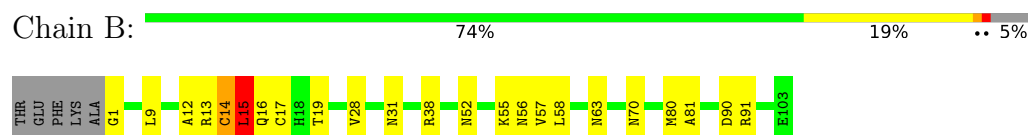
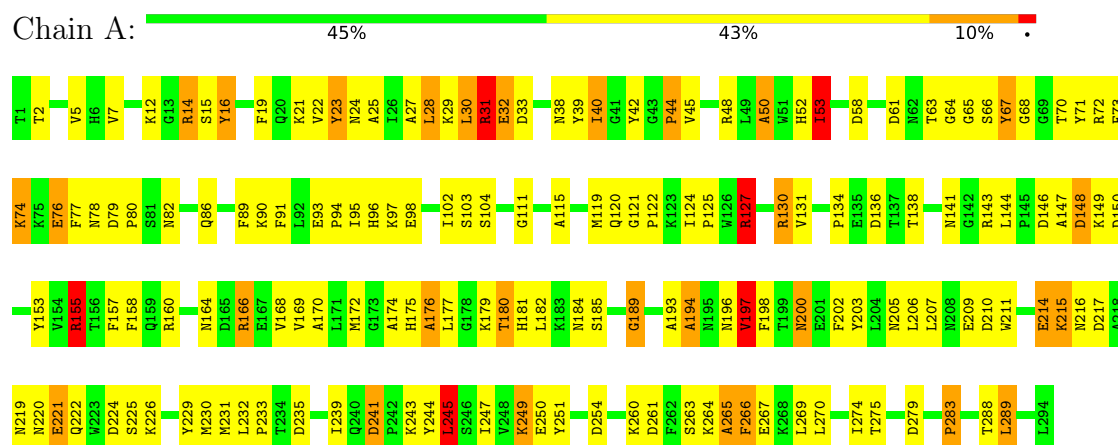


4.2.9 Score per residue for model 9

- Molecule 1: Cytochrome c peroxidase, mitochondrial



- Molecule 1: Cytochrome c peroxidase, mitochondrial



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 120 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

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

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, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.46±0.00	8±0/2438 (0.3± 0.0%)	2.19±0.00	138±0/3302 (4.2± 0.0%)
2	B	1.62±0.01	1±0/821 (0.1± 0.0%)	1.18±0.01	1±0/1097 (0.1± 0.0%)
All	All	1.50	90/32590 (0.3%)	1.99	1390/43990 (3.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	10.0±0.0
2	B	0.0±0.0	3.0±0.0
All	All	0	130

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	B	1	GLY	N-CA	7.19	1.57	1.45	6	10
1	A	265	ALA	C-N	7.04	1.42	1.33	1	10
1	A	264	LYS	N-CA	6.32	1.53	1.46	1	10
1	A	65	GLY	N-CA	5.77	1.50	1.45	1	10
1	A	111	GLY	C-O	5.31	1.30	1.23	1	10
1	A	180	THR	N-CA	5.31	1.52	1.45	1	10
1	A	266	PHE	CA-C	-5.29	1.45	1.52	1	10
1	A	125	PRO	CA-C	-5.28	1.46	1.52	1	10
1	A	251	TYR	C-N	-5.20	1.26	1.33	1	10

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
1	A	289	LEU	N-CA-C	-11.96	98.22	111.14	1	10
1	A	40	ILE	N-CA-C	-10.59	100.36	111.58	1	10
1	A	28	LEU	O-C-N	10.39	134.00	122.15	1	10
1	A	214	GLU	O-C-N	10.09	133.38	123.29	1	10
1	A	176	ALA	CA-C-N	8.70	134.46	122.19	1	10
1	A	176	ALA	C-N-CA	8.70	134.46	122.19	1	10
1	A	214	GLU	CA-C-O	-8.70	111.97	121.28	1	10
1	A	157	PHE	N-CA-C	-8.48	102.03	111.28	1	10
1	A	209	GLU	CA-C-N	8.40	135.81	123.13	1	10
1	A	209	GLU	C-N-CA	8.40	135.81	123.13	1	10
1	A	53	ILE	N-CA-C	-8.34	100.74	113.16	1	10
1	A	22	VAL	CA-C-N	8.27	131.19	120.44	1	10
1	A	22	VAL	C-N-CA	8.27	131.19	120.44	1	10
1	A	32	GLU	N-CA-C	8.17	119.96	111.14	1	10
1	A	76	GLU	CA-C-N	8.02	131.03	120.28	1	10
1	A	76	GLU	C-N-CA	8.02	131.03	120.28	1	10
1	A	53	ILE	O-C-N	8.02	131.64	122.18	1	10
1	A	181	HIS	CA-C-O	-7.81	111.73	120.32	1	10
1	A	217	ASP	O-C-N	7.79	133.13	122.46	1	10
1	A	23	TYR	CA-C-O	7.77	128.98	120.82	1	10
1	A	193	ALA	CA-C-O	-7.74	110.63	120.31	1	10
1	A	224	ASP	CA-C-O	-7.70	112.38	120.70	1	10
1	A	180	THR	CA-C-O	-7.64	112.26	121.28	1	10
1	A	141	ASN	CA-C-O	-7.59	113.28	121.56	1	10
1	A	30	LEU	N-CA-C	-7.55	102.40	111.69	1	10
1	A	25	ALA	CA-C-O	7.53	128.72	120.82	1	10
1	A	111	GLY	CA-C-N	-7.50	110.89	120.34	1	10
1	A	111	GLY	C-N-CA	-7.50	110.89	120.34	1	10
1	A	197	VAL	CA-C-O	-7.41	112.50	120.36	1	10
1	A	274	ILE	O-C-N	7.15	130.69	123.18	1	10
1	A	102	ILE	CA-C-O	-7.07	113.58	121.36	1	10
1	A	71	TYR	CA-C-O	7.04	128.01	119.49	1	10
1	A	89	PHE	CA-C-N	6.93	129.44	120.44	1	10
1	A	89	PHE	C-N-CA	6.93	129.44	120.44	1	10
1	A	175	HIS	CA-CB-CG	-6.89	106.91	113.80	2	10
1	A	189	GLY	O-C-N	6.88	128.65	121.77	1	10
1	A	121	GLY	O-C-N	6.80	128.57	121.77	1	10
1	A	283	PRO	O-C-N	6.72	131.35	123.01	1	10
1	A	52	HIS	N-CA-C	6.70	120.55	112.38	1	10
1	A	225	SER	N-CA-C	-6.69	99.77	110.14	1	10
1	A	31	ARG	O-C-N	-6.67	114.54	122.15	1	10
1	A	50	ALA	CA-C-N	6.66	129.09	120.44	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	50	ALA	C-N-CA	6.66	129.09	120.44	1	10
1	A	153	TYR	CA-C-N	6.65	128.94	120.56	1	10
1	A	153	TYR	C-N-CA	6.65	128.94	120.56	1	10
1	A	14	ARG	N-CA-C	-6.60	100.18	109.69	1	10
1	A	261	ASP	O-C-N	6.48	129.53	122.15	1	10
1	A	124	ILE	O-C-N	6.40	128.40	121.10	1	10
1	A	91	PHE	CA-C-N	-6.37	112.02	122.54	1	10
1	A	91	PHE	C-N-CA	-6.37	112.02	122.54	1	10
1	A	283	PRO	CA-C-O	-6.37	114.17	121.56	1	10
1	A	96	HIS	CA-C-N	6.36	128.81	120.28	1	10
1	A	96	HIS	C-N-CA	6.36	128.81	120.28	1	10
1	A	65	GLY	N-CA-C	-6.36	104.64	112.33	1	10
1	A	157	PHE	CA-C-N	-6.31	110.72	120.31	1	10
1	A	157	PHE	C-N-CA	-6.31	110.72	120.31	1	10
1	A	125	PRO	CA-C-O	-6.30	114.37	121.43	1	10
1	A	244	TYR	N-CA-C	-6.30	103.71	111.40	1	10
1	A	185	SER	CA-C-O	-6.28	112.61	119.08	1	10
1	A	64	GLY	CA-C-O	-6.24	113.71	122.58	1	10
1	A	215	LYS	O-C-N	6.24	131.14	123.21	1	10
1	A	216	ASN	O-C-N	6.24	129.81	121.83	1	10
1	A	216	ASN	CA-C-O	-6.16	113.80	121.50	1	10
1	A	138	THR	O-C-N	6.13	126.89	121.18	1	10
1	A	141	ASN	O-C-N	6.12	130.08	122.86	1	10
1	A	270	LEU	O-C-N	6.11	130.90	122.46	1	10
1	A	205	ASN	CA-C-N	6.09	129.26	120.79	1	10
1	A	205	ASN	C-N-CA	6.09	129.26	120.79	1	10
1	A	33	ASP	O-C-N	-6.03	113.28	122.08	1	10
1	A	16	TYR	CB-CA-C	5.99	122.35	110.42	2	10
1	A	265	ALA	CA-C-N	-5.96	112.49	120.54	1	10
1	A	265	ALA	C-N-CA	-5.96	112.49	120.54	1	10
1	A	73	PHE	CA-C-O	-5.95	114.26	121.28	1	10
1	A	73	PHE	CA-C-N	5.90	128.47	120.38	1	10
1	A	73	PHE	C-N-CA	5.90	128.47	120.38	1	10
1	A	216	ASN	N-CA-C	-5.90	100.71	109.86	1	10
1	A	202	PHE	CA-C-N	5.88	128.63	120.29	1	10
1	A	202	PHE	C-N-CA	5.88	128.63	120.29	1	10
1	A	98	GLU	O-C-N	-5.87	116.03	122.07	1	10
1	A	31	ARG	CA-C-O	5.84	126.61	120.42	1	10
1	A	241	ASP	CA-C-O	5.84	125.86	119.32	1	10
1	A	155	ARG	CA-C-O	5.82	126.72	120.55	1	10
1	A	68	GLY	N-CA-C	5.80	122.50	115.31	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	21	LYS	O-C-N	5.79	129.76	122.23	1	10
1	A	21	LYS	CA-C-O	-5.77	113.83	120.24	1	10
1	A	73	PHE	N-CA-C	-5.76	100.90	110.17	1	10
1	A	196	ASN	CA-C-O	-5.75	113.07	119.34	1	10
1	A	58	ASP	CA-C-O	-5.73	112.55	120.52	1	10
1	A	177	LEU	N-CA-C	5.70	118.92	109.46	1	10
1	A	157	PHE	CA-C-O	5.66	126.55	120.55	1	10
1	A	266	PHE	CA-C-N	-5.66	112.26	120.29	1	10
1	A	266	PHE	C-N-CA	-5.66	112.26	120.29	1	10
1	A	198	PHE	N-CA-C	5.63	117.92	108.23	1	10
1	A	158	PHE	CA-C-O	-5.63	113.49	119.97	1	10
1	A	103	SER	CA-C-O	-5.62	115.17	121.81	1	10
1	A	5	VAL	CA-C-N	5.58	131.55	123.13	1	10
1	A	5	VAL	C-N-CA	5.58	131.55	123.13	1	10
1	A	184	ASN	CA-C-O	5.54	126.77	120.00	1	10
1	A	224	ASP	O-C-N	5.54	130.44	123.23	1	10
1	A	77	PHE	O-C-N	5.54	127.99	122.12	1	10
1	A	179	LYS	CA-C-N	-5.54	113.23	122.64	1	10
1	A	179	LYS	C-N-CA	-5.54	113.23	122.64	1	10
1	A	104	SER	CA-C-N	5.51	126.10	119.98	1	10
1	A	104	SER	C-N-CA	5.51	126.10	119.98	1	10
1	A	225	SER	CA-C-O	-5.48	114.93	121.56	1	10
1	A	229	TYR	CA-C-N	5.43	131.12	122.59	1	10
1	A	229	TYR	C-N-CA	5.43	131.12	122.59	1	10
1	A	131	VAL	CA-C-N	5.43	129.18	121.42	1	10
1	A	131	VAL	C-N-CA	5.43	129.18	121.42	1	10
1	A	249	LYS	CA-C-O	5.43	126.26	120.24	1	10
1	A	274	ILE	CA-C-N	-5.39	115.50	123.05	1	10
1	A	274	ILE	C-N-CA	-5.39	115.50	123.05	1	10
1	A	245	LEU	O-C-N	-5.37	115.94	122.22	1	10
1	A	144	LEU	O-C-N	5.36	126.03	121.20	1	10
1	A	42	TYR	CA-C-N	5.36	130.28	121.87	1	10
1	A	42	TYR	C-N-CA	5.36	130.28	121.87	1	10
1	A	64	GLY	O-C-N	5.36	128.57	123.05	1	10
1	A	288	THR	CA-C-N	5.35	127.72	120.44	1	10
1	A	288	THR	C-N-CA	5.35	127.72	120.44	1	10
2	B	1	GLY	N-CA-C	5.35	128.81	113.30	2	10
1	A	65	GLY	CA-C-N	5.34	127.87	120.29	1	10
1	A	65	GLY	C-N-CA	5.34	127.87	120.29	1	10
1	A	150	ASP	CA-C-O	-5.34	115.30	121.49	1	10
1	A	194	ALA	CA-C-O	-5.25	114.55	122.38	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	16	TYR	N-CA-CB	-5.21	101.69	110.49	2	10
1	A	243	LYS	CA-C-N	5.15	129.31	120.71	1	10
1	A	243	LYS	C-N-CA	5.15	129.31	120.71	1	10
1	A	221	GLU	O-C-N	5.13	129.62	123.16	1	10
1	A	198	PHE	CA-C-O	5.13	126.52	120.98	1	10
1	A	225	SER	O-C-N	5.12	129.71	123.10	1	10
1	A	216	ASN	CA-C-N	5.10	130.64	121.66	1	10
1	A	216	ASN	C-N-CA	5.10	130.64	121.66	1	10
1	A	44	PRO	O-C-N	-5.09	116.68	122.18	1	10
1	A	197	VAL	O-C-N	5.09	128.70	123.20	1	10
1	A	247	ILE	N-CA-C	-5.08	105.46	111.00	1	10
1	A	170	ALA	O-C-N	5.08	127.30	122.07	1	10
1	A	149	LYS	CA-C-O	-5.06	115.35	121.32	1	10
1	A	122	PRO	CA-C-N	5.02	128.60	121.42	1	10
1	A	122	PRO	C-N-CA	5.02	128.60	121.42	1	10

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	14	ARG	Sidechain	10
1	A	31	ARG	Sidechain	10
1	A	48	ARG	Sidechain	10
1	A	72	ARG	Sidechain	10
1	A	127	ARG	Sidechain	10
1	A	130	ARG	Sidechain	10
1	A	143	ARG	Sidechain	10
1	A	155	ARG	Sidechain	10
1	A	160	ARG	Sidechain	10
1	A	166	ARG	Sidechain	10
2	B	13	ARG	Sidechain	10
2	B	38	ARG	Sidechain	10
2	B	91	ARG	Sidechain	10

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2371	2250	2252	51±1
2	B	804	805	809	13±1
4	B	43	32	25	6±1
All	All	32610	31170	31160	602

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:ALA:O	1:A:233:PRO:HG2	1.19	1.35	2	10
1:A:38:ASN:O	2:B:12:ALA:HB1	0.97	1.59	6	10
2:B:17:CYS:SG	4:B:104:HEC:C3C	0.92	2.58	1	10
1:A:93:GLU:N	1:A:94:PRO:HD2	0.90	1.82	2	10
2:B:14:CYS:SG	4:B:104:HEC:CBB	0.84	2.65	9	10
1:A:164:ASN:O	1:A:168:VAL:HG13	0.79	1.77	3	10
2:B:14:CYS:O	2:B:15:LEU:CB	0.75	2.34	4	10
1:A:16:TYR:O	1:A:19:PHE:N	0.67	2.28	1	10
1:A:93:GLU:N	1:A:94:PRO:CD	0.65	2.59	2	10
1:A:147:ALA:O	1:A:233:PRO:CG	0.65	2.30	2	10
1:A:200:ASN:H	1:A:200:ASN:HD22	0.64	1.33	1	10
2:B:80:MET:O	2:B:80:MET:HG3	0.62	1.94	2	10
2:B:14:CYS:O	2:B:15:LEU:HB3	0.60	1.97	7	10
2:B:80:MET:HB3	4:B:104:HEC:C1D	0.60	2.27	9	10
2:B:17:CYS:SG	4:B:104:HEC:CBC	0.59	2.89	2	10
1:A:119:MET:O	1:A:120:GLN:HB2	0.58	1.96	2	10
1:A:194:ALA:HB1	1:A:197:VAL:HG13	0.58	1.75	2	10
1:A:206:LEU:HG	1:A:239:ILE:CG2	0.57	2.29	2	10
1:A:180:THR:N	1:A:189:GLY:O	0.57	2.29	1	10
1:A:197:VAL:HG21	2:B:81:ALA:HB1	0.56	1.77	9	10
1:A:147:ALA:C	1:A:233:PRO:HG2	0.53	2.23	2	10
1:A:67:TYR:HA	1:A:130:ARG:HG2	0.53	1.79	2	10
1:A:200:ASN:HD22	1:A:200:ASN:N	0.53	2.00	1	10
1:A:193:ALA:HB1	2:B:17:CYS:SG	0.52	2.44	3	8
2:B:14:CYS:SG	4:B:104:HEC:C3B	0.52	2.97	2	10
1:A:115:ALA:O	1:A:119:MET:HG3	0.51	2.06	3	10
1:A:206:LEU:HG	1:A:239:ILE:HG21	0.51	1.80	2	10
1:A:79:ASP:O	1:A:82:ASN:HB2	0.51	2.06	2	10
1:A:127:ARG:HG3	1:A:283:PRO:HA	0.51	1.83	1	10
1:A:245:LEU:O	1:A:245:LEU:HD22	0.50	2.05	9	10
1:A:197:VAL:CG2	2:B:81:ALA:HB1	0.50	2.37	5	8
1:A:200:ASN:H	1:A:200:ASN:ND2	0.49	2.05	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:169:VAL:O	1:A:203:TYR:OH	0.49	2.31	6	10
1:A:23:TYR:O	1:A:27:ALA:N	0.48	2.36	1	10
1:A:215:LYS:HA	1:A:220:ASN:O	0.48	2.09	1	10
1:A:265:ALA:O	1:A:266:PHE:C	0.47	2.56	1	10
1:A:134:PRO:C	1:A:136:ASP:N	0.47	2.73	1	10
2:B:80:MET:HB3	4:B:104:HEC:C2D	0.46	2.41	3	5
1:A:74:LYS:O	1:A:78:ASN:HB2	0.45	2.11	1	10
1:A:40:ILE:CG2	1:A:44:PRO:HG3	0.45	2.42	2	10
1:A:232:LEU:O	1:A:235:ASP:N	0.45	2.47	1	10
1:A:239:ILE:HG22	1:A:245:LEU:HD23	0.44	1.87	9	9
1:A:230:MET:C	1:A:230:MET:SD	0.44	3.01	2	10
1:A:38:ASN:O	1:A:39:TYR:HB2	0.44	2.13	2	10
1:A:15:SER:O	1:A:16:TYR:C	0.43	2.61	1	10
1:A:66:SER:O	1:A:67:TYR:C	0.43	2.61	1	10
1:A:1:THR:O	1:A:2:THR:HG22	0.43	2.13	2	1
1:A:214:GLU:N	1:A:222:GLN:O	0.42	2.50	1	10
1:A:214:GLU:O	1:A:221:GLU:HA	0.42	2.14	9	10
1:A:79:ASP:OD1	1:A:80:PRO:HD2	0.42	2.14	2	10
1:A:90:LYS:O	1:A:94:PRO:HD2	0.42	2.15	1	10
1:A:200:ASN:N	1:A:200:ASN:ND2	0.42	2.67	1	10
1:A:2:THR:OG1	1:A:3:PRO:HD2	0.42	2.15	2	1
2:B:18:HIS:CD2	4:B:104:HEC:NB	0.41	2.89	5	8
1:A:148:ASP:HA	1:A:233:PRO:HG3	0.41	1.92	2	10
1:A:180:THR:OG1	1:A:230:MET:HE3	0.41	2.16	9	9
1:A:211:TRP:CH2	1:A:231:MET:HG2	0.41	2.50	1	10
1:A:174:ALA:C	1:A:176:ALA:H	0.41	2.24	1	10
1:A:249:LYS:O	1:A:250:GLU:C	0.41	2.62	1	10
1:A:174:ALA:C	1:A:176:ALA:N	0.40	2.79	1	10
1:A:7:VAL:HA	1:A:275:THR:O	0.40	2.16	1	10
1:A:50:ALA:O	1:A:53:ILE:HG13	0.40	2.17	1	9
1:A:90:LYS:O	1:A:94:PRO:CD	0.40	2.69	2	10
1:A:119:MET:O	1:A:120:GLN:CB	0.40	2.67	9	2
2:B:17:CYS:SG	4:B:104:HEC:HAC	0.40	2.46	4	1
1:A:250:GLU:O	1:A:253:ASN:HB2	0.40	2.17	9	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	292/294 (99%)	264±0 (90±0%)	27±0 (9±0%)	1±0 (0±0%)	37	78
2	B	101/108 (94%)	94±3 (93±3%)	6±3 (6±3%)	2±0 (2±0%)	9	52
All	All	3930/4020 (98%)	3576 (91%)	326 (8%)	28 (1%)	20	70

All 3 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	67	TYR	10
2	B	15	LEU	10
2	B	56	ASN	8

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	252/252 (100%)	212±0 (84±0%)	40±0 (16±0%)	4	40
2	B	84/88 (95%)	69±1 (83±1%)	15±1 (17±1%)	4	37
All	All	3360/3400 (99%)	2813 (84%)	547 (16%)	4	40

All 61 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	2	THR	10
1	A	12	LYS	10
1	A	24	ASN	10
1	A	28	LEU	10
1	A	30	LEU	10
1	A	31	ARG	10
1	A	32	GLU	10
1	A	45	VAL	10
1	A	53	ILE	10
1	A	61	ASP	10

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Mol	Chain	Res	Type	Models (Total)
1	A	63	THR	10
1	A	70	THR	10
1	A	74	LYS	10
1	A	86	GLN	10
1	A	97	LYS	10
1	A	127	ARG	10
1	A	146	ASP	10
1	A	148	ASP	10
1	A	166	ARG	10
1	A	172	MET	10
1	A	182	LEU	10
1	A	197	VAL	10
1	A	200	ASN	10
1	A	207	LEU	10
1	A	210	ASP	10
1	A	219	ASN	10
1	A	226	LYS	10
1	A	241	ASP	10
1	A	245	LEU	10
1	A	254	ASP	10
1	A	260	LYS	10
1	A	263	SER	10
1	A	267	GLU	10
1	A	269	LEU	10
1	A	279	ASP	10
1	A	289	LEU	10
2	B	9	LEU	10
2	B	14	CYS	10
2	B	15	LEU	10
2	B	16	GLN	10
2	B	19	THR	10
2	B	28	VAL	10
2	B	31	ASN	10
2	B	52	ASN	10
2	B	55	LYS	10
2	B	56	ASN	10
2	B	57	VAL	10
2	B	58	LEU	10
2	B	63	ASN	10
2	B	70	ASN	10
1	A	29	LYS	9
1	A	76	GLU	9

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Mol	Chain	Res	Type	Models (Total)
1	A	95	ILE	9
1	A	155	ARG	9
2	B	90	ASP	4
1	A	294	LEU	2
1	A	141	ASN	1
1	A	206	LEU	1
2	B	21	GLU	1
2	B	50	ASP	1
1	A	47	VAL	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	HEC	B	104	2	46,50,50	3.01±0.00	9±0 (18±0%)
3	HEM	A	295	1	50,50,50	1.73±0.00	12±0 (24±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
4	HEC	B	104	2	58,82,82	1.51±0.01	10±0 (16±0%)
3	HEM	A	295	1	67,82,82	1.31±0.00	9±0 (13±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
4	HEC	B	104	2	-	0±0,14,54,54	-
3	HEM	A	295	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
4	B	104	HEC	CBB-CAB	10.26	1.11	1.49	2	10
4	B	104	HEC	CAC-C3C	9.82	1.66	1.35	10	10
4	B	104	HEC	CBC-CAC	9.18	1.15	1.49	9	10
4	B	104	HEC	CAB-C3B	8.74	1.63	1.35	7	10
3	A	295	HEM	FE-NB	5.16	2.10	1.94	1	10
3	A	295	HEM	FE-ND	3.90	2.06	1.94	1	10
3	A	295	HEM	C3B-C2B	3.35	1.30	1.37	1	10
3	A	295	HEM	CAB-C3B	3.14	1.55	1.47	1	10
3	A	295	HEM	CMA-C3A	3.08	1.57	1.50	1	10
4	B	104	HEC	CMC-C2C	3.02	1.57	1.50	9	10
3	A	295	HEM	CMB-C2B	2.97	1.56	1.50	1	10
3	A	295	HEM	C2A-C3A	2.74	1.31	1.38	1	10
4	B	104	HEC	CAA-C2A	2.67	1.58	1.51	10	10
3	A	295	HEM	C3D-C2D	2.34	1.31	1.36	1	10
4	B	104	HEC	C3C-C2C	2.31	1.33	1.41	7	10
3	A	295	HEM	C1B-NB	2.27	1.36	1.40	1	10
3	A	295	HEM	CAA-C2A	2.25	1.57	1.51	1	10
4	B	104	HEC	CAD-C3D	2.20	1.57	1.51	10	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
4	B	104	HEC	CMA-C3A	2.15	1.55	1.50	4	7
3	A	295	HEM	CMD-C2D	2.13	1.55	1.50	1	10
3	A	295	HEM	C4D-ND	2.10	1.36	1.40	1	10

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
4	B	104	HEC	CBB-CAB-C3B	5.28	116.89	127.43	7	10
4	B	104	HEC	CBC-CAC-C3C	4.29	118.86	127.43	10	10
3	A	295	HEM	CBC-CAC-C3C	4.09	147.95	127.53	1	10
4	B	104	HEC	O2D-CGD-O1D	3.67	132.78	123.33	4	10
3	A	295	HEM	CAA-C2A-C1A	2.92	119.24	124.94	1	10
4	B	104	HEC	CMC-C2C-C1C	2.80	121.15	125.42	10	10
4	B	104	HEC	CMB-C2B-C1B	2.61	121.44	125.42	3	10
3	A	295	HEM	CHA-C1A-NA	2.39	128.19	123.86	1	10
3	A	295	HEM	CMB-C2B-C1B	2.37	121.33	125.03	1	10
3	A	295	HEM	CMA-C3A-C2A	2.35	130.61	125.62	1	10
3	A	295	HEM	CMD-C2D-C1D	2.32	121.41	125.03	1	10
4	B	104	HEC	O2A-CGA-O1A	2.32	129.29	123.33	9	10
3	A	295	HEM	O1D-CGD-CBD	2.28	115.85	123.09	1	10
4	B	104	HEC	C2A-C1A-NA	2.27	108.13	110.32	1	10
4	B	104	HEC	CHB-C4A-NA	2.24	122.02	124.45	10	10
3	A	295	HEM	CMD-C2D-C3D	2.11	131.85	126.15	1	10
3	A	295	HEM	CMA-C3A-C4A	2.08	122.25	125.42	1	10
4	B	104	HEC	O1A-CGA-CBA	2.07	116.53	123.09	7	9
4	B	104	HEC	O1D-CGD-CBD	2.03	116.65	123.09	3	9

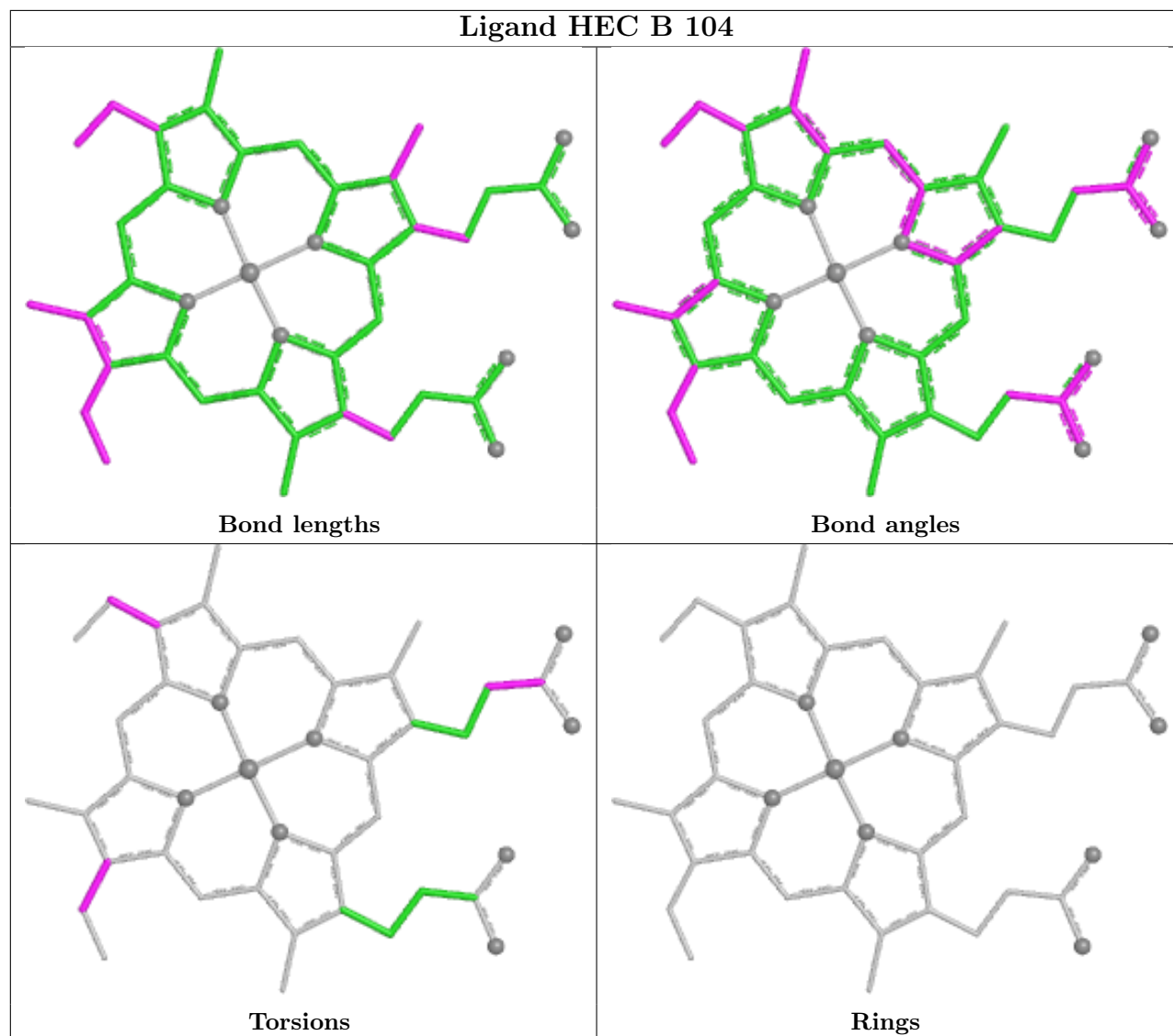
There are no chirality outliers.

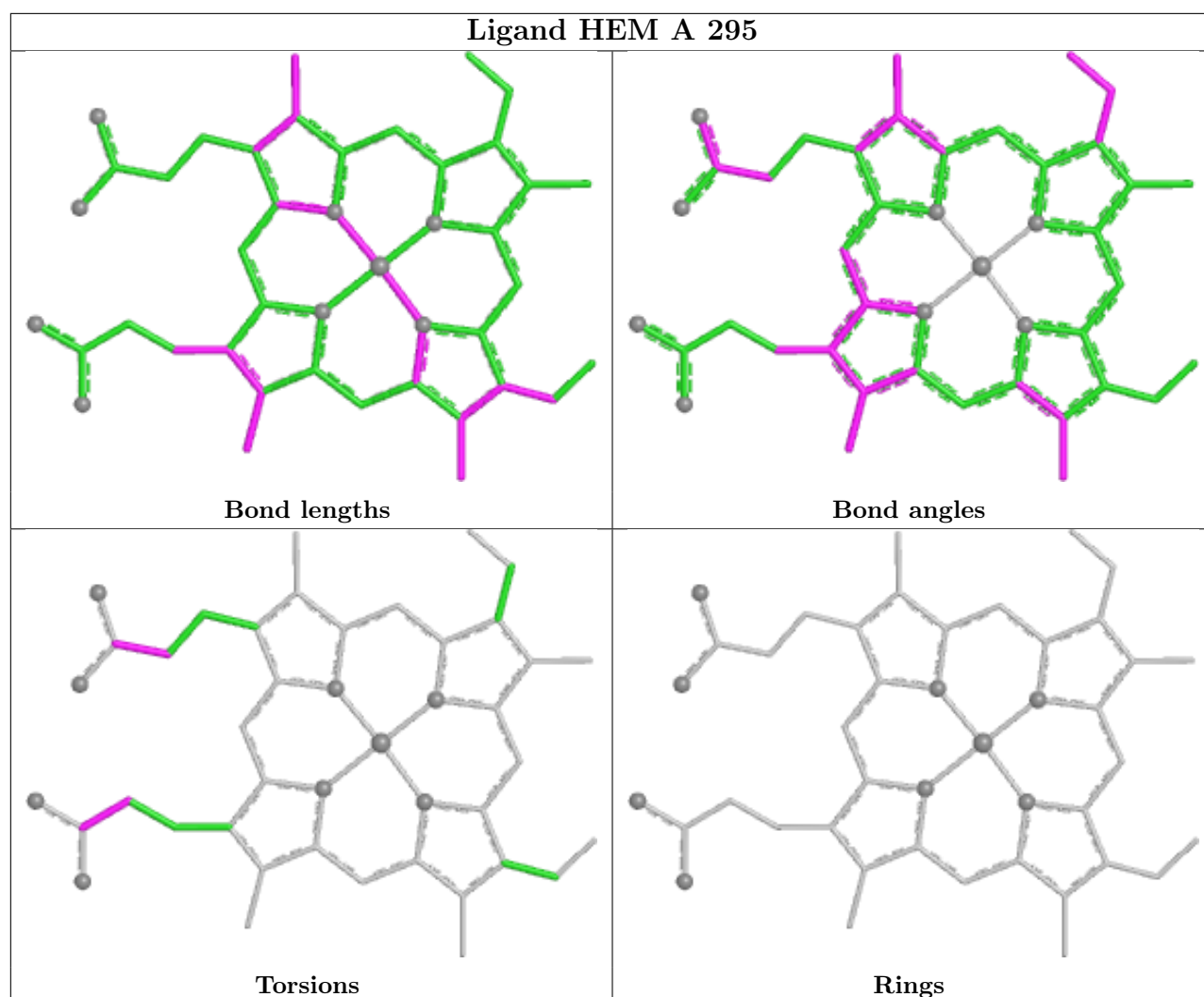
There are no torsion outliers.

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