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Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 09:11 PM BST

PDB ID	:	2GB8
Title	:	Solution structure of the complex between yeast iso-1-cytochrome c and yeast cytochrome c peroxidase
Authors	:	Volkov, A.N.; Worrall, J.A.R.; Ubbink, M.
Deposited on	:	2006-03-10

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

http://wwpdb.org/validation/2016/NMRValidationReportHelp

with specific help available everywhere you see the (i) symbol.

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

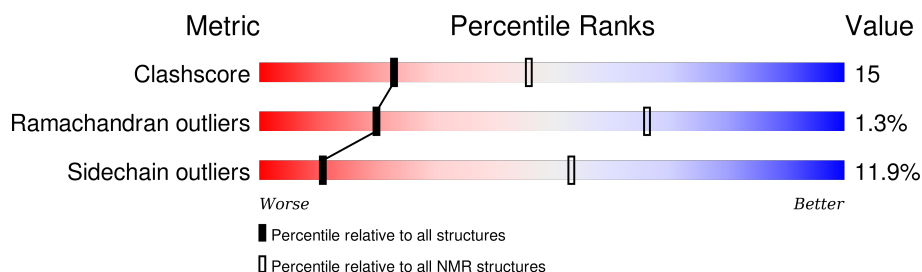|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		15
Ramachandran outliers		1.3%
Sidechain outliers		11.9%

Worse   *Better*

▮ Percentile relative to all structures

〗 Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	294	70%　　　　　27%　　　· ·
2	B	108	49%　　　　37%　　7%　·　5%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 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:291 (291)	-0.00	3
2	A:292-A:294, B:1-B:103 (106)	0.06	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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	2, 3, 4, 5, 6, 8, 10, 13, 15, 17
2	1, 7, 9, 11
3	14, 20
4	12, 16
Single-model clusters	18; 19

3 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6382 atoms, of which 3121 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cytochrome c peroxidase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	294	4622	1514	2252	395	455	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	THR	SEE REMARK 999	UNP P00431
A	152	GLY	ASP	SEE REMARK 999	UNP P00431

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	103	1612	507	807	145	148	5	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: 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
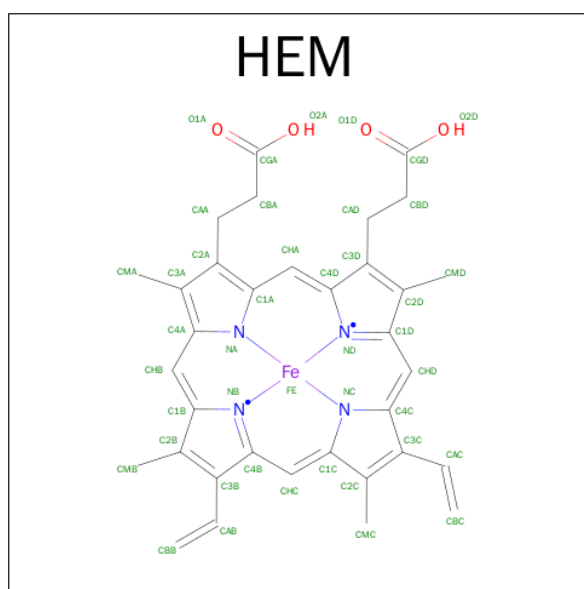
- Molecule 4 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).
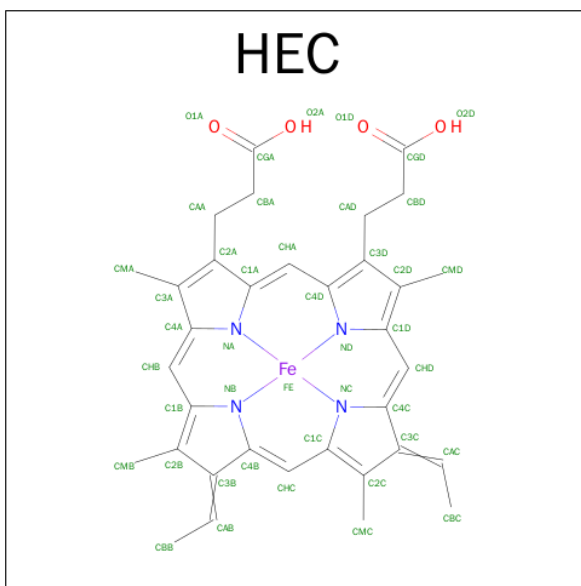
| Mol	Chain	Residues	Atoms					
			Total	C	Fe	H	N	O
4	B	1	75	34	1	32	4	4

4   Residue-property plots (i)

4.1   Average score per residue in the NMR ensemble

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

- Molecule 1: Cytochrome c peroxidase
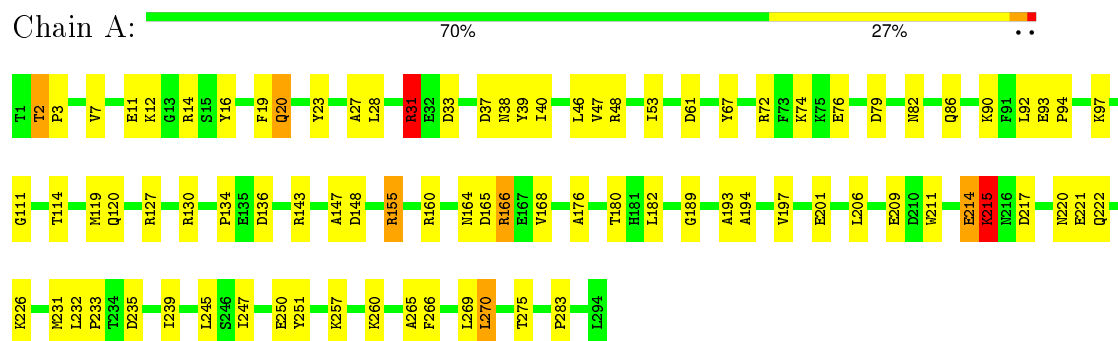
- Molecule 2: Cytochrome c iso-1
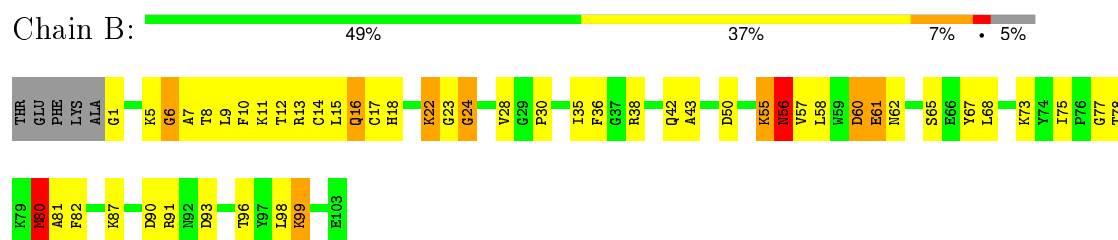
4.2   Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1   Score per residue for model 1

- Molecule 1: Cytochrome c peroxidase
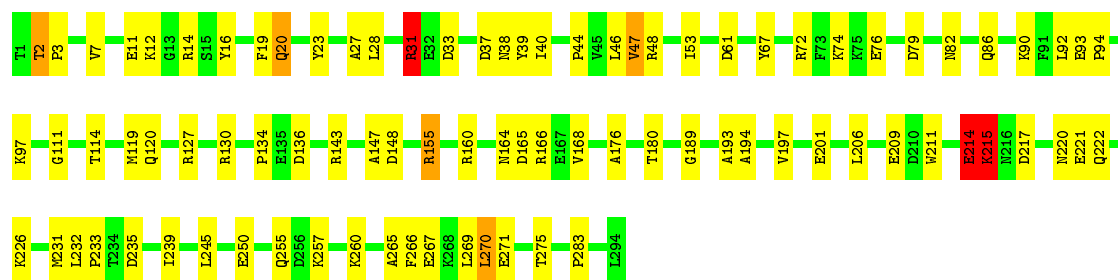
• Molecule 2: Cytochrome c iso-1
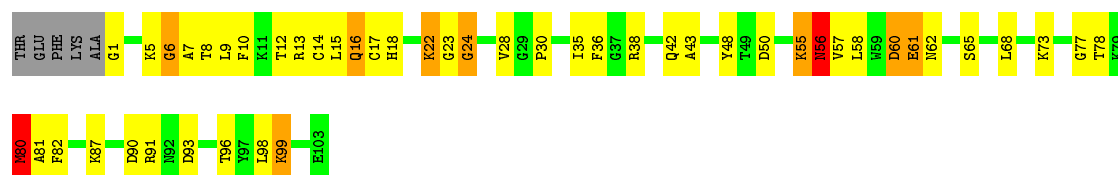
4.2.2 Score per residue for model 2

• Molecule 1: Cytochrome c peroxidase
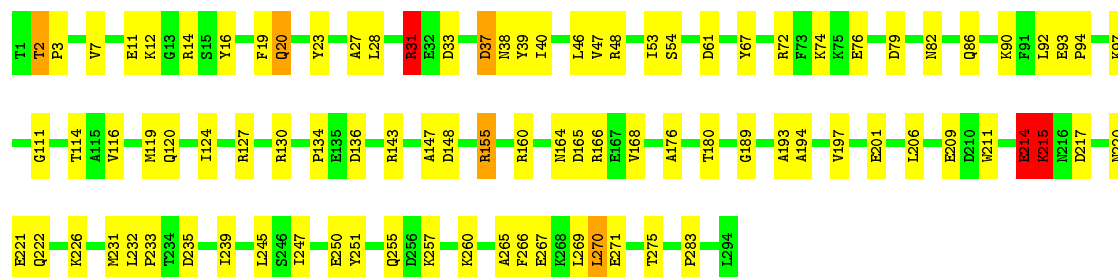
• Molecule 2: Cytochrome c iso-1

4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: Cytochrome c peroxidase

Chain A: 69% 29%

• Molecule 2: Cytochrome c iso-1

Chain B: 47% 39% 7% 5%

4.2.4 Score per residue for model 4

• Molecule 1: Cytochrome c peroxidase

Chain A: 71% 26%

• Molecule 2: Cytochrome c iso-1

Chain B: 48% 38% 7% 5%

4.2.5 Score per residue for model 5

• Molecule 1: Cytochrome c peroxidase

Chain A:

70%   27%

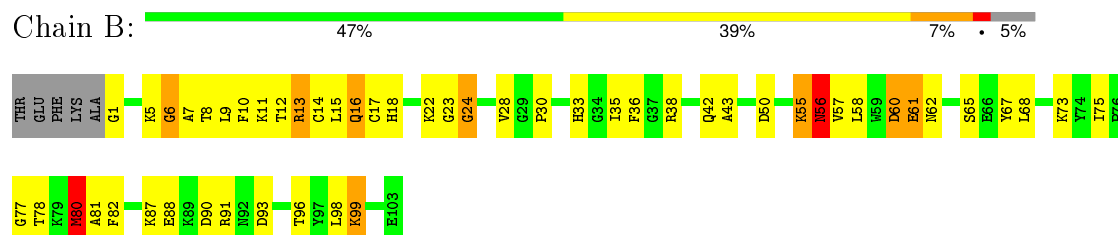T1 T2 P3 V7 E11 K12 G13 R14 S15 Y16 F19 Q20 Y23 A27 L28 R31 E32 D33 D37 N38 Y39 I40 L46 V47 R48 I53 D61 Y67 R72 F73 K74 K75 E76 D79 N82 Q86 K90 F91 L92 E93 P94 K97

G111 T114 M119 Q120 R127 R130 P134 E135 D136 R143 A147 D148 R155 R160 N164 D165 R166 E167 V168 A176 T180 H181 L182 G189 A193 A194 V197 E201 L206 E209 D210 W211 E214 K215 N216 D217 N220 E221 Q222

K226 M231 L232 P233 T234 D235 I239 L245 S246 I247 E250 Y251 K257 K260 A265 F266 L269 L270 T275 P283 E290 L294

• **Molecule 2: Cytochrome c iso-1**

Chain B:

48%   37%   8%   • 5%

THR GLU PHE LYS ALA G1 K5 G6 A7 T8 L9 F10 K11 T12 R13 C14 L15 Q16 C17 H18 K22 G23 G24 V28 G29 P30 I35 F36 G37 R38 Q42 A43 Y48 T49 D50 K55 N56 V57 L58 W59 D60 E61 N62 S65 E66 Y67 L68 K73 Y74 I75 P76

G77 T78 K79 M80 A81 F82 K87 E88 K89 D90 R91 N92 D93 T96 Y97 L98 K99 E103

4.2.6 Score per residue for model 6

• **Molecule 1: Cytochrome c peroxidase**

Chain A:

67%   31%   ••

T1 T2 P3 V7 E11 K12 G13 R14 S15 Y16 F19 Q20 Y23 A27 L28 K29 L30 R31 E32 D33 D37 N38 Y39 I40 L46 V47 R48 I53 D61 Y67 R72 F73 K74 K75 E76 D79 N82 Q86 K90 F91 L92 E93 P94 K97

G111 T114 A115 V116 M119 Q120 G121 I124 R127 R130 P134 E135 D136 R143 A147 D148 R155 R160 N164 D165 R166 E167 V168 A176 L177 T180 H181 L182 G189 A193 A194 V197 F198 E201 L206 E209 D210 W211 K212 L213

E214 K215 N216 D217 N220 E221 Q222 K226 M231 L232 P233 T234 D235 Y236 I239 L245 S246 I247 E250 Y251 K257 F258 F259 K260 A265 F266 L269 I270 T275 P283 E290 L294

• **Molecule 2: Cytochrome c iso-1**

Chain B:

49%   36%   8%   • 5%

THR GLU PHE LYS ALA G1 K5 G6 A7 T8 L9 F10 K11 T12 C14 L15 Q16 C17 H18 K22 G23 G24 V28 G29 P30 H33 G34 I35 F36 G37 R38 Q42 A43 D50 K55 N56 V57 L58 W59 D60 E61 N62 S65 E66 Y67 L68 K73 Y74 I75 P76

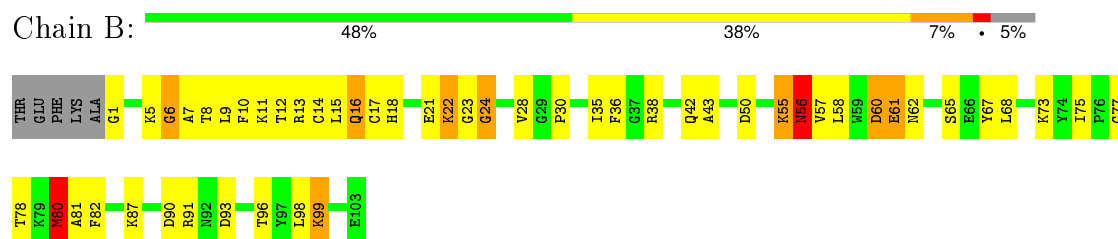G77 T78 K79 M80 A81 F82 K87 D90 R91 N92 D93 T96 Y97 L98 K99 E103

4.2.7 Score per residue for model 7

• **Molecule 1: Cytochrome c peroxidase**

Chain A: 71%   26%

T1 T2 P3 V7 E11 K12 G13 R14 S15 Y16 F19 Q20 Y23 A27 L28 R31 E32 D33 D37 N38 Y39 I40 L46 V47 R48 I53 D61 Y67 R72 E76 D79 N82 Q86 K90 F91 L92 E93 P94 K97 G111

T114 M119 Q120 R127 R130 P134 E135 D136 R143 A147 D148 R155 R160 N164 D165 R166 E167 V168 A176 T180 H181 L182 G189 A193 A194 V197 E201 L206 E209 D210 W211 E214 K215 N216 D217 N220 E221 Q222 K226
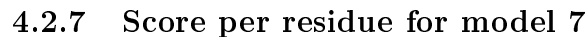
Y229 M230 M231 L232 P233 T234 D235 I239 L245 E250 K257 K260 A265 F266 L269 L270 T275 S282 P283 I294

• Molecule 2: Cytochrome c iso-1

Chain B: 49%   36%   8% • 5%

THR GLU PHE LYS ALA G1 K5 G6 A7 T8 L9 F10 K11 T12 R13 C14 L15 Q16 C17 H18 K22 G23 G24 V28 G29 P30 I35 F36 G37 R38 Q42 A43 D50 K55 N56 V57 L58 W59 D60 E61 N62 S65 E66 Y67 L68 K73 Y74 I75 P76 G77 T78

K79 M80 A81 F82 K87 D90 R91 N92 D93 T96 Y97 L98 K99 E103

4.2.8 Score per residue for model 8

• Molecule 1: Cytochrome c peroxidase

Chain A: 67%   29%

T1 T2 P3 V7 E11 K12 G13 R14 S15 Y16 E17 D18 F19 Q20 Y23 A27 L28 R31 E32 D33 D37 N38 Y39 I40 L46 V47 R48 I53 S54 D61 Y67 R72 F73 K74 K75 E76 D79 N82 Q86 K90 F91 L92 E93 P94 I95

H96 K97 G111 T114 A115 V116 M119 Q120 I124 R127 R130 P134 E135 D136 R143 A147 D148 R155 R160 N164 D165 R166 E167 V168 A176 T180 H181 L182 G189 A193 A194 V197 E201 L206 E209 D210 W211 E214 K215

M216 D217 N220 E221 Q222 K226 M231 L232 P233 T234 D235 Y236 I239 L245 S246 I247 E250 Y251 A252 N253 D256 K257 K260 A265 F266 E267 K268 L269 L270 T275 P283 E290 L294

• Molecule 2: Cytochrome c iso-1

Chain B: 51%   34%   8% • 5%

THR GLU PHE LYS ALA G1 K5 G6 A7 T8 L9 F10 K11 T12 C14 L15 Q16 C17 H18 K22 G23 G24 V28 G29 P30 I35 F36 G37 R38 H39 Q42 A43 D50 K55 N56 V57 L58 W59 D60 E61 N62 S65 E66 Y67 K73 Y74 I75 M80 A81

F82 K87 D90 R91 N92 D93 T96 Y97 L98 K99 E103

4.2.9 Score per residue for model 9

• Molecule 1: Cytochrome c peroxidase

Chain A:

• Molecule 2: Cytochrome c iso-1

Chain B:

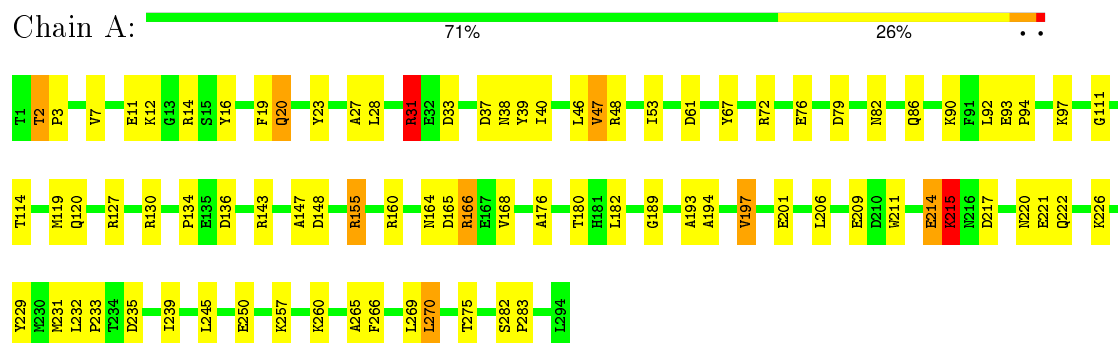### 4.2.10 Score per residue for model 10

• Molecule 1: Cytochrome c peroxidase

Chain A:

• Molecule 2: Cytochrome c iso-1

Chain B:
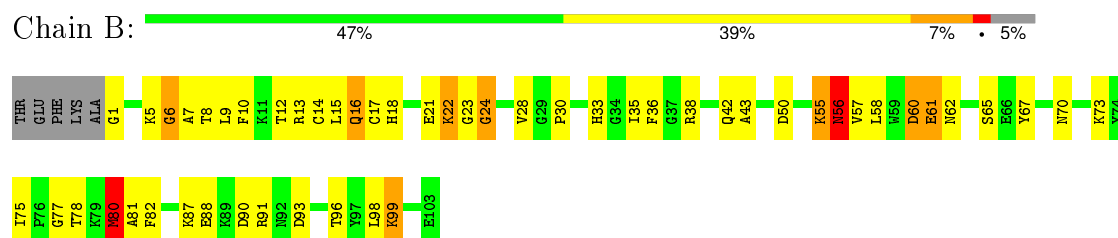
4.2.11 Score per residue for model 11

• Molecule 1: Cytochrome c peroxidase

Chain A:

68%   29%

T1 T2 P3 V7 E11 K12 G13 R14 S15 Y16 E17 D18 F19 Q20 Y23 A27 L28 R31 E32 D33 D37 N38 Y39 I40 L46 V47 R48 I53 D61 Y67 R72 F73 K74 K75 E76 D79 N82 Q86 K90 F91 L92 E93 P94 K97

G111 T114 M119 Q120 R127 R130 P134 E135 D136 R143 A147 D148 R155 R160 N164 D165 R166 E167 V168 A176 T180 H181 L182 G189 A193 A194 V197 E201 L206 E209 D210 W211 E214 K215 N216 D217 A218 N219 N220 E221

Q222 K226 Y229 M230 M231 L232 P233 T234 D235 Y236 I239 L245 S246 I247 E250 Y251 K257 K260 A265 F266 E267 K268 L269 L270 E271 T275 S282 P283 L294

• Molecule 2: Cytochrome c iso-1

Chain B:

52%   34%   7%   •   5%

THR GLU PHE LYS ALA G1 K5 G6 A7 T8 L9 F10 K11 T12 R13 C14 L15 Q16 C17 H18 K22 G23 G24 V28 G29 P30 I35 F36 G37 R38 Q42 A43 D50 K55 N56 V57 L58 W59 D60 E61 N62 S65 E66 Y67 K73 Y74 I75 P76 G77 T78 K79

M80 A81 F82 K87 D90 R91 N92 D93 T96 Y97 L98 K99 E103

4.2.12 Score per residue for model 12

• Molecule 1: Cytochrome c peroxidase

Chain A:

69%   28%   •   •

T1 T2 P3 V7 E11 K12 G13 R14 S15 Y16 F19 Q20 Y23 A27 L28 R31 E32 D33 D37 N38 Y39 I40 L46 V47 R48 I53 S54 D61 Y67 R72 F73 K74 K75 E76 D79 N82 Q86 K90 F91 L92 E93 P94 K97

G111 T114 A115 V116 M119 Q120 I124 R127 R130 P134 E135 D136 R143 A147 D148 R155 R160 D165 R166 A176 T180 H181 L182 G189 A193 A194 V197 E201 L206 E209 D210 W211 E214 K215 N216 D217 N220 E221

Q222 K226 Y229 M230 M231 L232 P233 T234 D235 Y236 I239 L245 S246 I247 E250 Y251 Q255 D256 K257 K260 A265 F266 L269 L270 T275 P283 L294

• Molecule 2: Cytochrome c iso-1

Chain B:

47%   40%   6%   •   5%

THR GLU PHE LYS ALA G1 K5 G6 A7 T8 L9 F10 K11 T12 R13 C14 L15 Q16 C17 H18 K22 G23 G24 V28 G29 P30 H33 G34 I35 F36 G37 R38 H39 Q42 A43 D50 K55 N56 V57 L58 W59 D60 E61 N62 S65 E66 Y67 K73 Y74 I75 P76

G77 T78 K79 M80 A81 F82 K87 E88 K89 D90 R91 N92 D93 T96 Y97 L98 K99 E103

4.2.13 Score per residue for model 13

• Molecule 1: Cytochrome c peroxidase

Chain A:

• Molecule 2: Cytochrome c iso-1

Chain B:
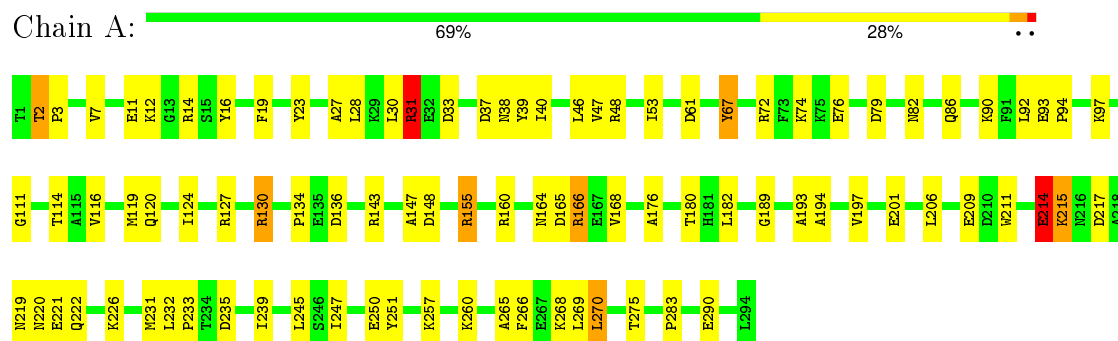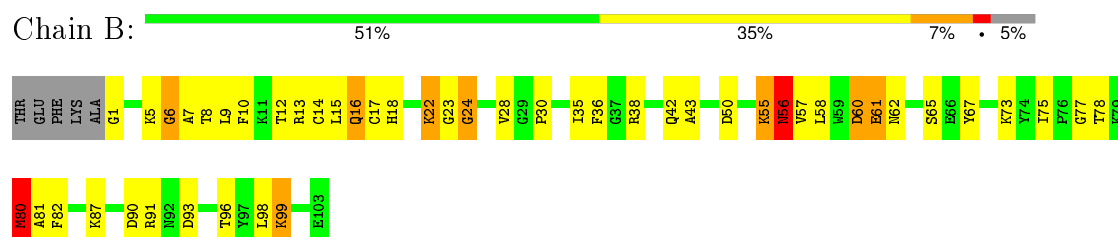
4.2.14 Score per residue for model 14

• Molecule 1: Cytochrome c peroxidase

Chain A:

• Molecule 2: Cytochrome c iso-1

Chain B:
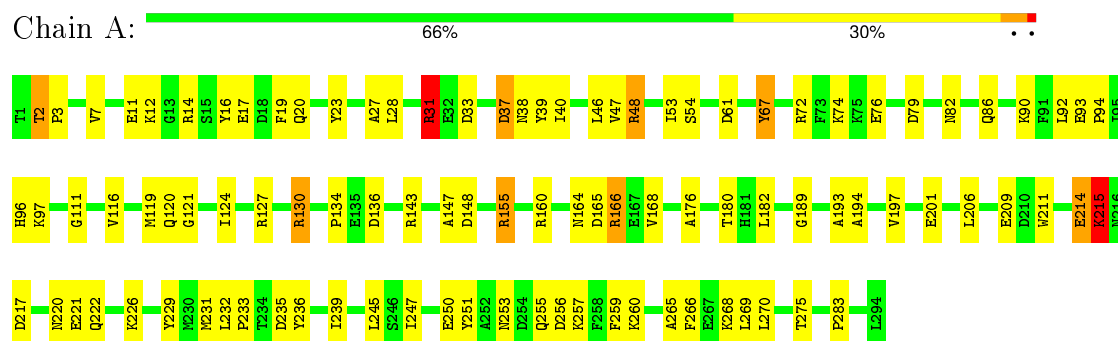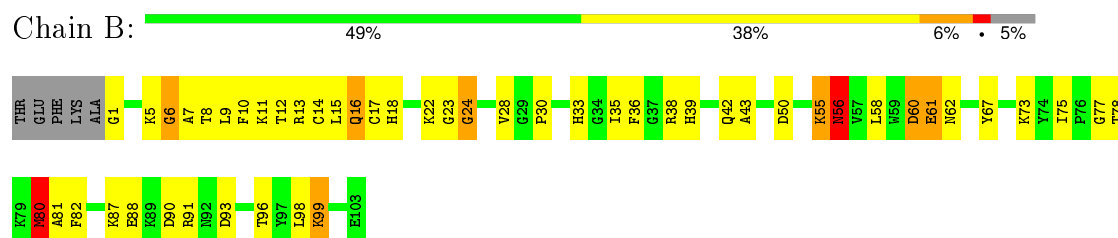
4.2.15 Score per residue for model 15

• Molecule 1: Cytochrome c peroxidase

Chain A:

71%   26%

T1 T2 P3 V7 E11 K12 G13 R14 S15 Y16 F19 Q20 Y23 A27 L28 R31 E32 D33 N38 Y39 L46 V47 R48 I53 D61 Y67 R72 F73 K74 K75 E76 D79 N82 Q86 K90 F91 L92 E93 P94 K97 G111

T114 M119 Q120 R127 R130 P134 E135 D136 R143 A147 D148 R155 R160 N164 D165 R166 E167 V168 A176 T180 H181 L182 G189 A193 A194 V197 E201 L206 E209 D210 W211 E214 K215 N216 D217 N220 E221 Q222 K226

M231 L232 P233 T234 D235 I239 L245 S246 I247 E250 Y251 K257 K260 A265 F266 L269 L270 T275 P283 L294

• Molecule 2: Cytochrome c iso-1

Chain B:

51%   34%   8% • 5%

THR GLU PHE LYS ALA G1 K5 G6 A7 T8 L9 F10 K11 T12 R13 C14 L15 Q16 C17 H18 K22 G23 G24 V28 G29 P30 I35 F36 G37 R38 Q42 A43 D50 K55 N56 V57 L58 W59 D60 E61 N62 S65 E66 Y67 L68 K73 Y74 I75 M80 A81

F82 K87 D90 R91 N92 D93 T96 Y97 L98 K99 E103

4.2.16   Score per residue for model 16

• Molecule 1: Cytochrome c peroxidase

Chain A:

68%   28%

T1 T2 P3 V7 E11 K12 G13 R14 S15 Y16 E17 D18 F19 Q20 Y23 A27 L28 R31 E32 D33 D37 N38 Y39 I40 L46 V47 R48 I53 S54 D61 Y67 R72 F73 K74 K75 E76 D79 N82 K90 F91 L92 E93 P94 I95 H96 K97

G111 T114 A115 V116 M119 Q120 I124 R127 R130 P134 E135 D136 R143 A147 D148 R155 R160 N164 D165 R166 E167 V168 A176 T180 G189 A193 A194 V197 L206 E209 D210 W211 E214 K215 N216 D217 N220 E221 Q222

K226 Y229 M230 M231 L232 P233 T234 D235 Y236 I239 L245 S246 I247 E250 Y251 D256 K257 K260 A265 F266 E267 K268 L269 L270 T275 P283 L294

• Molecule 2: Cytochrome c iso-1

Chain B:

48%   40%   6% • 5%

THR GLU PHE LYS ALA G1 K5 G6 A7 T8 L9 F10 K11 T12 R13 C14 L15 Q16 C17 H18 K22 G23 G24 V28 G29 P30 H33 G34 I35 F36 G37 R38 H39 Q42 A43 D50 K55 N56 V57 L58 W59 D60 E61 N62 S65 E66 Y67 K73 Y74 I75 P76

G77 T78 K79 M80 A81 F82 K87 D90 R91 N92 D93 T96 Y97 L98 K99 E103

4.2.17   Score per residue for model 17

• Molecule 1: Cytochrome c peroxidase

Chain A:

- Molecule 2: Cytochrome c iso-1

Chain B:
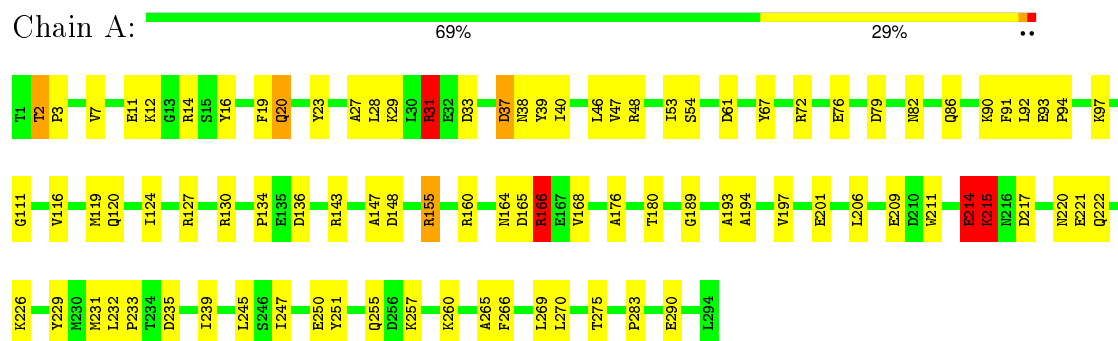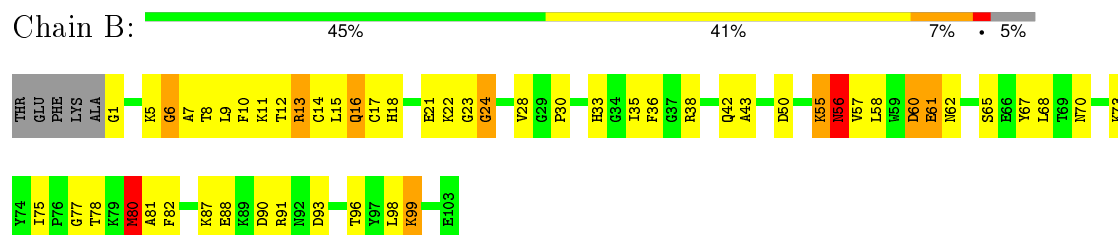
4.2.18 Score per residue for model 18

- Molecule 1: Cytochrome c peroxidase

Chain A:

- Molecule 2: Cytochrome c iso-1

Chain B:
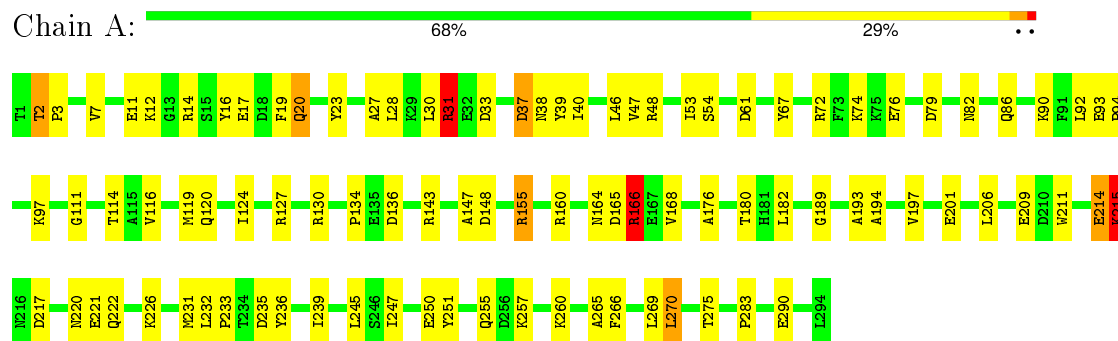
4.2.19 Score per residue for model 19

- Molecule 1: Cytochrome c peroxidase

Chain A:

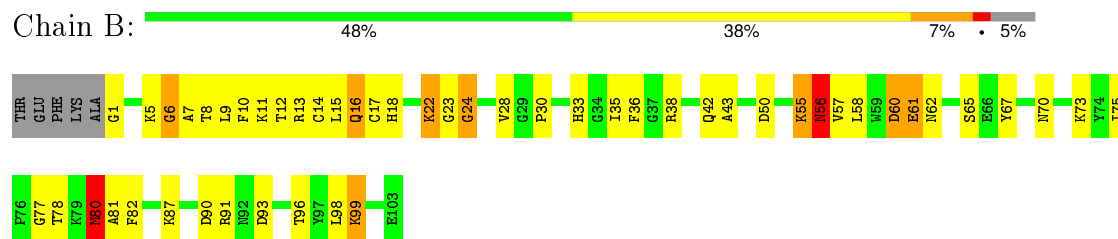
• Molecule 2: Cytochrome c iso-1

Chain B:
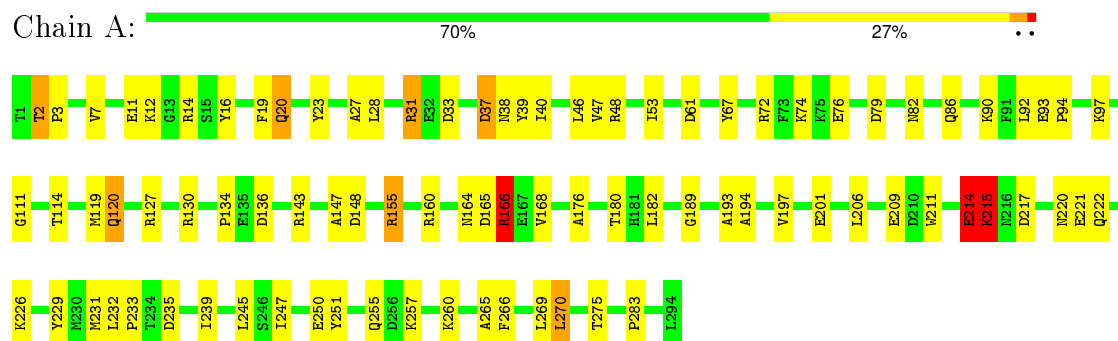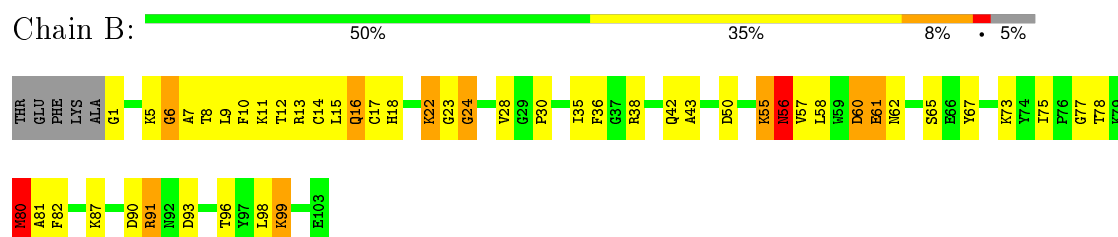
4.2.20 Score per residue for model 20

• Molecule 1: Cytochrome c peroxidase
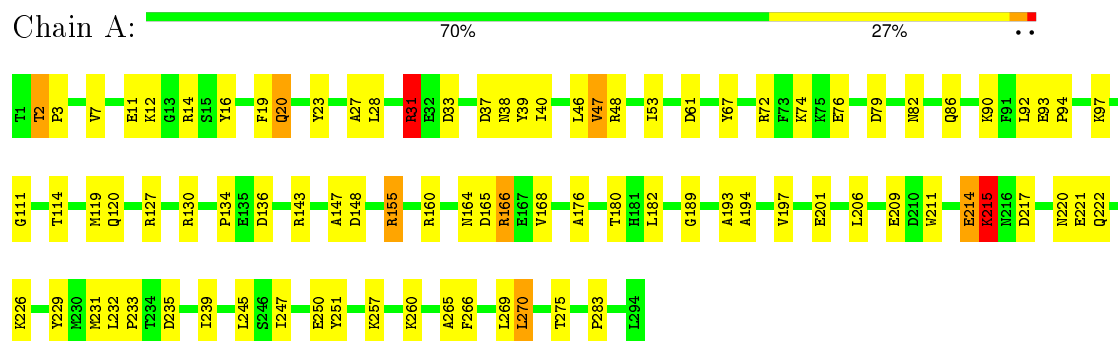
Chain A:

• Molecule 2: Cytochrome c iso-1
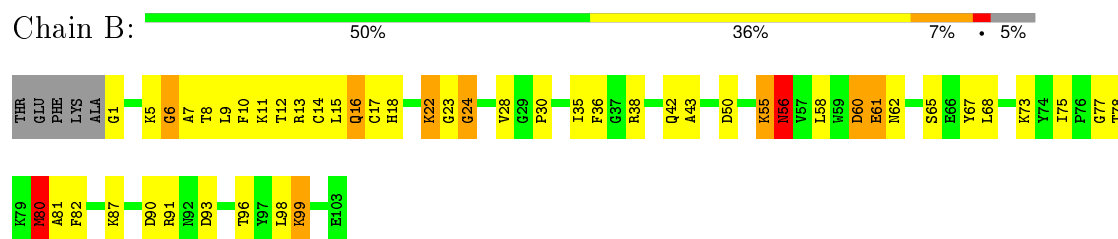
Chain B:

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *rigid-body docking solely on the basis of experimental data; sidechain dynamics.*.

Of the 100 calculated structures, 20 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
XPLOR-NIH	structure solution	2.13
XPLOR-NIH	refinement	2.13

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

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 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	1.11±0.00	0±0/2437 (0.0±0.0%)	1.45±0.00	12±0/3302 (0.4±0.0%)
2	B	0.92±0.00	0±0/822 (0.0±0.0%)	1.40±0.00	2±0/1100 (0.2±0.0%)
All	All	1.06	0/65180 (0.0%)	1.44	280/88040 (0.3%)

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	260

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	28	LEU	O-C-N	7.06	134.00	122.70	1	20
1	A	214	GLU	O-C-N	6.67	133.38	122.70	1	20
2	B	80	MET	CB-CA-C	6.63	123.66	110.40	1	20
1	A	217	ASP	O-C-N	6.52	133.13	122.70	1	20
1	A	33	ASP	O-C-N	-5.89	113.28	122.70	1	20
1	A	209	GLU	C-N-CA	5.64	135.81	121.70	1	20
1	A	53	ILE	O-C-N	5.59	131.64	122.70	1	20
2	B	80	MET	CG-SD-CE	-5.46	91.46	100.20	15	20
1	A	111	GLY	C-N-CA	-5.43	110.89	122.30	1	20
1	A	283	PRO	O-C-N	5.41	131.35	122.70	1	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models Worst	Models Total
1	A	215	LYS	O-C-N	5.27	131.14	122.70	1	20
1	A	270	LEU	O-C-N	5.12	130.90	122.70	1	20
1	A	176	ALA	C-N-CA	5.10	134.46	121.70	1	20
1	A	31	ARG	O-C-N	-5.10	114.54	122.70	1	20

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	143	ARG	Sidechain	20
1	A	160	ARG	Sidechain	20
2	B	13	ARG	Sidechain	20
1	A	31	ARG	Sidechain	20
1	A	14	ARG	Sidechain	20
1	A	166	ARG	Sidechain	20
2	B	91	ARG	Sidechain	20
2	B	38	ARG	Sidechain	20
1	A	155	ARG	Sidechain	20
1	A	127	ARG	Sidechain	20
1	A	72	ARG	Sidechain	20
1	A	48	ARG	Sidechain	20
1	A	130	ARG	Sidechain	20

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	2370	2252	2252	57±5
2	B	805	807	811	52±3
3	A	43	30	30	2±1
4	B	43	32	32	15±2
All	All	65220	62420	62500	1881

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:193:ALA:HB1	2:B:17:CYS:SG	1.04	1.92	4	20
1:A:193:ALA:HB2	2:B:28:VAL:HG21	1.04	1.30	16	20
1:A:193:ALA:CB	2:B:28:VAL:HG21	0.98	1.88	14	20
2:B:14:CYS:SG	4:B:104:HEC:CBB	0.93	2.57	20	20
1:A:194:ALA:HB2	2:B:81:ALA:HB3	0.87	1.44	17	20
1:A:194:ALA:CB	2:B:81:ALA:HB3	0.85	2.01	17	19
1:A:93:GLU:N	1:A:94:PRO:HD2	0.84	1.87	14	20
1:A:194:ALA:CB	2:B:81:ALA:CB	0.82	2.56	17	20
2:B:17:CYS:SG	4:B:104:HEC:C3C	0.81	2.69	6	20
1:A:147:ALA:O	1:A:233:PRO:HG2	0.81	1.75	12	20
1:A:197:VAL:HG11	2:B:82:PHE:CA	0.76	2.10	17	18
1:A:39:TYR:HB2	2:B:12:THR:HB	0.72	1.59	4	20
2:B:14:CYS:SG	4:B:104:HEC:HAB	0.72	2.25	1	20
1:A:194:ALA:HB2	2:B:81:ALA:CB	0.71	2.15	12	10
2:B:17:CYS:SG	4:B:104:HEC:CBC	0.71	2.79	19	20
1:A:38:ASN:O	2:B:12:THR:HB	0.70	1.86	8	15
1:A:239:ILE:HG22	1:A:245:LEU:HD23	0.68	1.64	18	20
1:A:194:ALA:HB2	4:B:104:HEC:HBC2	0.67	1.66	6	17
1:A:193:ALA:HB1	2:B:17:CYS:HG	0.67	1.49	4	10
1:A:16:TYR:O	1:A:19:PHE:N	0.67	2.28	15	20
1:A:194:ALA:N	4:B:104:HEC:HBC1	0.66	2.06	6	17
1:A:197:VAL:HG22	2:B:81:ALA:HB1	0.65	1.68	6	10
1:A:194:ALA:HB1	2:B:81:ALA:O	0.64	1.91	17	18
1:A:194:ALA:N	4:B:104:HEC:CBC	0.64	2.61	6	18
1:A:39:TYR:HB3	2:B:13:ARG:CG	0.64	2.21	17	4
1:A:193:ALA:C	4:B:104:HEC:CBC	0.64	2.66	17	15
1:A:39:TYR:HB3	2:B:13:ARG:HG3	0.63	1.70	17	7
1:A:245:LEU:HD13	1:A:245:LEU:O	0.62	1.93	3	10
2:B:14:CYS:SG	4:B:104:HEC:HBB3	0.62	2.34	4	20
2:B:87:LYS:O	2:B:90:ASP:HB2	0.62	1.95	8	20
1:A:194:ALA:CB	2:B:81:ALA:O	0.62	2.48	9	20
2:B:80:MET:CE	2:B:82:PHE:HB2	0.61	2.25	19	20
1:A:197:VAL:HG11	2:B:82:PHE:C	0.61	2.15	17	14
1:A:194:ALA:CA	4:B:104:HEC:CBC	0.61	2.79	6	11
1:A:93:GLU:N	1:A:94:PRO:CD	0.60	2.63	14	20
1:A:245:LEU:O	1:A:245:LEU:HD13	0.60	1.96	15	10
2:B:80:MET:HB2	4:B:104:HEC:C1D	0.59	2.28	15	20
1:A:194:ALA:HB2	4:B:104:HEC:CBC	0.58	2.28	6	10
1:A:194:ALA:CB	2:B:81:ALA:HB1	0.57	2.29	12	7
2:B:8:THR:O	2:B:12:THR:HG23	0.57	1.99	20	19
1:A:180:THR:N	1:A:189:GLY:O	0.57	2.29	15	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
2:B:17:CYS:SG	4:B:104:HEC:HBC3	0.57	2.40	19	20
1:A:194:ALA:HB1	1:A:197:VAL:HG12	0.57	1.77	1	1
1:A:119:MET:O	1:A:120:GLN:HB2	0.56	2.01	2	19
2:B:6:GLY:HA3	2:B:93:ASP:O	0.56	2.01	16	20
1:A:229:TYR:OH	2:B:28:VAL:HG22	0.56	2.00	19	9
2:B:5:LYS:O	2:B:7:ALA:N	0.55	2.40	6	20
1:A:193:ALA:HB2	2:B:28:VAL:CG2	0.55	2.20	16	6
1:A:47:VAL:HG23	3:A:295:HEM:HMD2	0.55	1.79	14	2
1:A:193:ALA:C	4:B:104:HEC:HBC1	0.55	2.23	16	4
1:A:197:VAL:HG11	2:B:82:PHE:N	0.54	2.17	17	3
2:B:10:PHE:CE1	2:B:98:LEU:HD21	0.54	2.37	20	20
1:A:46:LEU:CD2	1:A:92:LEU:HD11	0.54	2.32	18	20
1:A:47:VAL:HG22	3:A:295:HEM:HMD3	0.53	1.80	7	7
2:B:18:HIS:CE1	2:B:30:PRO:HD2	0.53	2.39	14	20
1:A:37:ASP:HB3	1:A:40:ILE:HD12	0.53	1.79	12	18
2:B:5:LYS:O	2:B:6:GLY:C	0.52	2.48	19	20
1:A:206:LEU:CD2	1:A:239:ILE:HG23	0.52	2.35	18	20
1:A:194:ALA:CB	4:B:104:HEC:HBC2	0.52	2.34	6	2
2:B:22:LYS:C	2:B:24:GLY:H	0.51	2.09	15	20
2:B:42:GLN:O	2:B:43:ALA:C	0.50	2.50	18	20
1:A:47:VAL:HG23	3:A:295:HEM:HMD3	0.50	1.83	12	5
2:B:23:GLY:O	2:B:24:GLY:O	0.50	2.30	18	20
2:B:14:CYS:SG	4:B:104:HEC:C3B	0.49	2.99	1	20
1:A:79:ASP:O	1:A:82:ASN:HB2	0.49	2.08	14	20
1:A:193:ALA:C	4:B:104:HEC:HBC3	0.49	2.28	17	4
2:B:55:LYS:O	2:B:56:ASN:C	0.48	2.52	18	20
1:A:215:LYS:HG2	1:A:221:GLU:HG2	0.48	1.84	9	20
1:A:39:TYR:HB2	2:B:12:THR:CB	0.48	2.37	10	7
2:B:68:LEU:HD21	4:B:104:HEC:HMB2	0.48	1.86	4	10
2:B:67:TYR:CE1	2:B:75:ILE:HD12	0.48	2.43	10	19
1:A:23:TYR:O	1:A:27:ALA:N	0.48	2.36	15	20
1:A:215:LYS:HA	1:A:220:ASN:O	0.48	2.09	15	20
2:B:80:MET:HE3	4:B:104:HEC:C1C	0.48	2.39	15	11
1:A:166:ARG:NH1	1:A:247:ILE:HG23	0.48	2.24	10	2
1:A:47:VAL:CG2	3:A:295:HEM:HMD3	0.47	2.39	19	16
2:B:22:LYS:HD2	2:B:33:HIS:CD2	0.47	2.44	6	9
2:B:18:HIS:HE1	2:B:30:PRO:HD2	0.46	1.70	6	20
1:A:39:TYR:CB	2:B:13:ARG:HG3	0.46	2.38	17	2
2:B:55:LYS:O	2:B:56:ASN:O	0.46	2.34	1	20
2:B:1:GLY:O	2:B:96:THR:HG21	0.46	2.11	19	20
2:B:23:GLY:O	2:B:24:GLY:C	0.46	2.54	18	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:197:VAL:HG11	2:B:82:PHE:HA	0.46	1.88	2	7
1:A:206:LEU:HG	1:A:239:ILE:HG21	0.46	1.86	17	15
2:B:15:LEU:O	2:B:16:GLN:C	0.46	2.54	8	20
1:A:166:ARG:NH2	1:A:247:ILE:HG23	0.45	2.27	14	6
2:B:35:ILE:HG23	2:B:36:PHE:H	0.45	1.71	19	20
1:A:180:THR:HG22	3:A:295:HEM:HAA2	0.45	1.88	14	8
1:A:197:VAL:CG2	2:B:81:ALA:HB1	0.45	2.40	6	4
1:A:90:LYS:O	1:A:93:GLU:HG2	0.45	2.12	12	14
1:A:164:ASN:O	1:A:168:VAL:HG13	0.45	2.12	11	18
2:B:80:MET:CE	2:B:82:PHE:CB	0.45	2.95	17	20
1:A:90:LYS:O	1:A:94:PRO:HD2	0.45	2.11	1	20
1:A:236:TYR:CE1	1:A:239:ILE:HD11	0.45	2.46	8	7
1:A:232:LEU:O	1:A:235:ASP:N	0.45	2.47	15	20
1:A:266:PHE:CE2	1:A:270:LEU:HD11	0.45	2.47	7	14
1:A:206:LEU:HD21	1:A:239:ILE:HG23	0.45	1.88	8	9
2:B:80:MET:HE2	2:B:82:PHE:CB	0.45	2.42	4	19
1:A:116:VAL:HG11	1:A:124:ILE:HD11	0.44	1.89	10	10
1:A:247:ILE:HG22	1:A:251:TYR:CE2	0.44	2.47	14	18
1:A:194:ALA:CB	4:B:104:HEC:CBC	0.44	2.94	6	1
1:A:2:THR:HG23	1:A:3:PRO:HD2	0.44	1.90	8	20
1:A:230:MET:C	1:A:230:MET:SD	0.44	2.96	16	1
2:B:55:LYS:HE2	2:B:57:VAL:HG11	0.44	1.90	19	17
1:A:121:GLY:HA2	1:A:259:PHE:CZ	0.44	2.48	6	2
1:A:211:TRP:CH2	1:A:231:MET:HG2	0.44	2.48	10	19
2:B:80:MET:HE1	4:B:104:HEC:CHC	0.44	2.43	18	2
1:A:193:ALA:CB	4:B:104:HEC:HBC1	0.44	2.42	12	2
1:A:38:ASN:O	1:A:39:TYR:HB2	0.43	2.13	19	16
1:A:265:ALA:O	1:A:266:PHE:C	0.43	2.56	15	20
1:A:38:ASN:C	2:B:12:THR:HB	0.43	2.34	5	2
2:B:8:THR:HA	2:B:11:LYS:HG2	0.43	1.89	19	2
1:A:20:GLN:HG3	1:A:20:GLN:O	0.43	2.13	1	6
1:A:46:LEU:HD21	1:A:92:LEU:HD11	0.43	1.91	18	2
1:A:211:TRP:CZ3	1:A:231:MET:HG2	0.43	2.49	11	20
1:A:67:TYR:HA	1:A:130:ARG:HG2	0.43	1.91	14	6
2:B:98:LEU:O	2:B:99:LYS:C	0.43	2.58	1	20
1:A:214:GLU:O	1:A:221:GLU:HA	0.43	2.14	10	20
1:A:23:TYR:CE2	1:A:114:THR:HA	0.43	2.48	20	18
2:B:5:LYS:O	2:B:8:THR:N	0.42	2.52	3	20
1:A:214:GLU:N	1:A:222:GLN:O	0.42	2.50	15	20
1:A:20:GLN:O	1:A:20:GLN:HG3	0.42	2.14	18	11
2:B:77:GLY:O	2:B:78:THR:C	0.42	2.58	1	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
2:B:11:LYS:HG2	2:B:12:THR:N	0.42	2.28	7	1
1:A:177:LEU:HD11	1:A:198:PHE:CD1	0.42	2.49	6	1
1:A:206:LEU:HG	1:A:239:ILE:CG2	0.42	2.45	1	6
1:A:119:MET:O	1:A:120:GLN:CB	0.42	2.66	19	2
1:A:239:ILE:HG22	1:A:245:LEU:CD2	0.42	2.41	14	3
1:A:7:VAL:HA	1:A:275:THR:O	0.41	2.15	19	20
2:B:60:ASP:O	2:B:62:ASN:N	0.41	2.54	9	20
1:A:39:TYR:CB	2:B:12:THR:HB	0.41	2.44	19	1
1:A:206:LEU:HD13	1:A:231:MET:CE	0.41	2.45	18	1
2:B:18:HIS:CD2	4:B:104:HEC:NB	0.41	2.88	20	17
1:A:29:LYS:HD3	1:A:91:PHE:CE1	0.41	2.50	17	3
1:A:194:ALA:HB2	2:B:81:ALA:O	0.41	2.13	12	1
1:A:134:PRO:C	1:A:136:ASP:N	0.41	2.73	15	20
2:B:68:LEU:HD21	4:B:104:HEC:CMB	0.41	2.46	17	4
1:A:2:THR:HG23	1:A:3:PRO:CD	0.41	2.46	8	4
2:B:35:ILE:HG23	2:B:36:PHE:N	0.41	2.31	20	2
1:A:40:ILE:CG2	1:A:44:PRO:HG3	0.40	2.46	1	1
1:A:271:GLU:HA	1:A:274:ILE:HD12	0.40	1.94	10	1
1:A:39:TYR:CG	2:B:12:THR:OG1	0.40	2.70	4	1
2:B:30:PRO:HG3	2:B:48:TYR:CE1	0.40	2.51	1	2
1:A:250:GLU:O	1:A:253:ASN:HB2	0.40	2.17	9	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	292/294 (99%)	264±0 (90±0%)	27±0 (9±0%)	1±0 (0±0%)	50	83
2	B	101/108 (94%)	88±0 (87±0%)	9±0 (9±0%)	4±0 (4±0%)	6	33
All	All	7860/8040 (98%)	7040 (90%)	720 (9%)	100 (1%)	20	66

All 5 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	20
2	B	6	GLY	20
2	B	24	GLY	20
2	B	61	GLU	20
2	B	56	ASN	20

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/252 (100%)	226±3 (90±1%)	26±3 (10±1%)	13	57
2	B	85/89 (96%)	71±1 (83±1%)	14±1 (17±1%)	6	43
All	All	6740/6820 (99%)	5937 (88%)	803 (12%)	11	53

All 63 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)
2	B	60	ASP	20
1	A	226	LYS	20
1	A	61	ASP	20
1	A	250	GLU	20
2	B	50	ASP	20
1	A	148	ASP	20
1	A	11	GLU	20
2	B	99	LYS	20
2	B	55	LYS	20
1	A	2	THR	20
1	A	76	GLU	20
1	A	155	ARG	20
2	B	73	LYS	20
2	B	58	LEU	20
2	B	61	GLU	20
2	B	56	ASN	20
1	A	257	LYS	20
1	A	260	LYS	20
1	A	97	LYS	20
1	A	269	LEU	20

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Mol	Chain	Res	Type	Models (Total)
1	A	12	LYS	20
2	B	80	MET	20
2	B	9	LEU	20
2	B	65	SER	19
1	A	165	ASP	19
1	A	20	GLN	19
1	A	201	GLU	19
1	A	86	GLN	19
2	B	16	GLN	19
1	A	74	LYS	18
1	A	31	ARG	18
1	A	215	LYS	17
2	B	22	LYS	15
1	A	182	LEU	14
1	A	166	ARG	12
2	B	11	LYS	12
1	A	37	ASP	11
1	A	255	GLN	10
1	A	54	SER	9
1	A	214	GLU	9
1	A	47	VAL	7
1	A	290	GLU	6
1	A	17	GLU	6
2	B	88	GLU	6
1	A	268	LYS	5
1	A	256	ASP	5
1	A	197	VAL	5
1	A	267	GLU	5
1	A	271	GLU	5
1	A	48	ARG	4
2	B	21	GLU	4
1	A	96	HIS	4
2	B	39	HIS	4
1	A	30	LEU	4
2	B	70	ASN	3
1	A	219	ASN	2
1	A	253	ASN	2
1	A	282	SER	2
1	A	4	LEU	1
2	B	91	ARG	1
1	A	143	ARG	1
1	A	120	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	212	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

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
3	HEM	A	295	1	24,50,50	2.61±0.00	1±0 (4±0%)
4	HEC	B	104	2	24,50,50	2.76±0.01	2±0 (8±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
3	HEM	A	295	1	16,82,82	3.42±0.00	1±0 (6±0%)
4	HEC	B	104	2	19,82,82	2.42±0.00	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	295	1	-	0±0,6,54,54	0±0,0,8,8
4	HEC	B	104	2	-	0±0,6,54,54	0±0,0,8,8

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	C3C-C2C	8.44	1.32	1.40	20	20
3	A	295	HEM	C3B-C2B	7.87	1.30	1.40	5	20
4	B	104	HEC	C3B-C2B	6.25	1.34	1.40	19	20

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
								Worst	Total
3	A	295	HEM	C3C-CAC-CBC	10.72	147.95	126.40	5	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided