



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 07:44 PM UTC

PDB ID : 1L3O / pdb_00001l3o
Title : SOLUTION STRUCTURE DETERMINATION OF THE FULLY OXIDIZED DOUBLE MUTANT K9-10A CYTOCHROME C7 FROM DESULFURIUMONAS ACETOXIDANS, ENSEMBLE OF 35 STRUCTURES
Authors : Assfalg, M.; Bertini, I.; Turano, P.; Bruschi, M.; Durand, M.C.; Giudici-Orticoni, M.T.; Dolla, A.
Deposited on : 2002-02-28

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

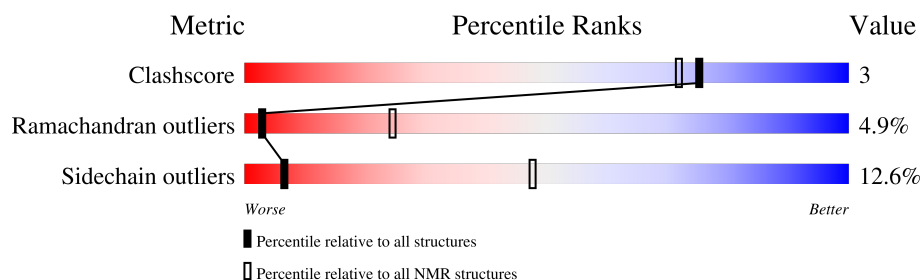
1 Overall quality at a glance

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	68	78% 12% 10%

2 Ensemble composition and analysis

This entry contains 35 models. Model 14 is the overall representative, medoid model (most similar to other models).

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:2-A:54, A:61-A:68 (61)	0.67	14

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 7 clusters and 4 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1198 atoms, of which 572 are hydrogens and 0 are deuteriums.

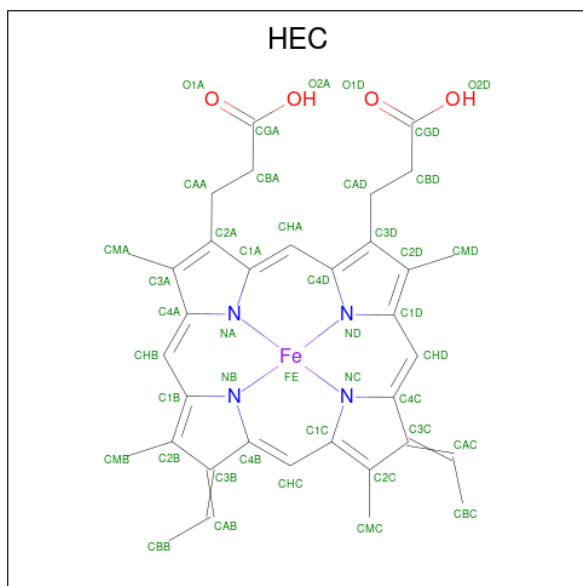
- Molecule 1 is a protein called cytochrome c7.

Mol	Chain	Residues	Atoms						Trace
1	A	68	Total	C	H	N	O	S	0
			973	300	476	94	97	6	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	ALA	LYS	engineered mutation	UNP P00137
A	10	ALA	LYS	engineered mutation	UNP P00137

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



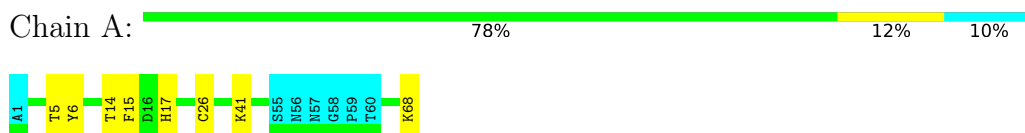
Mol	Chain	Residues	Atoms					
2	A	1	Total	C	Fe	H	N	O
			75	34	1	32	4	4
2	A	1	Total	C	Fe	H	N	O
			75	34	1	32	4	4
2	A	1	Total	C	Fe	H	N	O
			75	34	1	32	4	4

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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 c7

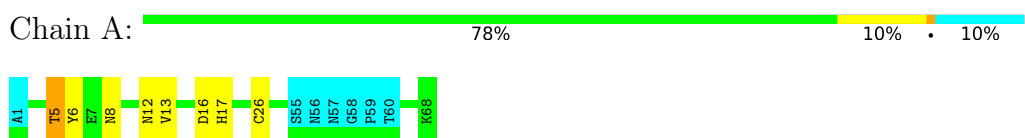


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

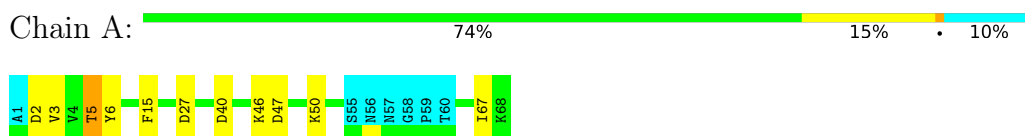
4.2.1 Score per residue for model 1

- Molecule 1: cytochrome c7



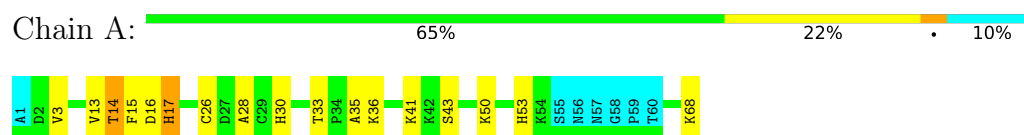
4.2.2 Score per residue for model 2

- Molecule 1: cytochrome c7



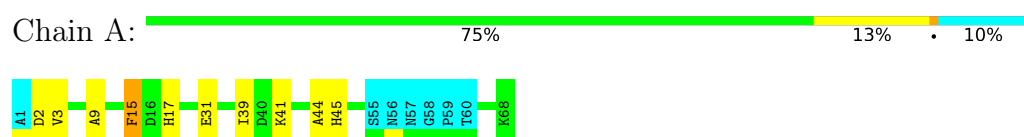
4.2.3 Score per residue for model 3

- Molecule 1: cytochrome c7



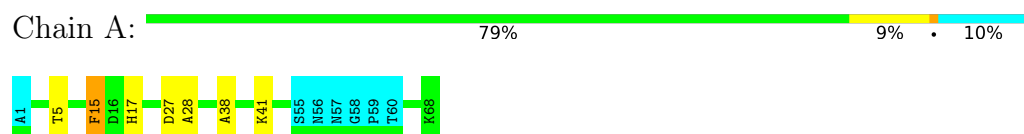
4.2.4 Score per residue for model 4

- Molecule 1: cytochrome c7



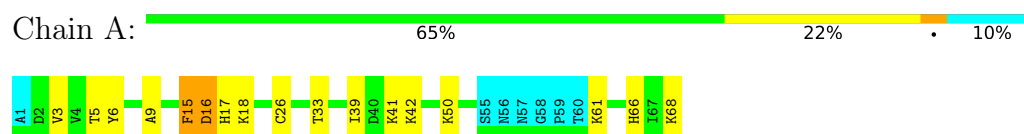
4.2.5 Score per residue for model 5

- Molecule 1: cytochrome c7



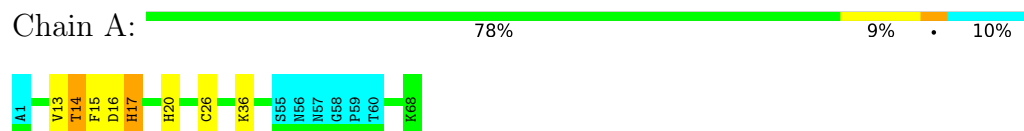
4.2.6 Score per residue for model 6

- Molecule 1: cytochrome c7



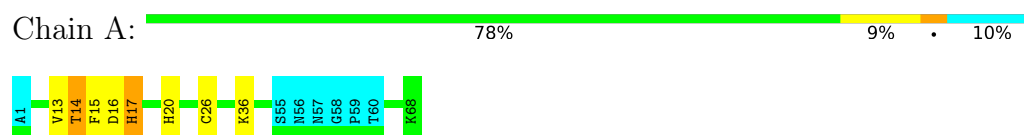
4.2.7 Score per residue for model 7

- Molecule 1: cytochrome c7



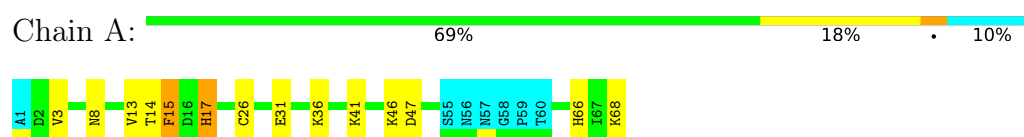
4.2.8 Score per residue for model 8

- Molecule 1: cytochrome c7



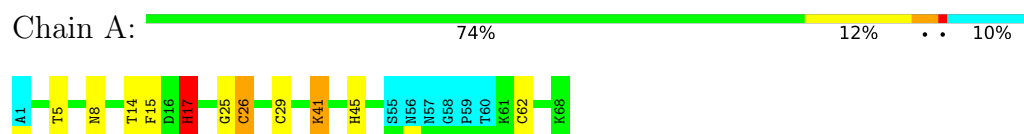
4.2.9 Score per residue for model 9

- Molecule 1: cytochrome c7



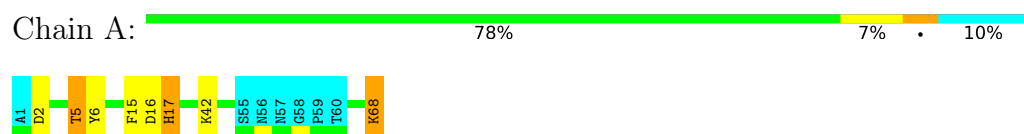
4.2.10 Score per residue for model 10

- Molecule 1: cytochrome c7



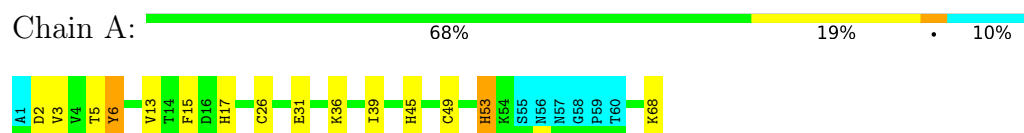
4.2.11 Score per residue for model 11

- Molecule 1: cytochrome c7



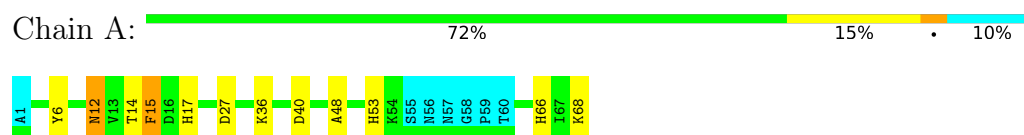
4.2.12 Score per residue for model 12

- Molecule 1: cytochrome c7



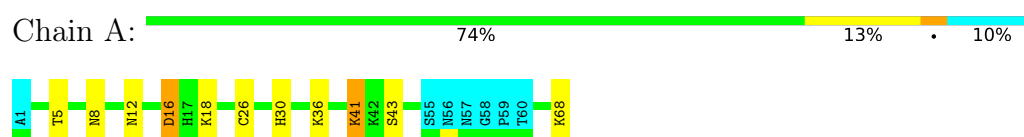
4.2.13 Score per residue for model 13

- Molecule 1: cytochrome c7



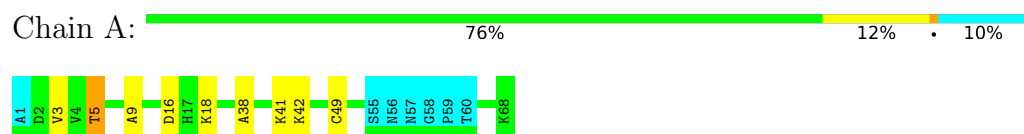
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: cytochrome c7



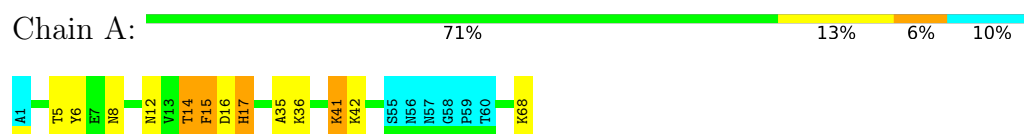
4.2.15 Score per residue for model 15

- Molecule 1: cytochrome c7



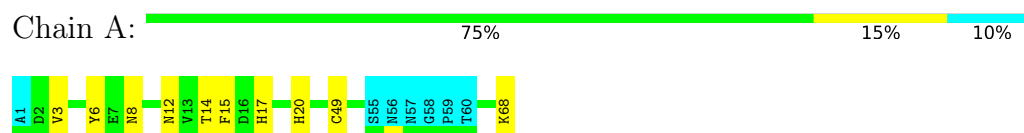
4.2.16 Score per residue for model 16

- Molecule 1: cytochrome c7



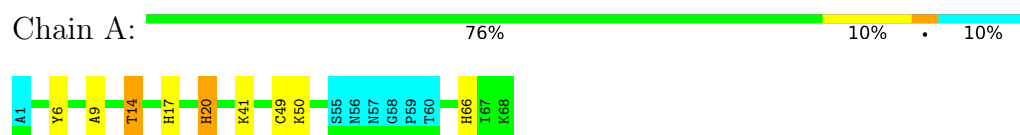
4.2.17 Score per residue for model 17

- Molecule 1: cytochrome c7



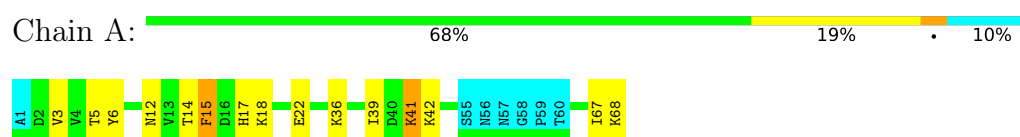
4.2.18 Score per residue for model 18

- Molecule 1: cytochrome c7



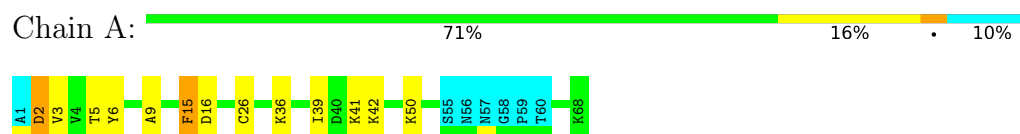
4.2.19 Score per residue for model 19

- Molecule 1: cytochrome c7



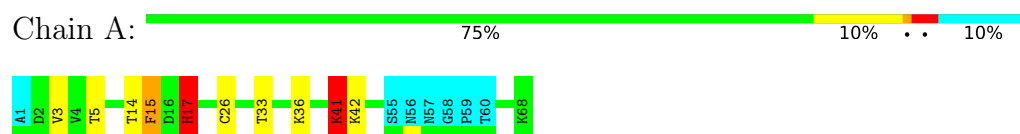
4.2.20 Score per residue for model 20

- Molecule 1: cytochrome c7



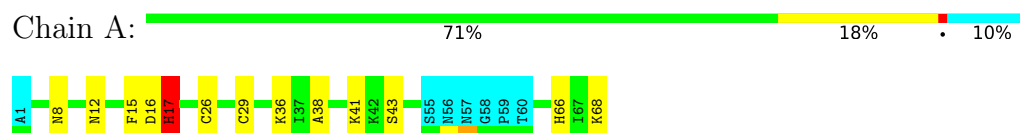
4.2.21 Score per residue for model 21

- Molecule 1: cytochrome c7



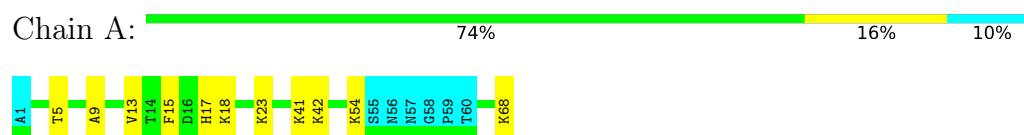
4.2.22 Score per residue for model 22

- Molecule 1: cytochrome c7



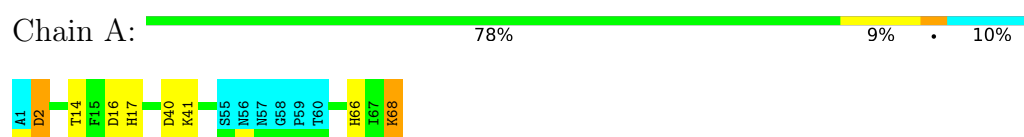
4.2.23 Score per residue for model 23

- Molecule 1: cytochrome c7



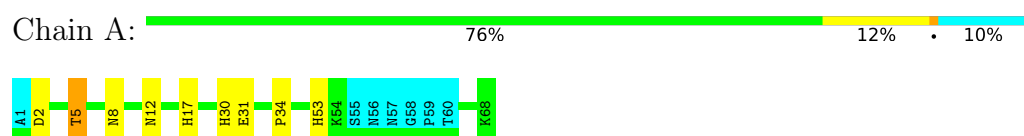
4.2.24 Score per residue for model 24

- Molecule 1: cytochrome c7



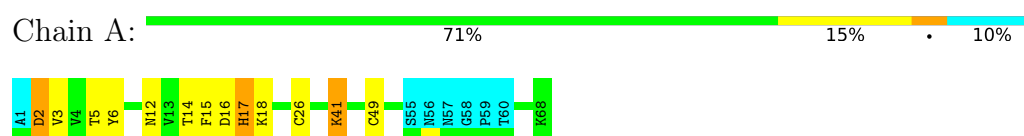
4.2.25 Score per residue for model 25

- Molecule 1: cytochrome c7



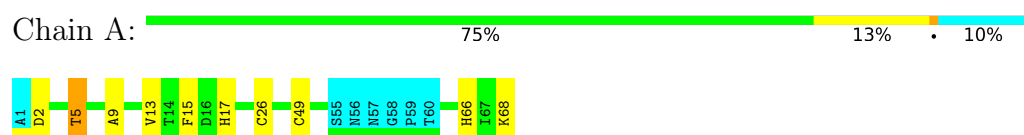
4.2.26 Score per residue for model 26

- Molecule 1: cytochrome c7



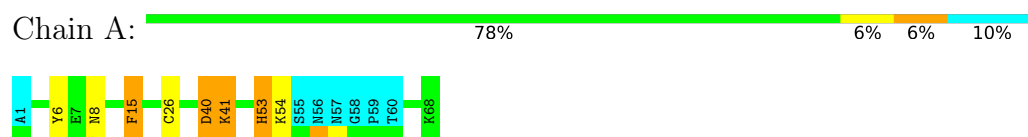
4.2.27 Score per residue for model 27

- Molecule 1: cytochrome c7



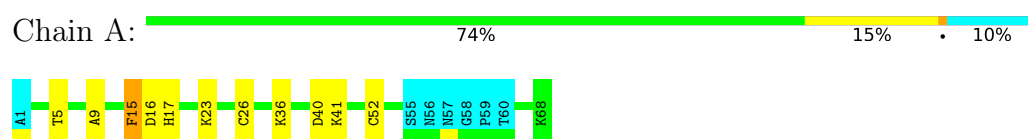
4.2.28 Score per residue for model 28

- Molecule 1: cytochrome c7



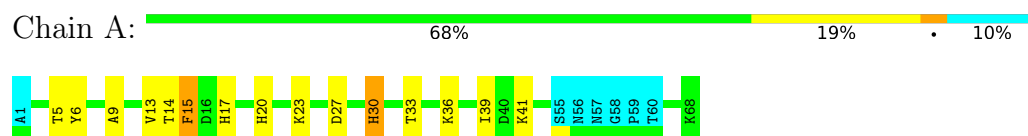
4.2.29 Score per residue for model 29

- Molecule 1: cytochrome c7



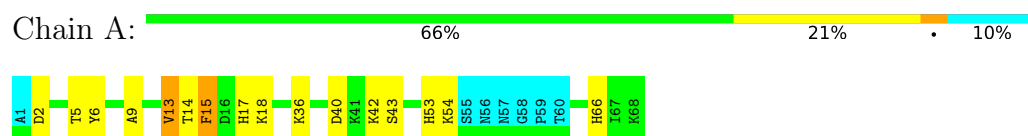
4.2.30 Score per residue for model 30

- Molecule 1: cytochrome c7



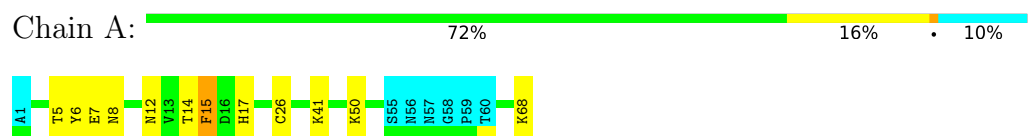
4.2.31 Score per residue for model 31

- Molecule 1: cytochrome c7



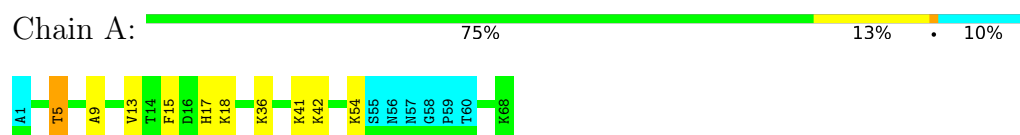
4.2.32 Score per residue for model 32

- Molecule 1: cytochrome c7



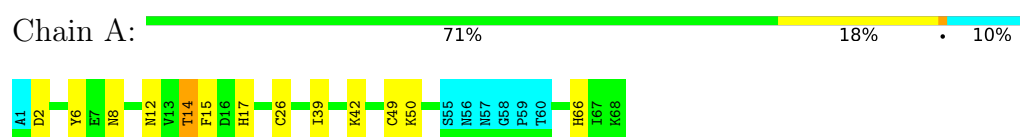
4.2.33 Score per residue for model 33

- Molecule 1: cytochrome c7



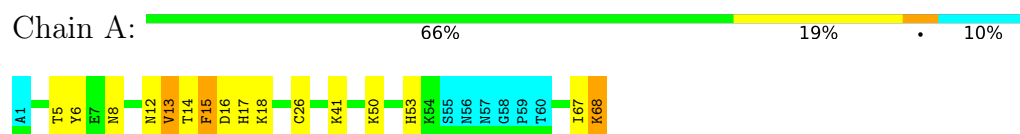
4.2.34 Score per residue for model 34

- Molecule 1: cytochrome c7



4.2.35 Score per residue for model 35

- Molecule 1: cytochrome c7



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing in torsion angle space and restrained energy minimization*.

Of the 500 calculated structures, 35 were deposited, based on the following criterion: *The submitted conformer models are the 35 structures with the lowest target function values*.

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

Software name	Classification	Version
PSEUDYANA	structure solution	1.5
Amber	refinement	5.0

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: 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	0.83±0.02	0±0/460 (0.0± 0.0%)	1.46±0.05	2±2/614 (0.4± 0.3%)
All	All	0.83	1/16100 (0.0%)	1.46	85/21490 (0.4%)

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	1.5±1.1
All	All	0	54

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	2	ASP	CA-C	5.17	1.55	1.52	25	1

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	15	PHE	CA-CB-CG	8.28	122.08	113.80	21	10
1	A	17	HIS	CB-CG-CD2	-7.84	121.01	131.20	16	8
1	A	2	ASP	CA-CB-CG	6.66	119.26	112.60	20	1
1	A	16	ASP	CA-CB-CG	6.08	118.68	112.60	6	5
1	A	26	CYS	CA-C-N	6.02	128.66	120.54	10	18
1	A	26	CYS	C-N-CA	6.02	128.66	120.54	10	18
1	A	13	VAL	N-CA-C	5.97	117.14	112.12	35	2
1	A	35	ALA	CA-C-N	5.95	132.91	121.54	16	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	35	ALA	C-N-CA	5.95	132.91	121.54	16	2
1	A	53	HIS	CA-CB-CG	5.76	119.56	113.80	31	1
1	A	25	GLY	CA-C-N	5.65	132.34	121.54	10	1
1	A	25	GLY	C-N-CA	5.65	132.34	121.54	10	1
1	A	13	VAL	N-CA-CB	-5.63	106.01	112.21	33	1
1	A	43	SER	CA-C-N	5.51	127.93	120.38	3	1
1	A	43	SER	C-N-CA	5.51	127.93	120.38	3	1
1	A	53	HIS	CA-C-N	5.30	127.64	120.38	25	2
1	A	53	HIS	C-N-CA	5.30	127.64	120.38	25	2
1	A	12	ASN	CA-CB-CG	5.25	117.84	112.60	13	1
1	A	53	HIS	CE1-NE2-CD2	-5.21	103.79	109.00	12	1
1	A	13	VAL	CA-C-N	5.14	130.89	123.13	30	1
1	A	13	VAL	C-N-CA	5.14	130.89	123.13	30	1
1	A	30	HIS	CB-CG-CD2	-5.13	124.53	131.20	14	2
1	A	62	CYS	CA-C-N	5.11	125.75	120.03	10	1
1	A	62	CYS	C-N-CA	5.11	125.75	120.03	10	1
1	A	40	ASP	CA-CB-CG	5.01	117.61	112.60	13	1

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	15	PHE	Sidechain,Peptide	24
1	A	6	TYR	Sidechain	15
1	A	17	HIS	Sidechain	9
1	A	30	HIS	Sidechain	3
1	A	16	ASP	Peptide	2

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	452	435	435	1±1
2	A	129	96	90	3±1
All	All	20335	18585	18375	119

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:153:HEC:HBB3	2:A:153:HEC:HMB1	0.65	1.68	5	9
2:A:153:HEC:HMB3	2:A:153:HEC:HBB2	0.62	1.71	35	5
2:A:166:HEC:CGA	2:A:166:HEC:HMA1	0.62	2.25	31	1
2:A:153:HEC:HBC3	2:A:153:HEC:HMC1	0.56	1.78	13	7
2:A:153:HEC:HMB1	2:A:153:HEC:CBB	0.55	2.32	12	10
2:A:166:HEC:HBC3	2:A:166:HEC:HMC1	0.54	1.80	29	1
2:A:153:HEC:HBC3	2:A:153:HEC:HMC3	0.53	1.80	18	7
2:A:153:HEC:HMC3	2:A:153:HEC:CBC	0.53	2.34	18	22
2:A:153:HEC:HMC3	2:A:153:HEC:HBC3	0.50	1.84	9	13
1:A:49:CYS:SG	2:A:153:HEC:HHC	0.49	2.48	18	6
1:A:41:LYS:NZ	2:A:166:HEC:O1A	0.49	2.45	14	2
2:A:153:HEC:HMB1	2:A:153:HEC:HBB2	0.47	1.86	15	2
1:A:15:PHE:CZ	1:A:39:ILE:HG21	0.47	2.45	19	7
2:A:153:HEC:HMB3	2:A:153:HEC:CBB	0.46	2.39	7	3
2:A:153:HEC:HBB2	2:A:153:HEC:CMB	0.46	2.41	18	2
1:A:15:PHE:HZ	1:A:39:ILE:HG21	0.45	1.72	4	1
1:A:40:ASP:CG	1:A:41:LYS:N	0.44	2.75	28	2
1:A:6:TYR:HB2	1:A:13:VAL:HG22	0.44	1.88	31	1
2:A:166:HEC:CGD	2:A:166:HEC:HHA	0.43	2.43	9	3
1:A:46:LYS:NZ	1:A:47:ASP:OD2	0.43	2.51	9	1
1:A:41:LYS:HZ3	2:A:166:HEC:CGD	0.43	2.25	16	1
1:A:36:LYS:NZ	2:A:130:HEC:O2A	0.43	2.50	21	1
1:A:68:LYS:NZ	1:A:68:LYS:C	0.42	2.78	24	2
1:A:20:HIS:CE1	2:A:153:HEC:NA	0.42	2.88	30	1
1:A:17:HIS:CE1	2:A:130:HEC:ND	0.42	2.88	10	1
1:A:39:ILE:HG23	1:A:44:ALA:HB2	0.41	1.91	4	1
1:A:6:TYR:HB2	1:A:13:VAL:HG12	0.41	1.92	12	1
1:A:13:VAL:HG23	1:A:14:THR:N	0.41	2.30	31	1
1:A:6:TYR:CE1	1:A:15:PHE:CE2	0.41	3.09	34	1
1:A:67:ILE:HG22	1:A:68:LYS:N	0.41	2.30	19	2
1:A:20:HIS:CE1	2:A:153:HEC:ND	0.40	2.89	18	1
1:A:23:LYS:NZ	2:A:153:HEC:O1D	0.40	2.54	30	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	60/68 (88%)	43±2 (71±4%)	14±2 (24±3%)	3±1 (5±2%)	3	24
All	All	2100/2380 (88%)	1494 (71%)	504 (24%)	102 (5%)	3	24

All 18 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	41	LYS	14
1	A	3	VAL	12
1	A	14	THR	12
1	A	9	ALA	11
1	A	2	ASP	9
1	A	42	LYS	9
1	A	5	THR	7
1	A	53	HIS	5
1	A	33	THR	4
1	A	31	GLU	4
1	A	27	ASP	3
1	A	38	ALA	3
1	A	28	ALA	2
1	A	26	CYS	2
1	A	54	LYS	2
1	A	48	ALA	1
1	A	15	PHE	1
1	A	34	PRO	1

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	47/52 (90%)	41±2 (87±4%)	6±2 (13±4%)	6	48
All	All	1645/1820 (90%)	1438 (87%)	207 (13%)	6	48

All 33 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	17	HIS	26
1	A	5	THR	23
1	A	36	LYS	15
1	A	68	LYS	15
1	A	8	ASN	12
1	A	12	ASN	12
1	A	41	LYS	12
1	A	14	THR	11
1	A	16	ASP	10
1	A	18	LYS	9
1	A	66	HIS	9
1	A	13	VAL	8
1	A	50	LYS	8
1	A	40	ASP	4
1	A	20	HIS	4
1	A	45	HIS	3
1	A	43	SER	3
1	A	2	ASP	3
1	A	29	CYS	2
1	A	42	LYS	2
1	A	23	LYS	2
1	A	54	LYS	2
1	A	15	PHE	2
1	A	46	LYS	1
1	A	47	ASP	1
1	A	67	ILE	1
1	A	61	LYS	1
1	A	6	TYR	1
1	A	22	GLU	1
1	A	52	CYS	1
1	A	27	ASP	1
1	A	7	GLU	1
1	A	49	CYS	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 oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

3 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
2	HEC	A	153	1	46,50,50	2.18±0.03	18±0 (38±0%)
2	HEC	A	166	1	46,50,50	2.16±0.03	18±1 (38±1%)
2	HEC	A	130	1	46,50,50	2.22±0.03	17±1 (36±2%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	HEC	A	153	1	58,82,82	1.63±0.07	10±1 (17±2%)
2	HEC	A	166	1	58,82,82	1.94±0.07	14±2 (23±3%)
2	HEC	A	130	1	58,82,82	1.97±0.05	12±1 (20±2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	166	1	-	0±0,14,54,54	-
2	HEC	A	153	1	-	0±0,14,54,54	-
2	HEC	A	130	1	-	0±0,14,54,54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	153	HEC	CAB-C3B	6.35	1.55	1.35	15	35
2	A	153	HEC	CAC-C3C	5.83	1.53	1.35	20	35
2	A	166	HEC	CAC-C3C	5.75	1.53	1.35	1	35
2	A	166	HEC	CAB-C3B	5.75	1.53	1.35	25	35
2	A	130	HEC	CAB-C3B	5.68	1.53	1.35	7	35
2	A	130	HEC	CAC-C3C	5.39	1.52	1.35	14	35
2	A	130	HEC	C1D-ND	4.36	1.31	1.39	23	35
2	A	166	HEC	C1C-NC	4.05	1.32	1.39	28	35
2	A	153	HEC	C1C-NC	4.00	1.32	1.39	23	35
2	A	130	HEC	CHD-C1D	3.95	1.30	1.39	5	35
2	A	166	HEC	C1B-NB	3.93	1.32	1.39	31	35
2	A	130	HEC	C1B-NB	3.92	1.32	1.39	7	35
2	A	130	HEC	C4A-NA	3.82	1.32	1.39	2	35
2	A	166	HEC	C1D-ND	3.80	1.32	1.39	2	35
2	A	130	HEC	C1C-NC	3.75	1.32	1.39	14	35
2	A	153	HEC	C4B-NB	3.73	1.32	1.39	23	35
2	A	130	HEC	C4C-NC	3.71	1.32	1.39	11	35
2	A	166	HEC	C4A-NA	3.65	1.32	1.39	6	35
2	A	153	HEC	C1B-NB	3.63	1.32	1.39	17	35
2	A	130	HEC	CHD-C4C	3.58	1.31	1.38	7	35
2	A	130	HEC	C4D-ND	3.49	1.33	1.39	26	35
2	A	153	HEC	C4A-NA	3.46	1.33	1.39	11	35
2	A	153	HEC	C4C-NC	3.44	1.33	1.39	17	35
2	A	166	HEC	C4B-NB	3.44	1.33	1.39	1	35
2	A	130	HEC	C4B-NB	3.44	1.33	1.39	10	35
2	A	153	HEC	C1D-ND	3.40	1.33	1.39	34	35
2	A	153	HEC	C4D-ND	3.23	1.33	1.39	18	35
2	A	166	HEC	CHC-C1C	3.15	1.32	1.39	28	35
2	A	166	HEC	C4C-NC	3.14	1.33	1.39	33	35
2	A	130	HEC	CHC-C1C	3.11	1.32	1.39	10	35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	166	HEC	C1A-NA	3.09	1.33	1.39	2	34
2	A	130	HEC	CHA-C4D	3.08	1.32	1.39	16	35
2	A	166	HEC	CHB-C1B	3.04	1.32	1.39	11	35
2	A	153	HEC	CHC-C1C	3.00	1.32	1.39	7	35
2	A	166	HEC	C4D-ND	3.00	1.34	1.39	27	35
2	A	166	HEC	CHD-C1D	2.92	1.32	1.39	34	35
2	A	153	HEC	C1A-NA	2.92	1.34	1.39	17	35
2	A	130	HEC	C1A-NA	2.91	1.34	1.39	25	32
2	A	153	HEC	CHD-C1D	2.88	1.33	1.39	35	35
2	A	166	HEC	CHA-C4D	2.85	1.33	1.39	2	35
2	A	166	HEC	CHB-C4A	2.84	1.32	1.38	11	34
2	A	166	HEC	CHA-C1A	2.78	1.32	1.38	2	21
2	A	130	HEC	CHC-C4B	2.78	1.32	1.38	10	33
2	A	153	HEC	CHA-C4D	2.70	1.33	1.39	33	35
2	A	153	HEC	CHB-C1B	2.70	1.33	1.39	19	35
2	A	153	HEC	CHB-C4A	2.70	1.33	1.38	16	35
2	A	130	HEC	CHB-C1B	2.69	1.33	1.39	32	35
2	A	153	HEC	CHC-C4B	2.67	1.33	1.38	34	33
2	A	166	HEC	CHD-C4C	2.64	1.33	1.38	33	32
2	A	153	HEC	CHD-C4C	2.63	1.33	1.38	29	35
2	A	153	HEC	CHA-C1A	2.62	1.33	1.38	31	33
2	A	166	HEC	CHC-C4B	2.59	1.33	1.38	14	34
2	A	130	HEC	CHB-C4A	2.52	1.33	1.38	32	19
2	A	166	HEC	CBD-CGD	2.43	1.56	1.50	11	10
2	A	130	HEC	CBA-CGA	2.25	1.55	1.50	24	10
2	A	130	HEC	CHA-C1A	2.22	1.34	1.38	2	8
2	A	130	HEC	CBD-CGD	2.05	1.55	1.50	7	3
2	A	153	HEC	CBA-CGA	2.01	1.55	1.50	23	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	130	HEC	CBB-CAB-C3B	7.80	111.84	127.43	4	35
2	A	166	HEC	CBB-CAB-C3B	7.45	112.54	127.43	7	35
2	A	130	HEC	CBC-CAC-C3C	7.30	112.84	127.43	3	35
2	A	153	HEC	CBB-CAB-C3B	6.96	113.53	127.43	21	35
2	A	166	HEC	CBC-CAC-C3C	6.86	113.73	127.43	31	35
2	A	153	HEC	CBC-CAC-C3C	5.98	115.49	127.43	29	35
2	A	166	HEC	CAD-C3D-C4D	4.59	133.91	124.94	22	28
2	A	130	HEC	CHD-C4C-NC	4.20	129.03	124.45	28	35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	130	HEC	CHA-C1A-NA	3.95	128.75	124.45	16	35
2	A	166	HEC	CHB-C4A-NA	3.80	128.59	124.45	17	35
2	A	166	HEC	CBD-CAD-C3D	3.76	122.92	112.53	18	20
2	A	130	HEC	CHB-C4A-NA	3.69	128.47	124.45	27	35
2	A	166	HEC	CHA-C1A-NA	3.39	128.15	124.45	35	35
2	A	153	HEC	CHC-C4B-NB	3.36	128.12	124.45	20	28
2	A	153	HEC	CHA-C1A-NA	3.35	128.10	124.45	18	34
2	A	153	HEC	CHB-C4A-NA	3.31	128.06	124.45	9	34
2	A	153	HEC	CHD-C1D-ND	3.11	129.49	123.86	20	34
2	A	130	HEC	CHD-C4C-C3C	3.04	120.09	125.21	7	35
2	A	130	HEC	CBA-CAA-C2A	3.01	120.86	112.53	25	4
2	A	166	HEC	CHD-C4C-NC	2.99	127.71	124.45	34	33
2	A	130	HEC	CAD-C3D-C4D	2.93	130.67	124.94	7	11
2	A	130	HEC	CHD-C1D-ND	2.88	129.08	123.86	7	34
2	A	166	HEC	CAD-C3D-C2D	2.82	120.75	127.07	33	10
2	A	130	HEC	CHD-C1D-C2D	2.80	119.31	127.43	5	35
2	A	166	HEC	CHD-C1D-ND	2.78	128.89	123.86	28	33
2	A	166	HEC	CMD-C2D-C1D	2.77	129.64	125.42	27	10
2	A	153	HEC	CHD-C4C-NC	2.77	127.47	124.45	25	29
2	A	153	HEC	CHC-C4B-C3B	2.76	120.55	125.21	20	19
2	A	153	HEC	CMD-C2D-C1D	2.75	129.60	125.42	26	3
2	A	166	HEC	CHC-C4B-NB	2.73	127.43	124.45	28	24
2	A	166	HEC	CHC-C1C-NC	2.65	128.67	123.86	26	30
2	A	166	HEC	CHB-C1B-NB	2.59	128.55	123.86	19	32
2	A	130	HEC	CHB-C1B-NB	2.55	128.49	123.86	25	21
2	A	153	HEC	CHB-C1B-NB	2.53	128.45	123.86	25	16
2	A	130	HEC	CHC-C1C-NC	2.51	128.41	123.86	16	31
2	A	130	HEC	CBD-CAD-C3D	2.51	119.47	112.53	10	4
2	A	153	HEC	CAD-C3D-C4D	2.46	129.74	124.94	32	6
2	A	166	HEC	CHC-C1C-C2C	2.44	120.33	127.43	26	30
2	A	153	HEC	CHA-C4D-ND	2.42	128.25	123.86	14	19
2	A	153	HEC	CBD-CAD-C3D	2.41	119.21	112.53	16	1
2	A	166	HEC	CAA-C2A-C1A	2.40	129.73	124.85	23	16
2	A	153	HEC	CHD-C1D-C2D	2.39	120.48	127.43	20	29
2	A	153	HEC	CMA-C3A-C4A	2.39	128.94	124.73	32	3
2	A	130	HEC	CHC-C4B-NB	2.36	127.02	124.45	30	10
2	A	166	HEC	CHB-C4A-C3A	2.35	120.61	125.49	1	16
2	A	166	HEC	CMA-C3A-C4A	2.34	128.85	124.73	19	2
2	A	153	HEC	CHC-C1C-NC	2.34	128.10	123.86	31	5
2	A	166	HEC	CHB-C1B-C2B	2.34	120.64	127.43	11	25
2	A	166	HEC	CHD-C1D-C2D	2.33	120.66	127.43	22	18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	166	HEC	O2D-CGD-CBD	2.33	121.36	114.00	16	2
2	A	153	HEC	O1D-CGD-CBD	2.30	115.78	123.09	20	2
2	A	130	HEC	CHA-C1A-C2A	2.30	121.23	124.86	16	4
2	A	130	HEC	O2A-CGA-CBA	2.30	121.26	114.00	4	6
2	A	130	HEC	CHC-C1C-C2C	2.29	120.77	127.43	16	11
2	A	153	HEC	O2D-CGD-CBD	2.28	121.20	114.00	6	4
2	A	130	HEC	CHB-C1B-C2B	2.26	120.85	127.43	25	13
2	A	166	HEC	O1D-CGD-CBD	2.27	115.91	123.09	12	5
2	A	130	HEC	CMC-C2C-C1C	2.25	128.84	125.42	23	7
2	A	153	HEC	CHC-C1C-C2C	2.22	120.97	127.43	31	6
2	A	130	HEC	O1A-CGA-CBA	2.21	116.08	123.09	34	3
2	A	166	HEC	O1A-CGA-CBA	2.20	116.11	123.09	35	3
2	A	166	HEC	CAA-C2A-C3A	2.20	123.75	127.87	34	4
2	A	130	HEC	CMA-C3A-C4A	2.20	128.59	124.73	18	3
2	A	130	HEC	CAA-C2A-C1A	2.14	129.20	124.85	13	4
2	A	153	HEC	CHB-C1B-C2B	2.13	121.23	127.43	25	3
2	A	130	HEC	O1D-CGD-CBD	2.11	116.41	123.09	22	4
2	A	166	HEC	CHA-C1A-C2A	2.11	121.54	124.86	35	2
2	A	153	HEC	O2D-CGD-O1D	2.09	117.96	123.33	22	1
2	A	166	HEC	CHC-C4B-C3B	2.08	121.70	125.21	28	1
2	A	153	HEC	CHD-C4C-C3C	2.08	121.70	125.21	35	3
2	A	130	HEC	CAA-C2A-C3A	2.08	123.97	127.87	9	1
2	A	153	HEC	O1A-CGA-CBA	2.08	116.51	123.09	32	2
2	A	130	HEC	O2A-CGA-O1A	2.06	118.03	123.33	4	2
2	A	130	HEC	CHB-C4A-C3A	2.04	121.25	125.49	16	1
2	A	153	HEC	CAA-C2A-C1A	2.03	128.99	124.85	31	1
2	A	153	HEC	CMC-C2C-C1C	2.02	128.50	125.42	20	1
2	A	153	HEC	CHA-C1A-C2A	2.00	121.70	124.86	18	1
2	A	166	HEC	CHD-C4C-C3C	2.00	121.83	125.21	34	1
2	A	130	HEC	CMD-C2D-C1D	2.00	128.47	125.42	27	1

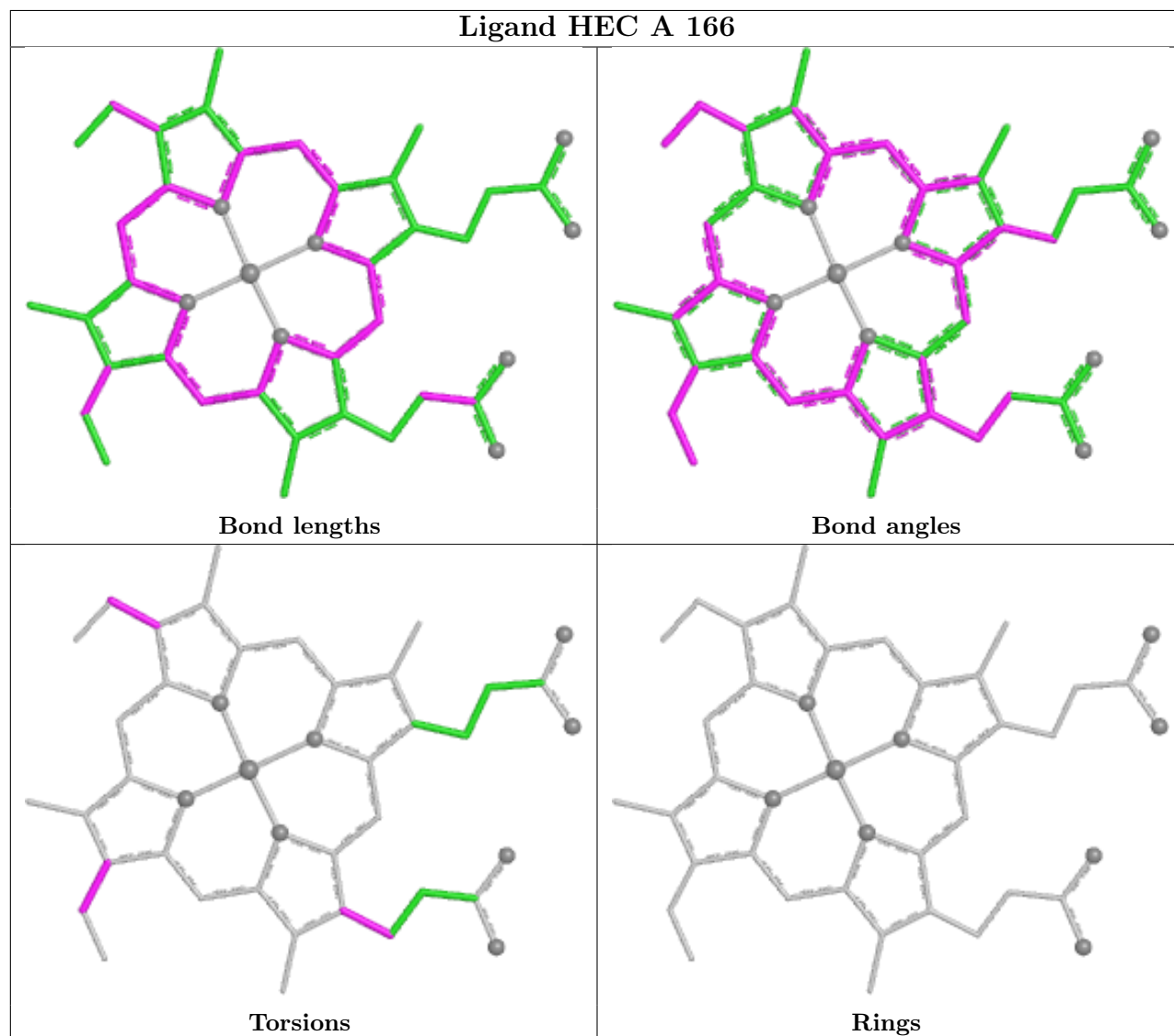
There are no chirality outliers.

There are no torsion outliers.

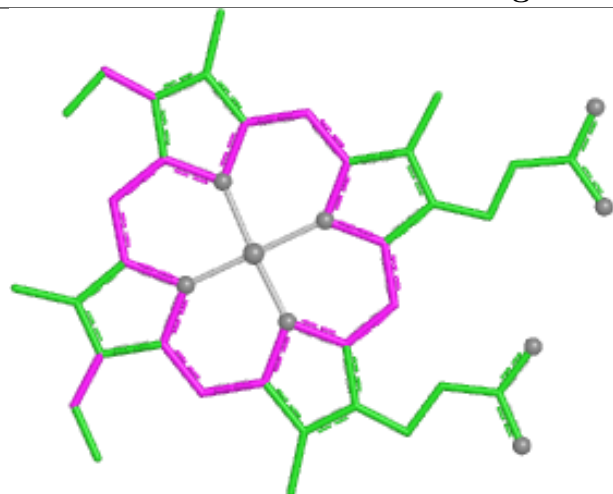
There are no ring outliers.

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

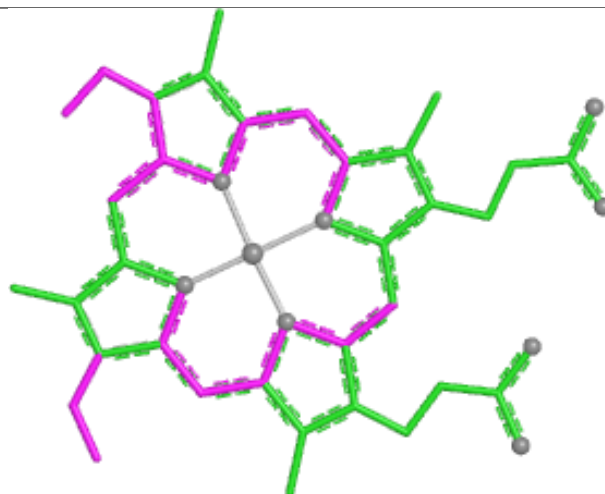
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



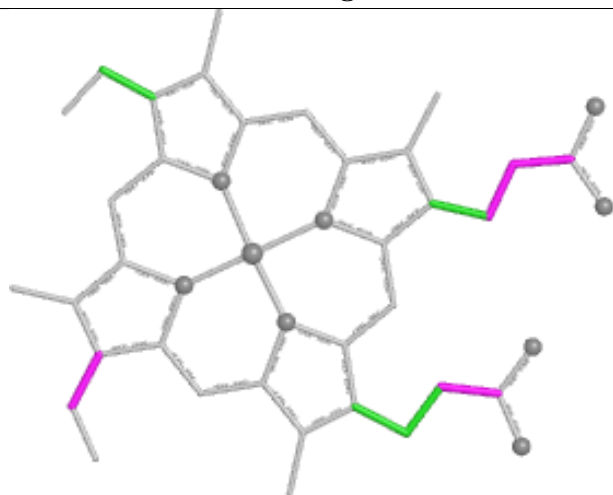
Ligand HEC A 153



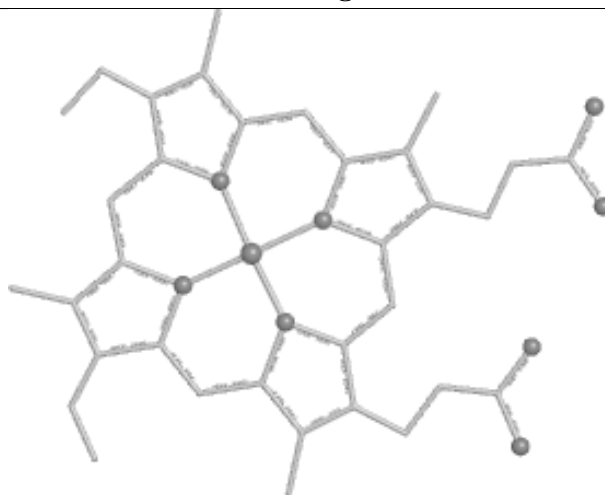
Bond lengths



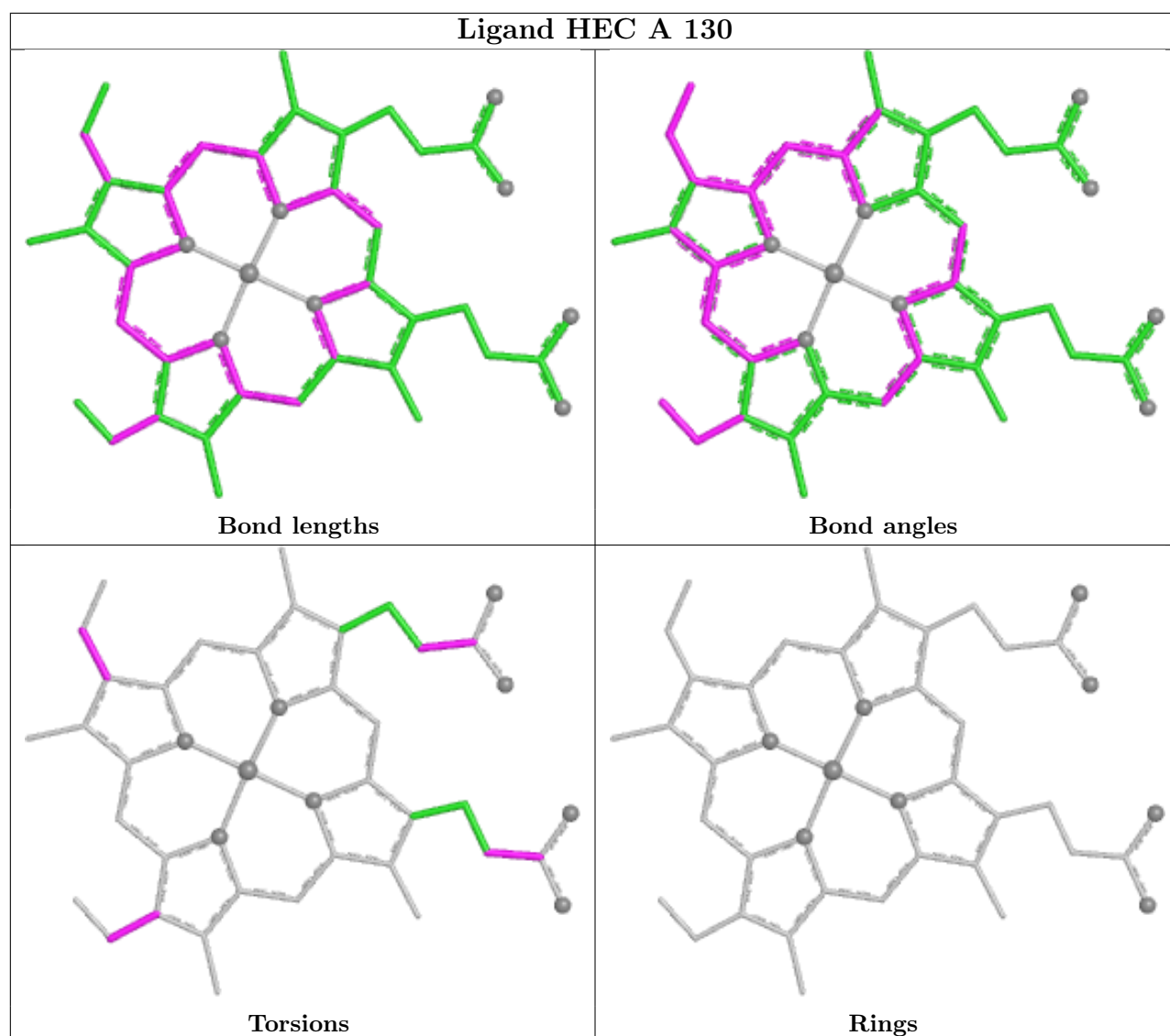
Bond angles



Torsions



Rings



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