



Full wwPDB NMR Structure Validation Report ⓘ

Sep 25, 2019 – 02:28 PM EDT

PDB ID : 2KMY
Title : NMR Solution structures of fully oxidised cytochrome c3 from *Desulfovibrio desulfuricans* ATCC 27774
Authors : Turner, D.L.; Paixao, V.B.; Vis, H.
Deposited on : 2009-08-05

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.0 (224370), CSD as540be (2019)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.4
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

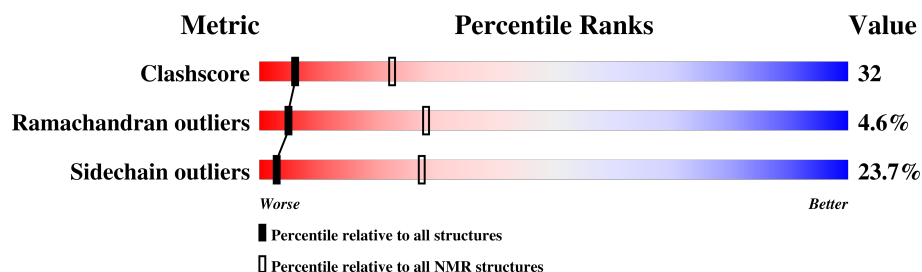
1 Overall quality at a glance

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	136327	12091
Ramachandran outliers	132723	10835
Sidechain outliers	132532	10811

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	107	<div> <div>45%</div> <div>48%</div> <div>7%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:107 (107)	0.24	2

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

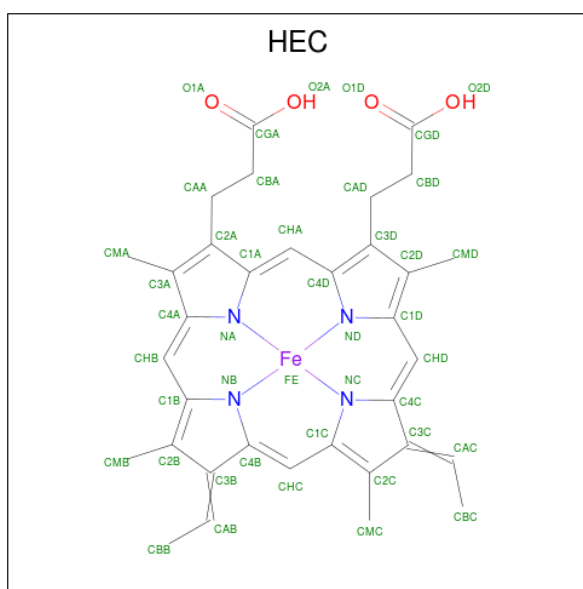
- Molecule 1 is a protein called Cytochrome c3.

Mol	Chain	Residues	Atoms						Trace
1	A	107	Total	C	H	N	O	S	0
			1602	503	796	144	150	9	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	ARG	LYS	SEE REMARK 999	UNP Q9L915

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



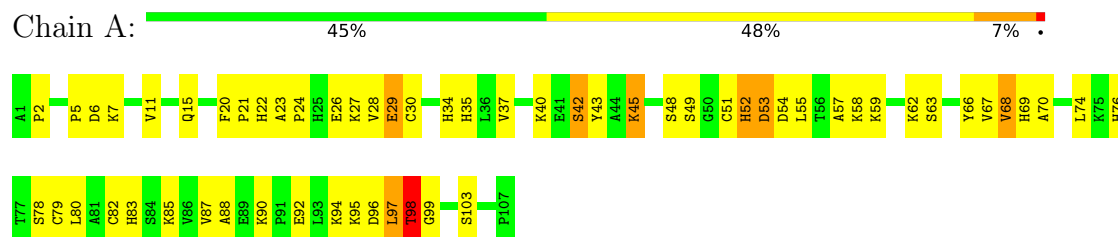
Mol	Chain	Residues	Atoms				
2	A	1	Total 43	C 34	Fe 1	N 4	O 4
2	A	1	Total 43	C 34	Fe 1	N 4	O 4
2	A	1	Total 43	C 34	Fe 1	N 4	O 4
2	A	1	Total 43	C 34	Fe 1	N 4	O 4

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Cytochrome c3

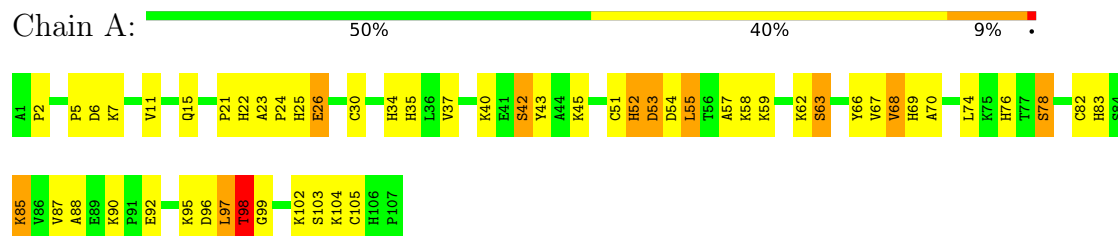


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

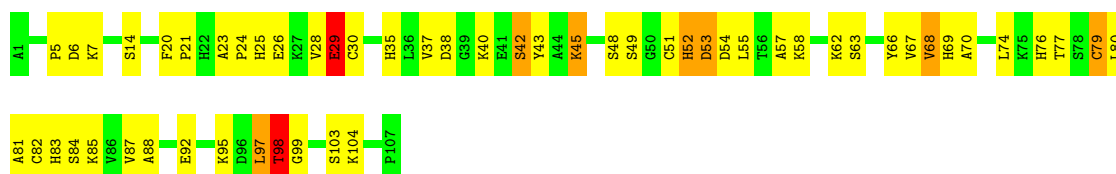
- Molecule 1: Cytochrome c3



4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Cytochrome c3

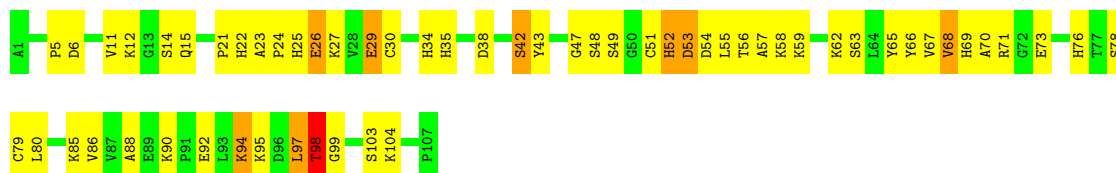




4.2.3 Score per residue for model 3

- Molecule 1: Cytochrome c3

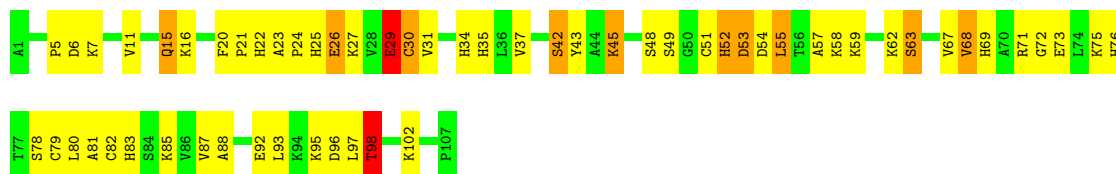
Chain A: 46% 46% 7% .



4.2.4 Score per residue for model 4

- Molecule 1: Cytochrome c3

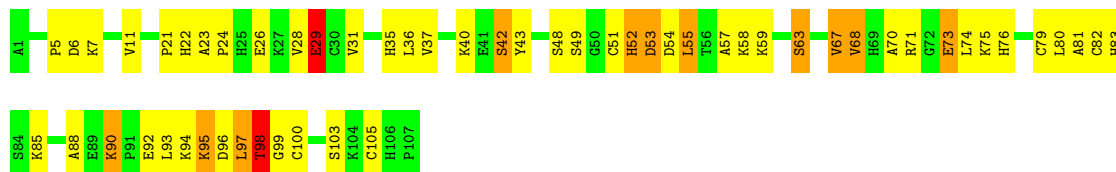
Chain A: 45% 44% 9% .



4.2.5 Score per residue for model 5

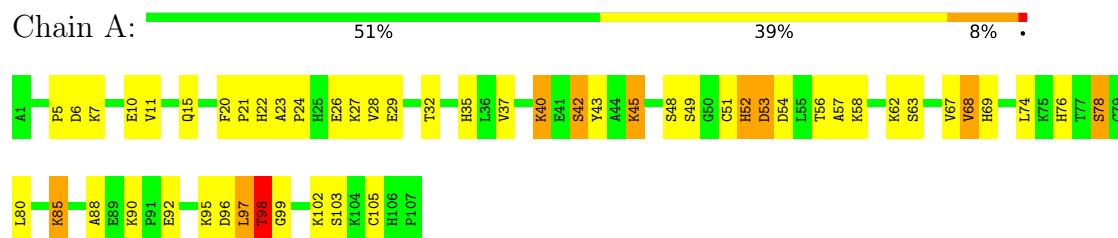
- Molecule 1: Cytochrome c3

Chain A: 48% 40% 10% .



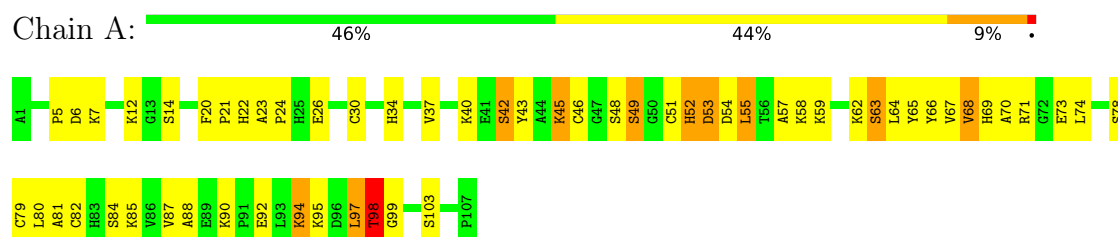
4.2.6 Score per residue for model 6

- Molecule 1: Cytochrome c3



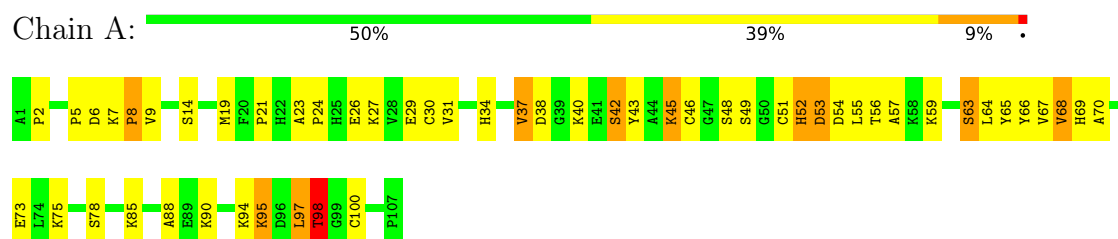
4.2.7 Score per residue for model 7

- Molecule 1: Cytochrome c3



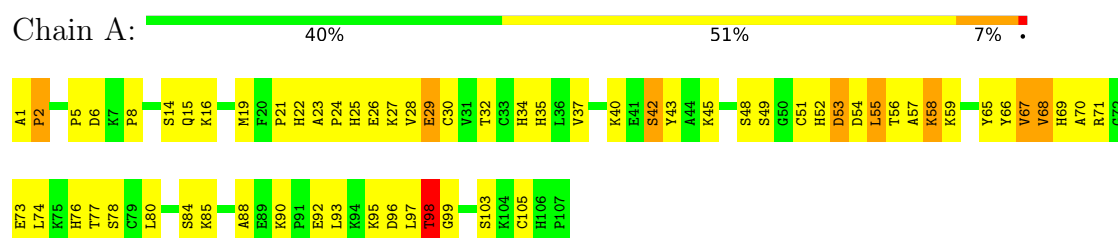
4.2.8 Score per residue for model 8

- Molecule 1: Cytochrome c3



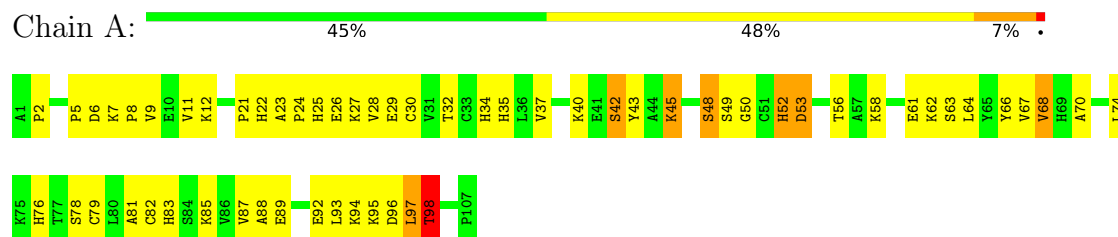
4.2.9 Score per residue for model 9

- Molecule 1: Cytochrome c3



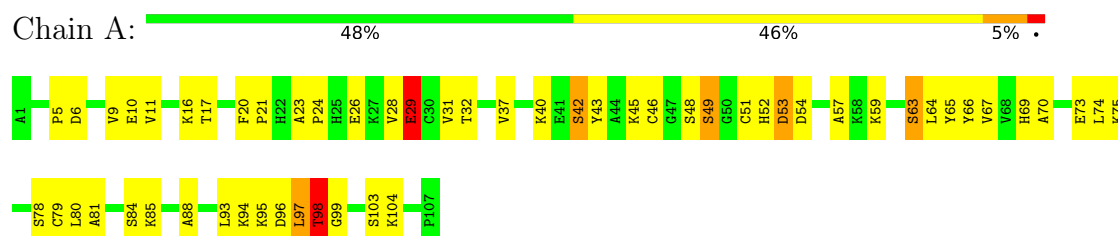
4.2.10 Score per residue for model 10

- Molecule 1: Cytochrome c3



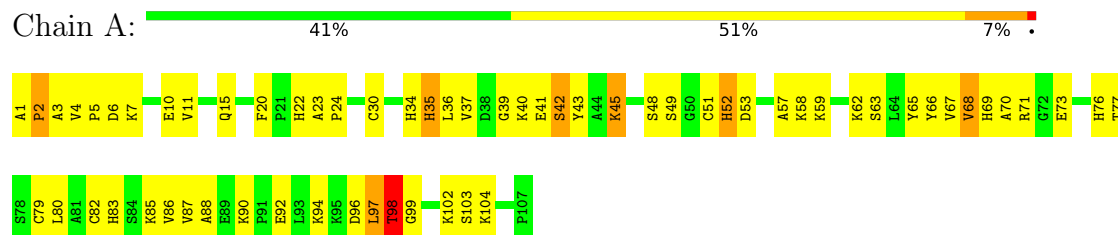
4.2.11 Score per residue for model 11

- Molecule 1: Cytochrome c3



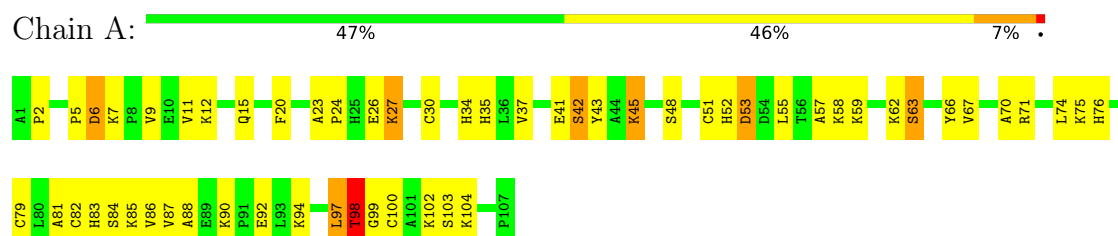
4.2.12 Score per residue for model 12

- Molecule 1: Cytochrome c3



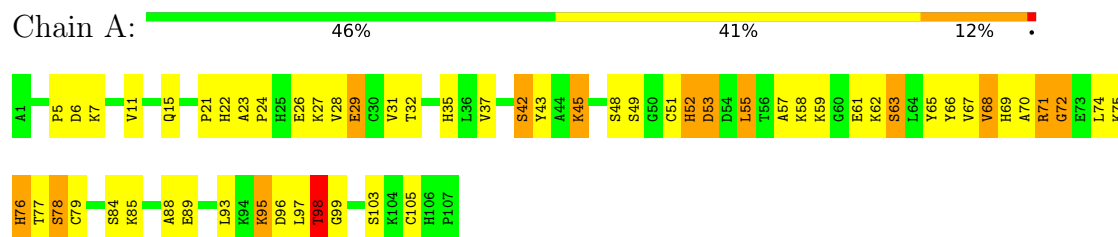
4.2.13 Score per residue for model 13

- Molecule 1: Cytochrome c3



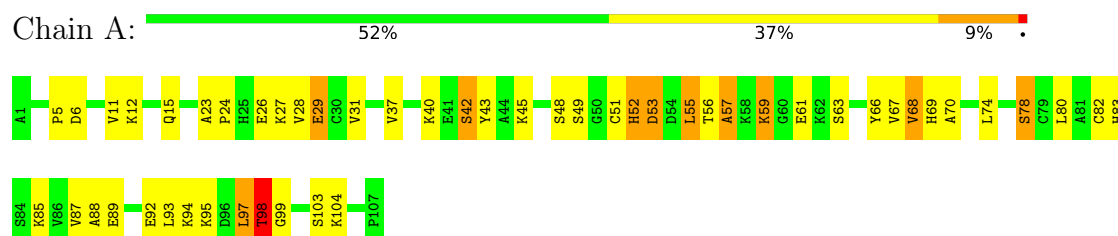
4.2.14 Score per residue for model 14

- Molecule 1: Cytochrome c3



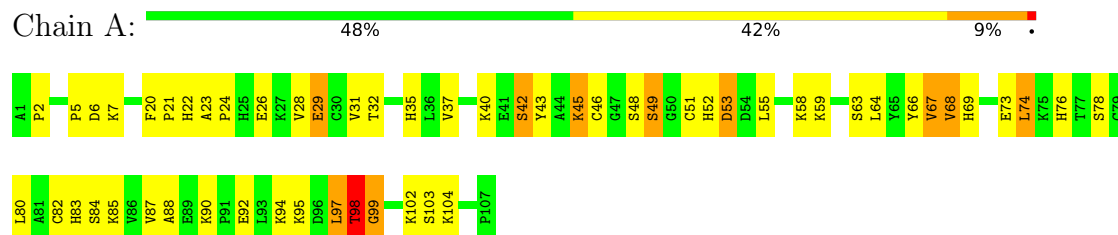
4.2.15 Score per residue for model 15

- Molecule 1: Cytochrome c3



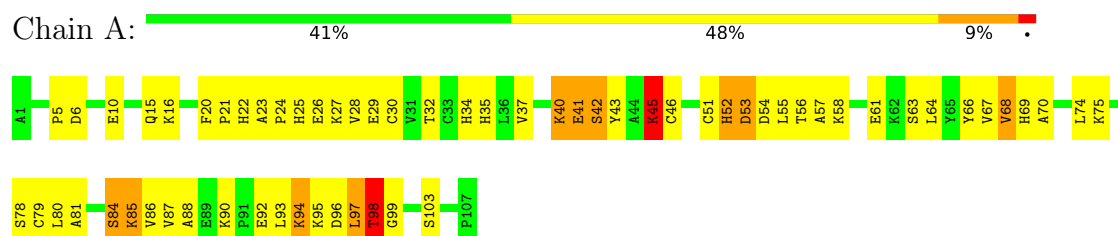
4.2.16 Score per residue for model 16

- Molecule 1: Cytochrome c3



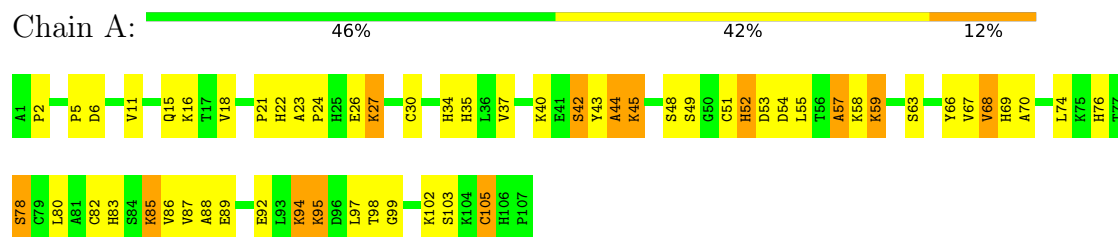
4.2.17 Score per residue for model 17

- Molecule 1: Cytochrome c3



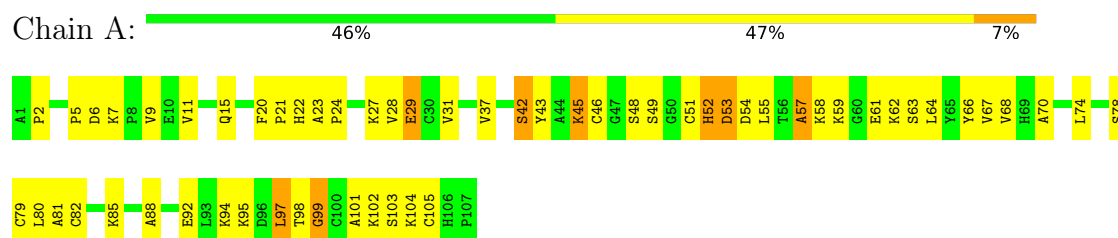
4.2.18 Score per residue for model 18

- Molecule 1: Cytochrome c3



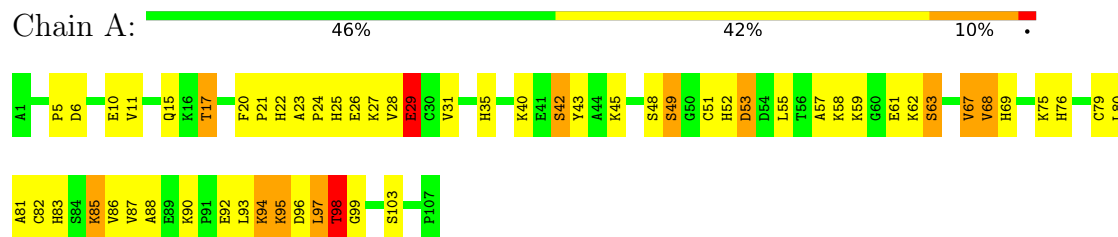
4.2.19 Score per residue for model 19

- Molecule 1: Cytochrome c3



4.2.20 Score per residue for model 20

- Molecule 1: Cytochrome c3



5 Refinement protocol and experimental data overview

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

Of the 600 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
PARADYANA	structure solution	
PARADYANA	refinement	

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

6 Model quality

6.1 Standard geometry

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	806	796	798	49±5
2	A	172	0	120	21±5
All	All	19560	15920	18360	1197

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 32.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:LEU:HD11	2:A:282:HEC:CHA	0.96	1.91	4	15
1:A:23:ALA:HB3	1:A:24:PRO:HD3	0.94	1.39	12	20
1:A:9:VAL:HG11	2:A:233:HEC:CGA	0.93	1.93	10	5
1:A:83:HIS:CE1	1:A:97:LEU:HD13	0.92	1.99	15	4
1:A:68:VAL:O	1:A:80:LEU:HD23	0.90	1.66	16	1
1:A:23:ALA:HB3	1:A:24:PRO:CD	0.88	1.98	5	20
2:A:282:HEC:HBC3	2:A:282:HEC:HMC1	0.87	1.47	15	10
1:A:67:VAL:O	1:A:67:VAL:HG22	0.86	1.70	16	1
1:A:52:HIS:CE1	1:A:67:VAL:HG11	0.86	2.04	5	15
2:A:282:HEC:HMC1	2:A:282:HEC:HBC3	0.85	1.46	19	10
1:A:67:VAL:HG22	1:A:67:VAL:O	0.84	1.70	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:LEU:O	1:A:98:THR:HG23	0.84	1.73	4	5
2:A:305:HEC:HBC3	2:A:305:HEC:HMC1	0.84	1.49	6	10
2:A:282:HEC:HMB1	2:A:282:HEC:HBB3	0.84	1.50	15	10
1:A:74:LEU:HD22	2:A:251:HEC:O2A	0.83	1.71	10	1
2:A:282:HEC:HBB3	2:A:282:HEC:HMB1	0.82	1.49	18	10
1:A:45:LYS:O	2:A:251:HEC:HMC3	0.82	1.74	18	18
2:A:305:HEC:HMC1	2:A:305:HEC:HBC3	0.82	1.49	18	9
1:A:65:TYR:CE2	1:A:69:HIS:CE1	0.81	2.69	12	3
1:A:68:VAL:O	1:A:80:LEU:HD13	0.80	1.77	4	6
2:A:305:HEC:CBC	2:A:305:HEC:HMC1	0.80	2.05	13	4
2:A:305:HEC:HMC1	2:A:305:HEC:CBC	0.80	2.06	16	6
1:A:67:VAL:O	1:A:68:VAL:HG23	0.79	1.77	16	15
2:A:233:HEC:HMB1	2:A:233:HEC:HBB3	0.77	1.54	16	14
1:A:74:LEU:HD22	2:A:251:HEC:O1A	0.75	1.81	19	1
1:A:35:HIS:CD2	1:A:76:HIS:CD2	0.74	2.76	16	11
1:A:54:ASP:OD1	1:A:57:ALA:HB3	0.73	1.84	9	4
1:A:11:VAL:HG22	2:A:233:HEC:O1D	0.72	1.85	19	3
2:A:233:HEC:HBB3	2:A:233:HEC:HMB1	0.72	1.61	11	5
1:A:87:VAL:HG11	1:A:94:LYS:HA	0.72	1.60	20	5
1:A:97:LEU:N	1:A:97:LEU:HD23	0.72	1.99	6	7
1:A:11:VAL:HG22	2:A:233:HEC:O2D	0.71	1.86	4	2
1:A:67:VAL:CG2	1:A:67:VAL:O	0.70	2.38	9	3
1:A:67:VAL:O	1:A:67:VAL:CG2	0.70	2.38	16	2
1:A:5:PRO:HG2	1:A:22:HIS:CE1	0.70	2.22	18	15
2:A:282:HEC:HMC1	2:A:282:HEC:CBC	0.69	2.17	16	13
2:A:282:HEC:CBC	2:A:282:HEC:HMC1	0.69	2.17	18	7
1:A:66:TYR:O	1:A:70:ALA:HB2	0.69	1.87	10	12
1:A:96:ASP:C	1:A:97:LEU:HD22	0.69	2.08	10	2
1:A:20:PHE:CE2	2:A:233:HEC:CHD	0.68	2.75	17	4
1:A:23:ALA:CB	1:A:24:PRO:CD	0.68	2.71	14	20
1:A:85:LYS:O	1:A:88:ALA:HB3	0.68	1.89	11	19
2:A:251:HEC:HBC3	2:A:251:HEC:HMC1	0.68	1.66	4	8
1:A:9:VAL:HG11	2:A:233:HEC:O2A	0.67	1.89	13	2
1:A:67:VAL:HG12	2:A:251:HEC:C3A	0.67	2.20	5	5
1:A:67:VAL:O	1:A:67:VAL:HG23	0.67	1.90	13	1
1:A:97:LEU:HD11	2:A:282:HEC:C1A	0.67	2.19	4	3
1:A:29:GLU:O	2:A:233:HEC:HMC3	0.66	1.91	4	3
1:A:96:ASP:C	1:A:97:LEU:HD23	0.65	2.11	12	4
1:A:67:VAL:HG23	1:A:67:VAL:O	0.65	1.90	11	1
1:A:35:HIS:CG	1:A:76:HIS:CD2	0.65	2.84	16	11
1:A:93:LEU:O	1:A:97:LEU:N	0.65	2.29	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:CYS:O	1:A:64:LEU:HD13	0.65	1.90	8	6
1:A:37:VAL:HG21	2:A:251:HEC:HBC2	0.65	1.67	6	10
1:A:66:TYR:CZ	1:A:74:LEU:CD2	0.64	2.80	16	8
1:A:65:TYR:CD2	1:A:69:HIS:CE1	0.64	2.85	12	2
1:A:42:SER:O	1:A:43:TYR:CD1	0.64	2.50	14	20
1:A:83:HIS:O	1:A:87:VAL:HG22	0.64	1.92	12	5
2:A:282:HEC:HMB1	2:A:282:HEC:CBB	0.64	2.22	12	6
1:A:37:VAL:HG12	1:A:37:VAL:O	0.64	1.92	19	3
1:A:68:VAL:HG12	1:A:69:HIS:CE1	0.64	2.28	20	9
1:A:20:PHE:CZ	2:A:233:HEC:CHD	0.63	2.82	20	9
1:A:68:VAL:CG1	1:A:69:HIS:CE1	0.63	2.82	20	10
1:A:20:PHE:CE2	2:A:233:HEC:C1D	0.63	2.82	17	1
2:A:233:HEC:O1D	2:A:233:HEC:HMD1	0.62	1.94	2	1
1:A:21:PRO:HG3	2:A:282:HEC:HBA1	0.62	1.71	2	1
1:A:97:LEU:CD1	2:A:282:HEC:CHA	0.62	2.77	20	14
1:A:70:ALA:HB3	1:A:78:SER:OG	0.62	1.94	15	1
2:A:251:HEC:HMB1	2:A:251:HEC:HBB3	0.62	1.71	14	14
2:A:251:HEC:HMC1	2:A:251:HEC:HBC3	0.62	1.72	6	10
1:A:97:LEU:CD2	1:A:97:LEU:N	0.61	2.63	1	11
1:A:97:LEU:CD2	2:A:282:HEC:CHA	0.61	2.78	18	1
1:A:11:VAL:HG12	1:A:11:VAL:O	0.61	1.96	18	9
1:A:97:LEU:N	1:A:97:LEU:CD2	0.61	2.63	6	7
1:A:63:SER:O	1:A:67:VAL:HG22	0.61	1.95	5	3
1:A:97:LEU:HD11	2:A:282:HEC:HBD1	0.60	1.71	17	1
1:A:54:ASP:OD2	1:A:57:ALA:HB3	0.60	1.95	3	2
1:A:37:VAL:CG2	2:A:251:HEC:HBC2	0.60	2.26	19	2
1:A:23:ALA:CB	1:A:24:PRO:HD3	0.60	2.23	12	20
1:A:63:SER:O	1:A:67:VAL:CG1	0.60	2.50	13	2
1:A:85:LYS:O	1:A:88:ALA:CB	0.60	2.50	15	17
1:A:83:HIS:CE1	1:A:97:LEU:CD1	0.59	2.82	15	1
1:A:28:VAL:CG1	1:A:32:THR:HG21	0.59	2.27	14	5
2:A:233:HEC:HMC1	2:A:233:HEC:HBC3	0.58	1.74	10	13
2:A:233:HEC:CHA	2:A:233:HEC:O1A	0.58	2.51	8	1
1:A:90:LYS:HD3	1:A:93:LEU:HD12	0.58	1.74	20	1
1:A:73:GLU:O	1:A:74:LEU:HD23	0.58	1.98	5	1
1:A:98:THR:O	1:A:99:GLY:C	0.58	2.41	19	6
1:A:57:ALA:HB3	1:A:63:SER:OG	0.58	1.99	13	5
1:A:21:PRO:HG2	1:A:24:PRO:HG2	0.58	1.75	18	11
2:A:251:HEC:HBB3	2:A:251:HEC:HMB1	0.58	1.75	1	5
1:A:37:VAL:O	1:A:37:VAL:HG12	0.57	1.99	16	7
1:A:11:VAL:HG22	2:A:233:HEC:CGD	0.57	2.30	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:ALA:HB3	1:A:78:SER:HG	0.57	1.58	15	1
1:A:65:TYR:CZ	1:A:69:HIS:CG	0.57	2.93	12	2
1:A:67:VAL:HG21	2:A:251:HEC:CHB	0.57	2.30	20	1
2:A:282:HEC:CBB	2:A:282:HEC:HMB1	0.56	2.28	3	8
1:A:21:PRO:CG	1:A:24:PRO:HG2	0.56	2.31	18	17
1:A:67:VAL:HG12	2:A:251:HEC:O1A	0.56	2.01	15	1
1:A:74:LEU:HD22	2:A:251:HEC:CGA	0.56	2.31	10	2
1:A:67:VAL:O	1:A:68:VAL:CG2	0.55	2.54	9	13
1:A:70:ALA:HB1	1:A:74:LEU:HD11	0.55	1.78	14	4
1:A:66:TYR:CD2	2:A:251:HEC:O1A	0.55	2.59	10	1
1:A:97:LEU:O	1:A:98:THR:CB	0.55	2.53	1	13
2:A:233:HEC:HBC3	2:A:233:HEC:HMC1	0.55	1.77	17	5
1:A:5:PRO:HG3	2:A:233:HEC:C3A	0.55	2.32	13	6
1:A:30:CYS:O	1:A:34:HIS:N	0.54	2.40	8	11
1:A:53:ASP:O	1:A:55:LEU:CD2	0.54	2.55	17	10
2:A:233:HEC:HBC1	2:A:282:HEC:CHC	0.54	2.33	17	5
1:A:9:VAL:HG11	2:A:233:HEC:O1A	0.54	2.01	10	2
1:A:80:LEU:CD1	1:A:98:THR:HG22	0.54	2.32	16	1
1:A:67:VAL:HG12	2:A:251:HEC:C4A	0.54	2.33	5	1
2:A:251:HEC:O1A	2:A:251:HEC:CHA	0.54	2.56	14	1
1:A:97:LEU:HD11	2:A:282:HEC:C4D	0.53	2.32	8	10
1:A:83:HIS:O	1:A:87:VAL:HG13	0.53	2.04	4	1
1:A:97:LEU:HD22	1:A:97:LEU:N	0.53	2.18	10	1
2:A:305:HEC:CBC	2:A:305:HEC:CMC	0.53	2.86	6	5
1:A:28:VAL:HG11	1:A:32:THR:HG21	0.52	1.81	6	5
1:A:70:ALA:CB	1:A:74:LEU:HD11	0.52	2.35	5	6
1:A:36:LEU:HD22	1:A:40:LYS:O	0.52	2.05	5	1
2:A:233:HEC:O2A	2:A:233:HEC:CHA	0.52	2.57	11	2
1:A:80:LEU:HD13	1:A:98:THR:HG22	0.52	1.82	16	1
1:A:97:LEU:HD21	2:A:282:HEC:CHA	0.52	2.35	18	1
1:A:18:VAL:HG11	1:A:105:CYS:SG	0.52	2.45	18	1
1:A:36:LEU:HD13	1:A:39:GLY:HA2	0.51	1.80	12	1
1:A:51:CYS:O	1:A:53:ASP:N	0.51	2.43	5	19
1:A:21:PRO:HB2	1:A:24:PRO:HG2	0.51	1.83	11	3
1:A:52:HIS:CE1	1:A:67:VAL:CG1	0.51	2.87	5	1
1:A:65:TYR:CE2	1:A:69:HIS:ND1	0.51	2.77	12	2
1:A:97:LEU:O	1:A:98:THR:CG2	0.51	2.56	4	4
1:A:54:ASP:OD1	1:A:57:ALA:CB	0.51	2.58	11	4
1:A:5:PRO:CG	2:A:233:HEC:C3A	0.51	2.89	11	5
1:A:35:HIS:HB3	1:A:76:HIS:CD2	0.51	2.41	14	1
1:A:70:ALA:O	1:A:78:SER:CB	0.51	2.58	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:LEU:CD1	1:A:78:SER:OG	0.51	2.58	16	6
1:A:37:VAL:HG22	2:A:251:HEC:HBC2	0.50	1.83	19	1
1:A:10:GLU:OE1	1:A:17:THR:CG2	0.50	2.60	20	2
1:A:75:LYS:CG	2:A:251:HEC:O2A	0.50	2.59	20	1
1:A:84:SER:O	1:A:87:VAL:HG22	0.50	2.07	17	3
1:A:66:TYR:O	1:A:70:ALA:CB	0.50	2.60	11	9
1:A:23:ALA:O	1:A:26:GLU:N	0.49	2.45	6	12
1:A:82:CYS:O	1:A:86:VAL:CG2	0.49	2.60	13	2
1:A:67:VAL:CG1	2:A:251:HEC:CGA	0.49	2.90	15	2
1:A:5:PRO:HD3	2:A:233:HEC:CHB	0.49	2.38	14	7
1:A:95:LYS:O	1:A:95:LYS:CD	0.49	2.60	5	3
1:A:97:LEU:HD23	1:A:97:LEU:N	0.49	2.21	3	5
1:A:95:LYS:CD	1:A:95:LYS:O	0.49	2.59	20	2
1:A:99:GLY:O	1:A:103:SER:CB	0.49	2.61	14	17
1:A:82:CYS:HB3	2:A:282:HEC:C2C	0.49	2.37	5	8
1:A:67:VAL:CG1	2:A:251:HEC:O2A	0.49	2.61	14	1
1:A:97:LEU:CD1	2:A:282:HEC:C4D	0.49	2.91	16	6
1:A:68:VAL:HG12	1:A:69:HIS:ND1	0.49	2.22	20	4
1:A:37:VAL:HG12	1:A:38:ASP:N	0.49	2.23	8	1
1:A:66:TYR:CZ	1:A:74:LEU:HD21	0.49	2.41	11	5
1:A:66:TYR:OH	1:A:74:LEU:CD2	0.49	2.61	14	3
1:A:43:TYR:O	1:A:44:ALA:C	0.49	2.51	18	1
1:A:23:ALA:O	1:A:26:GLU:HB2	0.48	2.07	17	2
1:A:67:VAL:HG12	2:A:251:HEC:CGA	0.48	2.38	15	1
1:A:93:LEU:O	1:A:96:ASP:N	0.48	2.47	4	5
1:A:42:SER:C	1:A:43:TYR:CD1	0.48	2.87	5	18
1:A:83:HIS:O	1:A:86:VAL:N	0.48	2.47	18	1
1:A:82:CYS:O	1:A:86:VAL:HG23	0.48	2.09	18	1
1:A:94:LYS:CD	1:A:98:THR:OG1	0.48	2.62	18	1
1:A:54:ASP:OD1	1:A:57:ALA:N	0.48	2.46	19	7
1:A:37:VAL:O	1:A:37:VAL:CG1	0.48	2.62	19	2
1:A:54:ASP:OD2	1:A:57:ALA:N	0.48	2.47	6	3
1:A:20:PHE:O	1:A:20:PHE:CD2	0.48	2.66	13	2
1:A:67:VAL:CG1	2:A:251:HEC:O1A	0.48	2.62	15	2
1:A:25:HIS:CD2	2:A:233:HEC:HBC2	0.47	2.44	17	2
1:A:9:VAL:CG1	2:A:233:HEC:CGA	0.47	2.90	11	2
1:A:65:TYR:C	1:A:65:TYR:CD1	0.47	2.86	7	1
1:A:64:LEU:O	1:A:67:VAL:HG23	0.47	2.10	7	1
1:A:59:LYS:HD3	1:A:66:TYR:CE1	0.47	2.45	12	3
1:A:97:LEU:CD2	2:A:282:HEC:C4D	0.47	2.92	18	1
1:A:67:VAL:CG1	2:A:251:HEC:C4A	0.47	2.93	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:VAL:CG1	1:A:97:LEU:CD1	0.47	2.93	18	1
1:A:80:LEU:HD21	1:A:98:THR:HA	0.46	1.85	7	1
1:A:69:HIS:O	1:A:70:ALA:C	0.46	2.53	12	2
1:A:97:LEU:HD21	2:A:282:HEC:C4D	0.46	2.40	18	1
1:A:82:CYS:O	1:A:85:LYS:N	0.46	2.48	16	4
1:A:37:VAL:O	1:A:40:LYS:CG	0.46	2.63	6	1
1:A:29:GLU:CG	1:A:32:THR:OG1	0.46	2.64	11	1
2:A:233:HEC:HMB1	2:A:233:HEC:CBB	0.46	2.34	16	2
1:A:65:TYR:CE1	1:A:69:HIS:HB2	0.46	2.45	8	4
1:A:67:VAL:HG12	2:A:251:HEC:O2A	0.46	2.11	14	1
1:A:28:VAL:HG11	2:A:282:HEC:HBC2	0.46	1.85	15	2
1:A:96:ASP:C	1:A:97:LEU:CD2	0.46	2.84	12	5
1:A:35:HIS:CG	1:A:76:HIS:NE2	0.46	2.83	16	5
1:A:64:LEU:HA	1:A:67:VAL:CG2	0.46	2.41	7	3
1:A:37:VAL:HG12	1:A:38:ASP:H	0.45	1.71	8	1
1:A:67:VAL:C	1:A:68:VAL:HG23	0.45	2.31	3	4
1:A:54:ASP:OD2	1:A:57:ALA:HB2	0.45	2.11	7	2
1:A:94:LYS:O	1:A:98:THR:OG1	0.45	2.34	7	1
1:A:21:PRO:CB	1:A:24:PRO:HG2	0.45	2.42	11	3
1:A:78:SER:O	1:A:81:ALA:HB3	0.45	2.11	4	2
1:A:50:GLY:N	1:A:53:ASP:OD1	0.45	2.50	10	1
1:A:27:LYS:NZ	2:A:282:HEC:O1D	0.45	2.50	18	1
1:A:100:CYS:SG	2:A:305:HEC:HMB1	0.45	2.51	5	3
1:A:74:LEU:HD12	1:A:78:SER:OG	0.45	2.11	16	4
1:A:79:CYS:C	1:A:81:ALA:N	0.45	2.70	20	9
1:A:94:LYS:CD	1:A:94:LYS:C	0.45	2.86	7	1
1:A:6:ASP:CG	1:A:7:LYS:N	0.44	2.69	13	1
1:A:95:LYS:CE	1:A:101:ALA:O	0.44	2.64	19	1
1:A:25:HIS:CD2	2:A:233:HEC:CBC	0.44	3.00	1	2
1:A:48:SER:O	1:A:49:SER:C	0.44	2.56	11	17
1:A:87:VAL:O	1:A:90:LYS:N	0.44	2.50	20	2
1:A:2:PRO:CG	1:A:43:TYR:CD2	0.44	3.00	8	1
1:A:66:TYR:CE2	2:A:251:HEC:O1A	0.44	2.70	19	1
1:A:42:SER:O	1:A:43:TYR:CG	0.44	2.71	2	2
1:A:94:LYS:O	1:A:99:GLY:N	0.44	2.50	3	2
1:A:20:PHE:CD2	2:A:233:HEC:HMD2	0.44	2.46	20	1
2:A:305:HEC:CMC	2:A:305:HEC:CBC	0.44	2.86	5	3
1:A:18:VAL:HB	2:A:305:HEC:HMD3	0.44	1.90	18	1
1:A:82:CYS:O	1:A:86:VAL:HG21	0.44	2.12	13	1
1:A:45:LYS:O	2:A:251:HEC:CMC	0.44	2.59	18	1
1:A:79:CYS:HB3	2:A:282:HEC:C4B	0.44	2.43	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:VAL:C	1:A:39:GLY:N	0.43	2.71	12	1
1:A:97:LEU:CD1	2:A:282:HEC:C1A	0.43	2.95	4	1
1:A:26:GLU:CD	1:A:26:GLU:O	0.43	2.56	9	3
2:A:282:HEC:HMD1	2:A:282:HEC:CGD	0.43	2.43	11	1
1:A:54:ASP:OD2	1:A:57:ALA:CB	0.43	2.66	7	1
2:A:282:HEC:CBC	2:A:282:HEC:CMC	0.43	2.94	4	4
1:A:54:ASP:CG	1:A:57:ALA:HB3	0.43	2.32	9	2
2:A:233:HEC:HMD1	2:A:233:HEC:O1D	0.43	2.14	13	1
1:A:40:LYS:O	1:A:41:GLU:C	0.43	2.57	12	2
1:A:80:LEU:HD11	1:A:98:THR:HA	0.43	1.90	15	1
1:A:81:ALA:O	1:A:85:LYS:CD	0.43	2.67	7	1
1:A:104:LYS:HE3	2:A:282:HEC:CGA	0.43	2.44	19	2
1:A:21:PRO:HG3	2:A:282:HEC:CBA	0.43	2.44	2	1
1:A:29:GLU:OE1	1:A:30:CYS:N	0.43	2.51	2	1
1:A:85:LYS:O	1:A:88:ALA:N	0.43	2.49	20	2
1:A:66:TYR:CG	1:A:66:TYR:O	0.42	2.71	7	1
1:A:10:GLU:HB3	1:A:17:THR:HG23	0.42	1.91	20	1
1:A:23:ALA:O	1:A:26:GLU:CG	0.42	2.68	1	1
1:A:94:LYS:O	1:A:98:THR:N	0.42	2.52	10	1
1:A:37:VAL:O	1:A:40:LYS:N	0.42	2.48	12	2
1:A:67:VAL:C	1:A:68:VAL:CG2	0.42	2.87	7	1
1:A:69:HIS:CD2	2:A:305:HEC:NB	0.42	2.87	8	1
1:A:2:PRO:CG	1:A:43:TYR:CE2	0.42	3.02	18	1
1:A:2:PRO:CG	1:A:43:TYR:CZ	0.42	3.03	18	1
1:A:28:VAL:O	1:A:29:GLU:O	0.42	2.38	20	8
1:A:20:PHE:HD2	2:A:282:HEC:HMB2	0.42	1.75	20	1
2:A:282:HEC:CMC	2:A:282:HEC:CBC	0.42	2.95	13	3
1:A:75:LYS:N	2:A:251:HEC:O2A	0.42	2.50	11	1
1:A:43:TYR:O	1:A:44:ALA:O	0.42	2.38	18	1
1:A:86:VAL:HG11	1:A:97:LEU:CD1	0.42	2.45	18	1
1:A:97:LEU:C	1:A:98:THR:OG1	0.42	2.57	14	1
1:A:80:LEU:O	1:A:80:LEU:HD13	0.41	2.15	9	1
1:A:9:VAL:HG21	2:A:233:HEC:O1A	0.41	2.14	10	1
1:A:27:LYS:NZ	2:A:282:HEC:HMD2	0.41	2.30	13	1
1:A:51:CYS:O	1:A:53:ASP:OD1	0.41	2.38	7	2
1:A:56:THR:O	1:A:57:ALA:C	0.41	2.58	15	1
1:A:90:LYS:HE3	1:A:93:LEU:HD12	0.41	1.92	5	1
1:A:66:TYR:CE2	2:A:251:HEC:CGA	0.41	3.03	19	1
1:A:25:HIS:CE1	2:A:282:HEC:NA	0.41	2.89	4	6
1:A:11:VAL:O	1:A:11:VAL:HG12	0.41	2.15	12	2
1:A:7:LYS:O	1:A:8:PRO:C	0.41	2.58	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:VAL:CG2	2:A:233:HEC:O2D	0.41	2.68	5	1
1:A:1:ALA:O	1:A:2:PRO:O	0.41	2.39	9	2
1:A:25:HIS:CG	2:A:233:HEC:HBC2	0.41	2.51	1	2
1:A:86:VAL:C	1:A:88:ALA:N	0.41	2.73	17	3
1:A:68:VAL:O	1:A:80:LEU:CD1	0.41	2.62	4	1
1:A:3:ALA:O	1:A:4:VAL:C	0.41	2.58	12	1
1:A:23:ALA:O	1:A:25:HIS:N	0.41	2.54	17	1
1:A:63:SER:O	1:A:67:VAL:CG2	0.41	2.68	7	1
1:A:93:LEU:CD1	2:A:282:HEC:O2D	0.41	2.69	15	1
1:A:35:HIS:HB2	1:A:76:HIS:CE1	0.41	2.51	20	1
2:A:251:HEC:O1D	2:A:251:HEC:O2A	0.41	2.38	4	1
1:A:65:TYR:CD2	1:A:69:HIS:ND1	0.41	2.89	12	1
1:A:78:SER:OG	1:A:79:CYS:N	0.41	2.54	14	1
1:A:93:LEU:HD13	2:A:282:HEC:CGD	0.41	2.46	15	1
1:A:98:THR:HA	2:A:305:HEC:HMC2	0.41	1.93	15	1
1:A:82:CYS:O	1:A:83:HIS:C	0.41	2.59	16	1
1:A:68:VAL:O	1:A:80:LEU:CB	0.41	2.68	17	1
2:A:233:HEC:CBB	2:A:233:HEC:HMB1	0.41	2.40	19	1
1:A:47:GLY:HA2	1:A:52:HIS:O	0.41	2.16	3	1
1:A:45:LYS:O	1:A:48:SER:OG	0.41	2.38	14	2
1:A:79:CYS:O	1:A:81:ALA:N	0.40	2.54	2	1
1:A:71:ARG:O	1:A:72:GLY:O	0.40	2.39	14	1
1:A:71:ARG:HB3	1:A:80:LEU:HD12	0.40	1.94	9	1
1:A:79:CYS:O	1:A:80:LEU:C	0.40	2.59	2	2
1:A:99:GLY:O	1:A:103:SER:OG	0.40	2.39	15	1
1:A:96:ASP:CB	1:A:97:LEU:HD23	0.40	2.46	1	1
1:A:11:VAL:O	1:A:12:LYS:C	0.40	2.60	3	2
1:A:64:LEU:O	1:A:67:VAL:HG13	0.40	2.16	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	105/107 (98%)	75±2 (72±2%)	25±3 (24±2%)	5±1 (5±1%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2100/2140 (98%)	1505 (72%)	499 (24%)	96 (5%)	5	28

All 15 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	52	HIS	20
1	A	98	THR	18
1	A	68	VAL	17
1	A	29	GLU	14
1	A	2	PRO	7
1	A	57	ALA	4
1	A	8	PRO	3
1	A	15	GLN	3
1	A	99	GLY	2
1	A	35	HIS	2
1	A	72	GLY	2
1	A	58	LYS	1
1	A	45	LYS	1
1	A	44	ALA	1
1	A	37	VAL	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	91/91 (100%)	69±2 (76±2%)	22±2 (24±2%)	3	27
All	All	1820/1820 (100%)	1388 (76%)	432 (24%)	3	27

All 51 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	6	ASP	20
1	A	42	SER	20
1	A	63	SER	19
1	A	53	ASP	18

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Mol	Chain	Res	Type	Models (Total)
1	A	98	THR	18
1	A	95	LYS	17
1	A	58	LYS	17
1	A	92	GLU	17
1	A	97	LEU	16
1	A	59	LYS	15
1	A	27	LYS	13
1	A	40	LYS	13
1	A	55	LEU	13
1	A	45	LYS	13
1	A	62	LYS	12
1	A	15	GLN	11
1	A	94	LYS	11
1	A	7	LYS	11
1	A	90	LYS	10
1	A	78	SER	10
1	A	31	VAL	9
1	A	73	GLU	9
1	A	102	LYS	8
1	A	71	ARG	7
1	A	104	LYS	7
1	A	105	CYS	7
1	A	26	GLU	6
1	A	56	THR	6
1	A	29	GLU	6
1	A	61	GLU	6
1	A	84	SER	6
1	A	75	LYS	6
1	A	16	LYS	5
1	A	14	SER	5
1	A	85	LYS	5
1	A	49	SER	4
1	A	67	VAL	4
1	A	89	GLU	4
1	A	77	THR	4
1	A	10	GLU	3
1	A	74	LEU	3
1	A	80	LEU	3
1	A	12	LYS	3
1	A	48	SER	2
1	A	19	MET	2
1	A	41	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	38	ASP	2
1	A	79	CYS	1
1	A	17	THR	1
1	A	30	CYS	1
1	A	76	HIS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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6.6 Other polymers [i](#)

There are no such molecules in this entry.

6.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided