Full wwPDB NMR Structure Validation Report (i)

Aug 4, 2026 – 10:47 AM EDT

PDB ID	:	1F22 / pdb_00001f22
Title	:	A PROTON-NMR INVESTIGATION OF THE FULLY REDUCED CYTOCHROME C7 FROM DESULFUROMONAS ACETOXIDANS. COMPARISON BETWEEN THE REDUCED AND THE OXIDIZED FORMS.
Authors	:	Assfalg, M.; Banci, L.; Bertini, I.; Bruschi, M.; Giudici-Orticoni, M.T.
Deposited on	:	2000-05-23

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 (i) 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 (i)) were used in the production of this report:

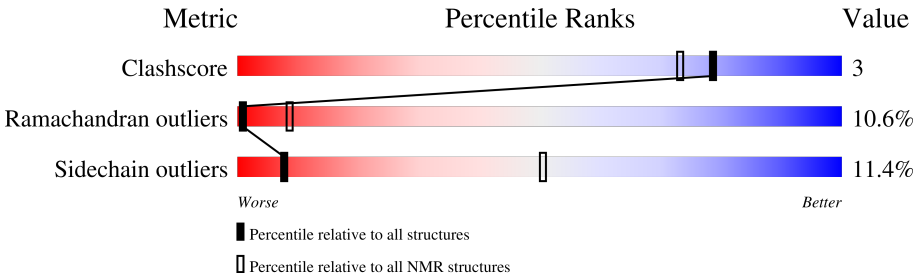
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	68	88% 10% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	A	HEC	69	35	-
2	A	HEC	70	35	-
2	A	HEC	71	35	-

2 Ensemble composition and analysis (i)

This entry contains 35 models. Model 31 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:68 (67)	1.09	31

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 1 single-model cluster was found.

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

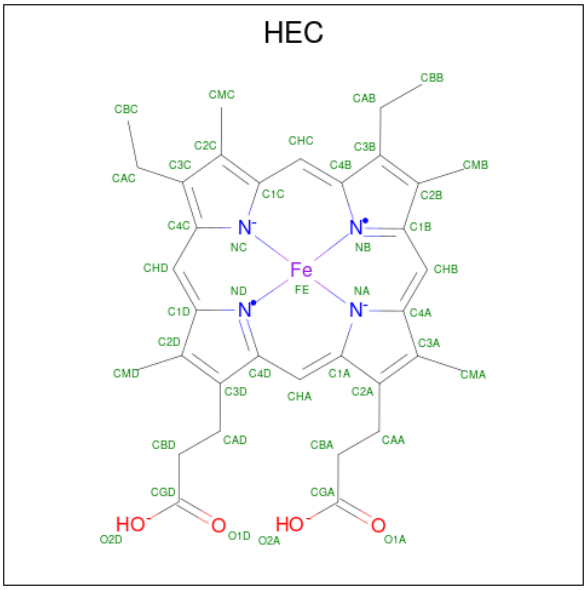
3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1222 atoms, of which 588 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CYTOCHROME C7.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	68	997	306	492	96	97	6	0

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					
			Total	C	Fe	H	N	O
2	A	1	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

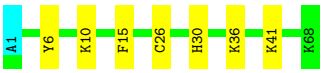
4.1 Average score per residue in the NMR ensemble

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

Chain A:





4.2 Scores per residue for each member of the ensemble

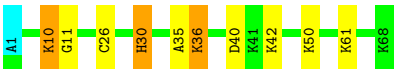
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: CYTOCHROME C7

Chain A:



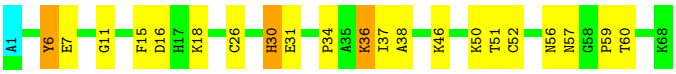


4.2.2 Score per residue for model 2

• Molecule 1: CYTOCHROME C7

Chain A:

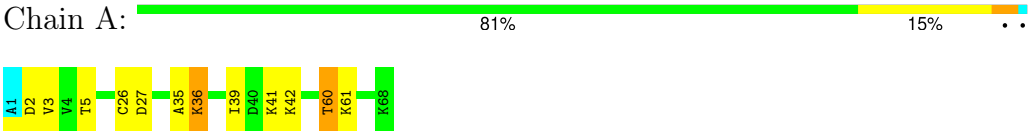




4.2.3 Score per residue for model 3

• Molecule 1: CYTOCHROME C7

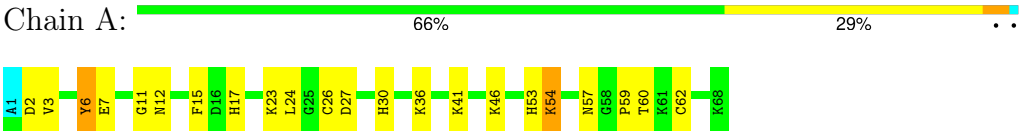
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: CYTOCHROME C7

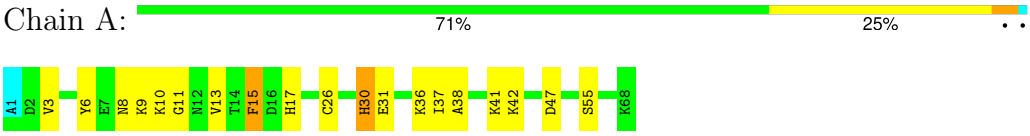
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: CYTOCHROME C7

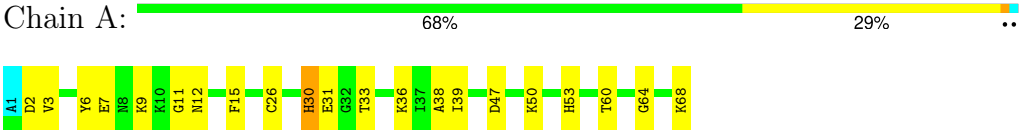
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: CYTOCHROME C7

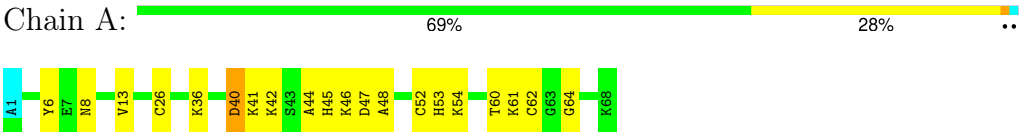
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: CYTOCHROME C7

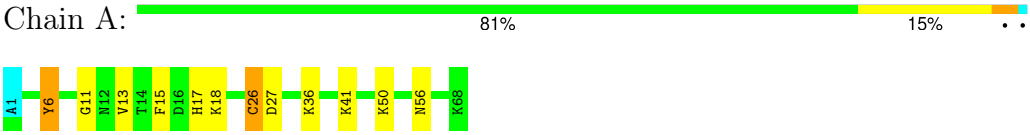
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: CYTOCHROME C7

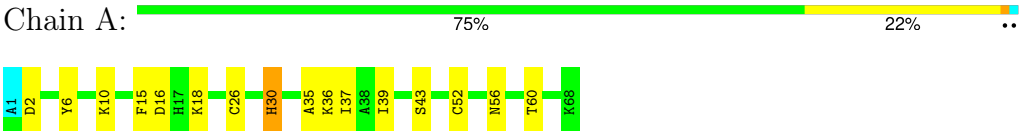
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: CYTOCHROME C7

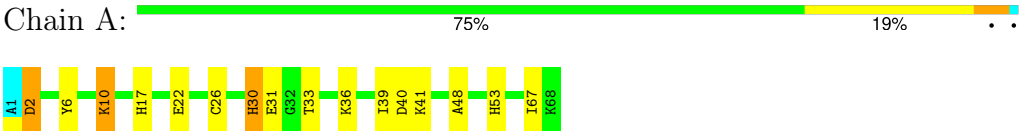
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: CYTOCHROME C7

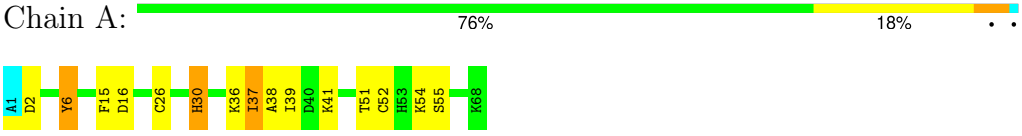
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: CYTOCHROME C7

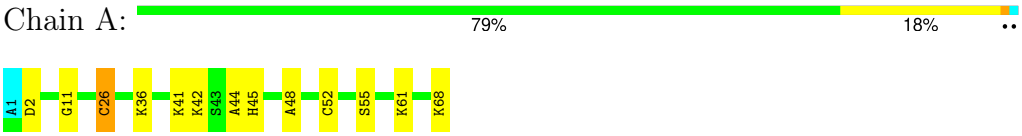
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: CYTOCHROME C7

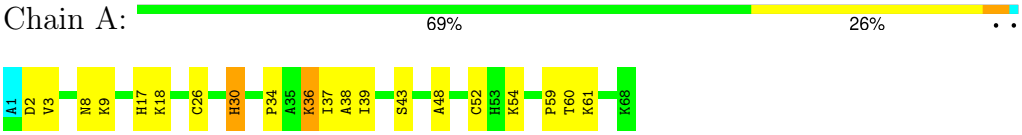
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: CYTOCHROME C7

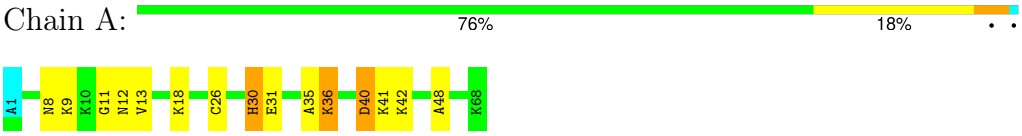
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: CYTOCHROME C7

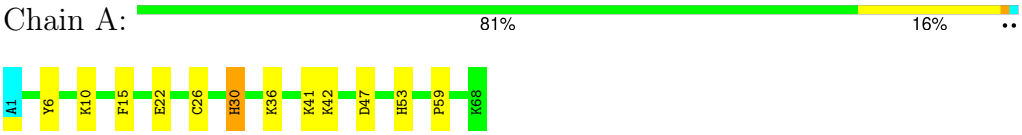
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: CYTOCHROME C7

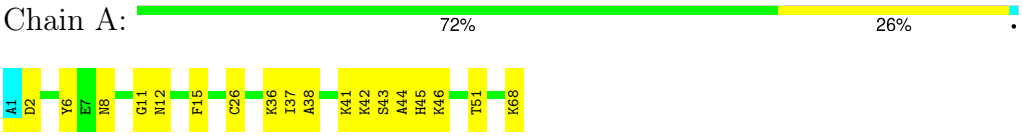
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: CYTOCHROME C7

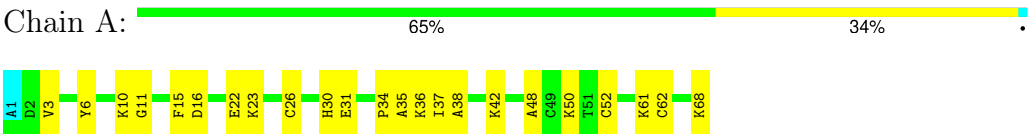
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: CYTOCHROME C7

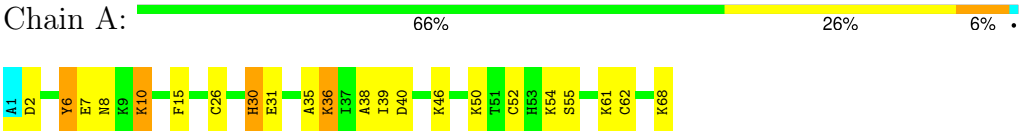
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: CYTOCHROME C7

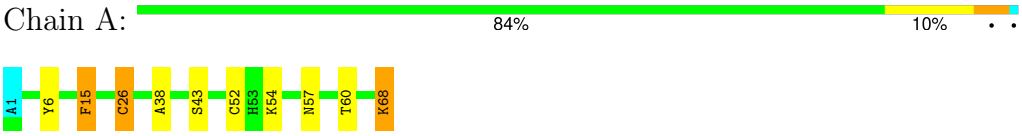
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: CYTOCHROME C7

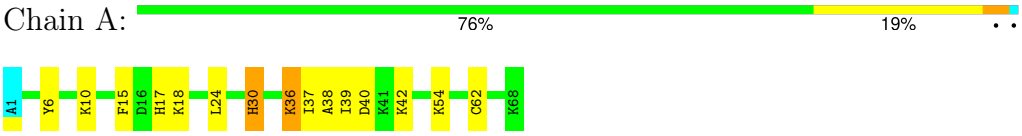
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: CYTOCHROME C7

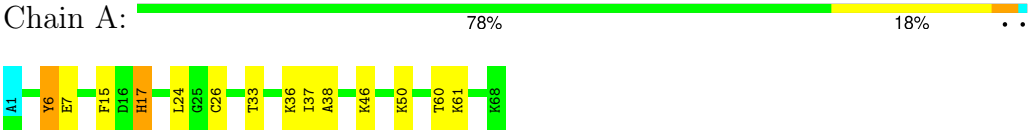
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: CYTOCHROME C7

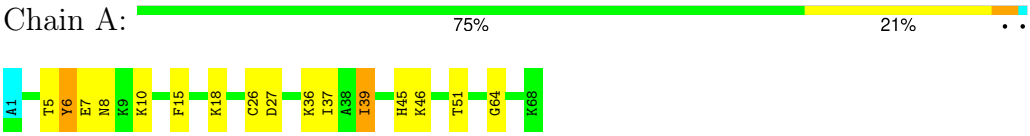
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: CYTOCHROME C7

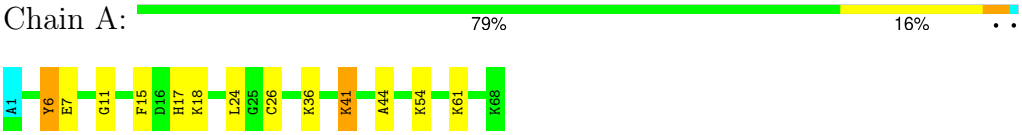
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: CYTOCHROME C7

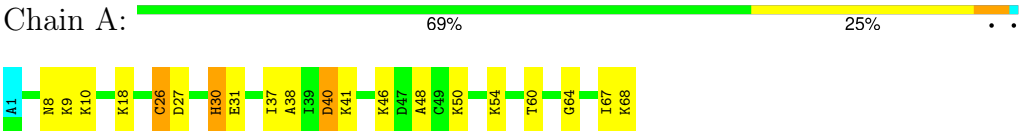
Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: CYTOCHROME C7

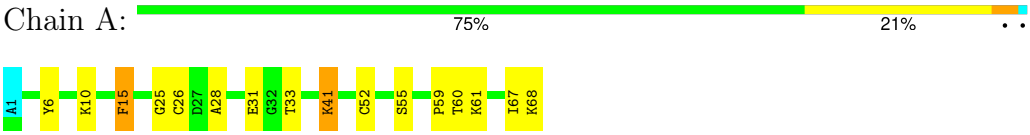
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: CYTOCHROME C7

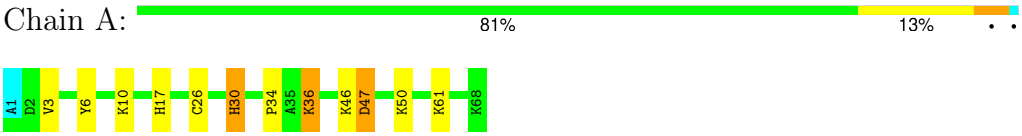
Chain A:



4.2.26 Score per residue for model 26

• Molecule 1: CYTOCHROME C7

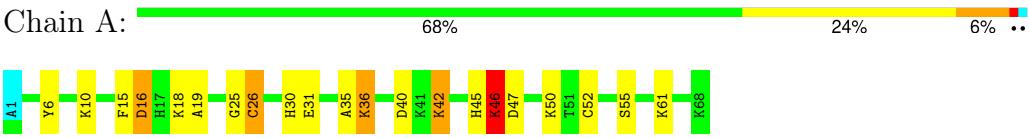
Chain A:



4.2.27 Score per residue for model 27

• Molecule 1: CYTOCHROME C7

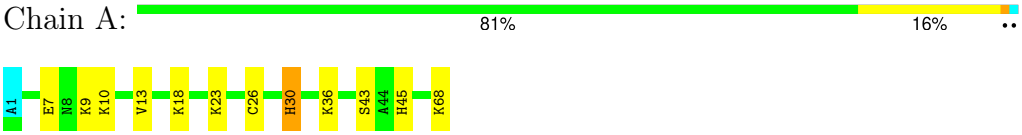
Chain A:



4.2.28 Score per residue for model 28

• Molecule 1: CYTOCHROME C7

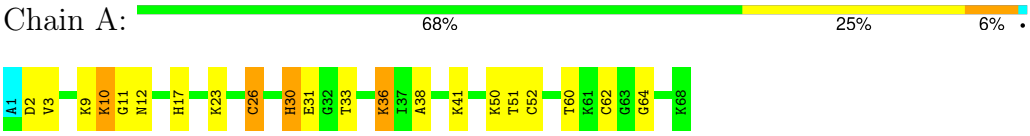
Chain A:



4.2.29 Score per residue for model 29

• Molecule 1: CYTOCHROME C7

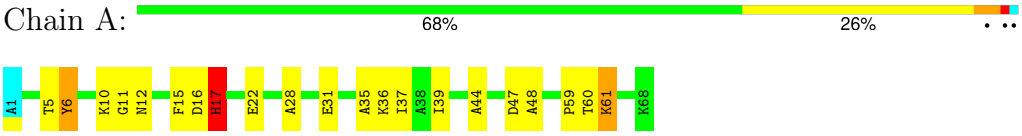
Chain A:



4.2.30 Score per residue for model 30

• Molecule 1: CYTOCHROME C7

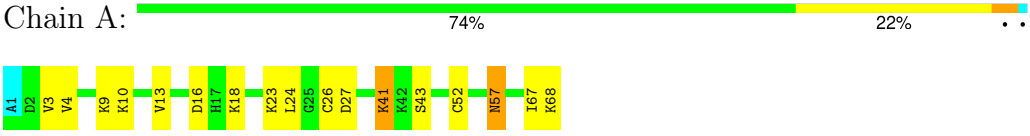
Chain A:



4.2.31 Score per residue for model 31 (medoid)

• Molecule 1: CYTOCHROME C7

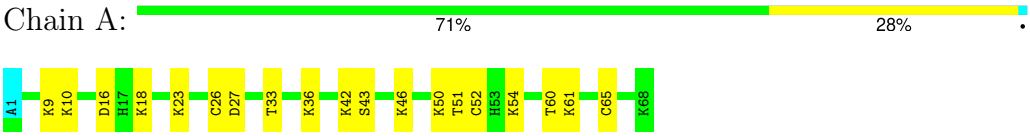
Chain A:



4.2.32 Score per residue for model 32

• Molecule 1: CYTOCHROME C7

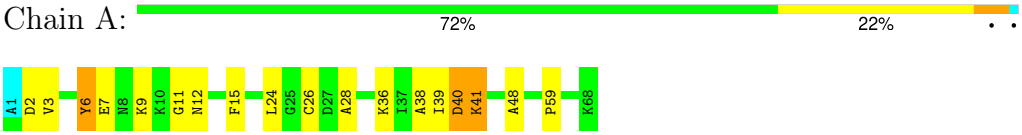
Chain A:



4.2.33 Score per residue for model 33

• Molecule 1: CYTOCHROME C7

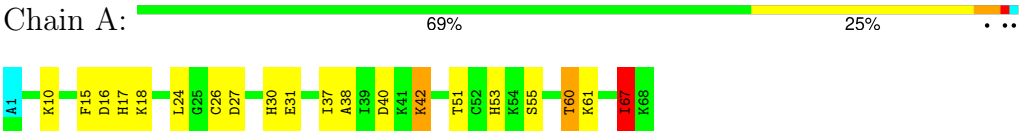
Chain A:



4.2.34 Score per residue for model 34

• Molecule 1: CYTOCHROME C7

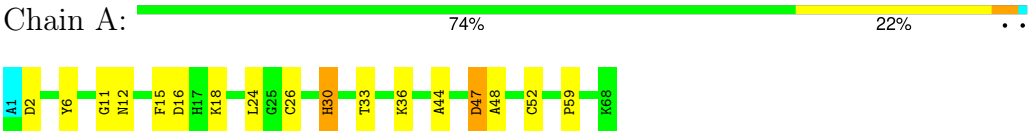
Chain A:



4.2.35 Score per residue for model 35

• Molecule 1: CYTOCHROME C7

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 35 calculated structures, 35 were deposited, based on the following criterion: *all calculated structures submitted.*

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

Software name	Classification	Version
DYANA	refinement	1.5

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	0.72±0.02	0±0/509 (0.0± 0.0%)	1.43±0.04	2±1/679 (0.3± 0.2%)
All	All	0.72	0/17815 (0.0%)	1.43	78/23765 (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	1.3±0.8
All	All	0	44

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	40	ASP	CA-CB-CG	8.94	121.54	112.60	33	3
1	A	30	HIS	CB-CG-CD2	-8.62	120.00	131.20	5	21
1	A	53	HIS	CA-CB-CG	7.94	121.74	113.80	34	3
1	A	26	CYS	CA-C-N	7.36	130.46	120.38	29	8
1	A	26	CYS	C-N-CA	7.36	130.46	120.38	29	8
1	A	47	ASP	CA-CB-CG	7.00	119.60	112.60	26	1
1	A	43	SER	CA-C-N	6.29	129.53	120.79	13	4
1	A	43	SER	C-N-CA	6.29	129.53	120.79	13	4
1	A	47	ASP	CB-CA-C	6.17	120.03	111.63	30	1
1	A	46	LYS	CA-C-N	5.86	132.72	121.54	27	1
1	A	46	LYS	C-N-CA	5.86	132.72	121.54	27	1
1	A	17	HIS	CB-CG-CD2	-5.75	123.72	131.20	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	35	ALA	CA-C-N	5.75	132.53	121.54	14	1
1	A	35	ALA	C-N-CA	5.75	132.53	121.54	14	1
1	A	45	HIS	CA-CB-CG	5.70	119.50	113.80	16	2
1	A	25	GLY	CA-C-N	5.58	132.20	121.54	27	1
1	A	25	GLY	C-N-CA	5.58	132.20	121.54	27	1
1	A	40	ASP	CA-C-N	5.30	129.82	121.56	18	1
1	A	40	ASP	C-N-CA	5.30	129.82	121.56	18	1
1	A	12	ASN	CA-CB-CG	5.27	117.87	112.60	6	1
1	A	25	GLY	N-CA-C	-5.27	105.53	111.85	25	1
1	A	17	HIS	CA-C-N	5.26	127.64	120.54	21	2
1	A	17	HIS	C-N-CA	5.26	127.64	120.54	21	2
1	A	60	THR	CA-CB-CG2	5.15	119.25	110.50	34	1
1	A	34	PRO	CA-C-N	5.14	131.37	121.54	17	1
1	A	34	PRO	C-N-CA	5.14	131.37	121.54	17	1
1	A	17	HIS	CA-CB-CG	5.05	118.85	113.80	8	1
1	A	41	LYS	CA-C-N	5.04	127.35	120.54	3	1
1	A	41	LYS	C-N-CA	5.04	127.35	120.54	3	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	30	HIS	Sidechain	17
1	A	6	TYR	Sidechain	13
1	A	59	PRO	Peptide	8
1	A	15	PHE	Sidechain,Peptide	4
1	A	47	ASP	Peptide	1
1	A	61	LYS	Peptide	1

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	500	485	485	2±1
2	A	129	96	90	2±1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	22015	20335	20125	117

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
1:A:44:ALA:HB1	2:A:71:HEC:HMD2	0.73	1.61	7	2
2:A:69:HEC:HBB3	2:A:69:HEC:HMB1	0.61	1.72	6	17
2:A:69:HEC:HBD2	2:A:69:HEC:HMD1	0.59	1.73	4	1
1:A:39:ILE:HG21	2:A:70:HEC:HBB1	0.57	1.74	22	4
2:A:69:HEC:HBB3	2:A:69:HEC:HMB3	0.53	1.80	30	9
1:A:24:LEU:HD21	2:A:70:HEC:HMD2	0.53	1.81	23	1
1:A:13:VAL:HG11	2:A:71:HEC:HMD2	0.53	1.79	14	4
1:A:6:TYR:CE1	1:A:15:PHE:CE1	0.51	2.98	4	8
1:A:24:LEU:HD13	2:A:70:HEC:HBC2	0.49	1.84	33	2
1:A:6:TYR:CZ	1:A:15:PHE:CE1	0.49	3.01	33	9
1:A:44:ALA:HA	1:A:48:ALA:HB3	0.49	1.85	35	2
1:A:52:CYS:SG	2:A:70:HEC:HMC1	0.48	2.49	11	6
1:A:8:ASN:HD21	1:A:13:VAL:HG23	0.48	1.68	14	1
2:A:71:HEC:HMB1	2:A:71:HEC:HBB3	0.48	1.85	29	3
1:A:6:TYR:CE2	1:A:15:PHE:CE1	0.47	3.02	25	5
1:A:6:TYR:CD1	1:A:15:PHE:CZ	0.47	3.02	17	1
1:A:41:LYS:NZ	2:A:71:HEC:O1A	0.47	2.47	31	2
2:A:71:HEC:CGA	2:A:71:HEC:HMA1	0.46	2.41	1	1
1:A:60:THR:HG23	1:A:61:LYS:H	0.46	1.71	30	1
1:A:10:LYS:CD	1:A:10:LYS:C	0.45	2.89	1	1
2:A:71:HEC:CBD	2:A:71:HEC:HHA	0.45	2.41	22	3
1:A:46:LYS:HD3	1:A:47:ASP:CB	0.45	2.41	26	1
1:A:40:ASP:OD2	1:A:42:LYS:NZ	0.45	2.49	27	2
1:A:40:ASP:CG	1:A:41:LYS:N	0.45	2.75	10	2
1:A:46:LYS:CD	1:A:47:ASP:HB3	0.44	2.42	26	1
1:A:40:ASP:OD2	1:A:41:LYS:NZ	0.44	2.51	14	1
1:A:6:TYR:CE2	1:A:15:PHE:CD1	0.43	3.06	19	1
1:A:13:VAL:CG1	2:A:71:HEC:HMD2	0.43	2.43	31	1
1:A:23:LYS:NZ	2:A:70:HEC:CGD	0.43	2.82	31	1
1:A:8:ASN:ND2	1:A:13:VAL:HG23	0.42	2.30	7	1
1:A:36:LYS:NZ	2:A:69:HEC:O2D	0.42	2.52	7	3
1:A:10:LYS:NZ	2:A:71:HEC:O1A	0.42	2.51	29	2
1:A:22:GLU:OE2	1:A:23:LYS:NZ	0.42	2.53	17	1
1:A:36:LYS:NZ	2:A:69:HEC:O1D	0.42	2.53	29	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:LYS:NZ	1:A:68:LYS:C	0.42	2.78	19	1
2:A:71:HEC:HMA3	2:A:71:HEC:CGA	0.41	2.45	24	1
1:A:36:LYS:CE	2:A:69:HEC:CGD	0.41	2.98	32	1
1:A:67:ILE:HD12	1:A:67:ILE:H	0.41	1.75	34	1
1:A:23:LYS:NZ	2:A:70:HEC:O1D	0.41	2.53	29	1
1:A:6:TYR:CD2	2:A:71:HEC:HMD2	0.41	2.51	21	1
1:A:10:LYS:NZ	2:A:71:HEC:O2A	0.41	2.53	18	1
1:A:41:LYS:NZ	2:A:71:HEC:O1D	0.41	2.51	14	1
2:A:69:HEC:HBB3	2:A:69:HEC:CMB	0.41	2.46	11	3
1:A:45:HIS:CD2	1:A:50:LYS:NZ	0.41	2.89	27	1
2:A:69:HEC:CMD	2:A:69:HEC:HBD2	0.41	2.45	34	1
1:A:16:ASP:CB	1:A:19:ALA:HB3	0.40	2.46	27	1
1:A:39:ILE:HD12	1:A:48:ALA:HB2	0.40	1.93	33	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	66/68 (97%)	38±3 (57±5%)	21±3 (32±4%)	7±2 (11±4%)	1	8
All	All	2310/2380 (97%)	1325 (57%)	741 (32%)	244 (11%)	1	8

All 37 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	26	CYS	31
1	A	36	LYS	25
1	A	11	GLY	15
1	A	38	ALA	15
1	A	2	ASP	12
1	A	61	LYS	9
1	A	31	GLU	9
1	A	3	VAL	9
1	A	37	ILE	8

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Mol	Chain	Res	Type	Models (Total)
1	A	35	ALA	7
1	A	7	GLU	7
1	A	12	ASN	7
1	A	55	SER	7
1	A	33	THR	7
1	A	48	ALA	7
1	A	42	LYS	6
1	A	39	ILE	6
1	A	27	ASP	5
1	A	54	LYS	5
1	A	47	ASP	5
1	A	64	GLY	5
1	A	67	ILE	5
1	A	62	CYS	4
1	A	41	LYS	4
1	A	34	PRO	3
1	A	56	ASN	3
1	A	60	THR	3
1	A	28	ALA	3
1	A	53	HIS	2
1	A	44	ALA	2
1	A	46	LYS	2
1	A	51	THR	1
1	A	17	HIS	1
1	A	8	ASN	1
1	A	16	ASP	1
1	A	57	ASN	1
1	A	65	CYS	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	54/54 (100%)	48±2 (89±5%)	6±2 (11±5%)	8 50
All	All	1890/1890 (100%)	1674 (89%)	216 (11%)	8 50

All 38 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	10	LYS	19
1	A	18	LYS	15
1	A	60	THR	12
1	A	50	LYS	11
1	A	41	LYS	11
1	A	9	LYS	10
1	A	68	LYS	10
1	A	36	LYS	9
1	A	16	ASP	9
1	A	46	LYS	9
1	A	52	CYS	9
1	A	42	LYS	7
1	A	17	HIS	7
1	A	54	LYS	6
1	A	37	ILE	6
1	A	51	THR	6
1	A	24	LEU	5
1	A	8	ASN	5
1	A	40	ASP	5
1	A	61	LYS	5
1	A	57	ASN	4
1	A	31	GLU	4
1	A	5	THR	3
1	A	27	ASP	3
1	A	23	LYS	3
1	A	45	HIS	3
1	A	22	GLU	3
1	A	43	SER	3
1	A	39	ILE	2
1	A	2	ASP	2
1	A	7	GLU	2
1	A	62	CYS	2
1	A	3	VAL	1
1	A	13	VAL	1
1	A	53	HIS	1
1	A	4	VAL	1
1	A	67	ILE	1
1	A	47	ASP	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.6 Ligand geometry (i)

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	70	1	50,50,50	1.15±0.03	5±1 (9±1%)
2	HEC	A	69	1	50,50,50	1.12±0.02	5±1 (9±1%)
2	HEC	A	71	1	50,50,50	1.19±0.04	5±1 (10±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	70	1	68,82,82	1.69±0.03	14±1 (21±1%)
2	HEC	A	69	1	68,82,82	1.69±0.04	15±2 (21±2%)
2	HEC	A	71	1	68,82,82	1.70±0.06	15±2 (21±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	70	1	1±0,1,7,7	0±0,14,54,54	-
2	HEC	A	71	1	1±0,1,7,7	0±0,14,54,54	-
2	HEC	A	69	1	1±0,1,7,7	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	71	HEC	FE-NC	4.88	2.11	1.95	27	35
2	A	70	HEC	FE-NC	4.23	2.09	1.95	9	29
2	A	70	HEC	FE-ND	3.95	2.07	1.94	4	35
2	A	71	HEC	FE-ND	3.90	2.06	1.94	14	31
2	A	71	HEC	FE-NB	3.82	2.06	1.94	23	32
2	A	70	HEC	FE-NB	3.73	2.06	1.94	17	16
2	A	69	HEC	FE-ND	3.71	2.06	1.94	21	32
2	A	70	HEC	C1D-ND	3.43	1.34	1.40	33	26
2	A	69	HEC	FE-NA	3.12	2.05	1.95	30	29
2	A	71	HEC	C1C-NC	3.09	1.33	1.39	29	31
2	A	69	HEC	FE-NB	3.05	2.04	1.94	19	9
2	A	69	HEC	C1D-ND	3.03	1.35	1.40	17	31
2	A	71	HEC	C4B-NB	2.97	1.35	1.40	4	23
2	A	70	HEC	FE-NA	2.80	2.04	1.95	13	18
2	A	69	HEC	FE-NC	2.78	2.04	1.95	14	17
2	A	71	HEC	C1D-ND	2.71	1.35	1.40	22	16
2	A	71	HEC	FE-NA	2.67	2.04	1.95	13	4
2	A	70	HEC	C1C-NC	2.56	1.34	1.39	30	15
2	A	70	HEC	C4C-NC	2.55	1.34	1.39	33	2
2	A	69	HEC	C4A-NA	2.40	1.35	1.39	16	25
2	A	70	HEC	C4B-NB	2.33	1.36	1.40	11	18
2	A	69	HEC	C1C-NC	2.21	1.35	1.39	5	12
2	A	71	HEC	C4A-NA	2.14	1.35	1.39	1	9
2	A	69	HEC	C4B-NB	2.12	1.36	1.40	33	4
2	A	71	HEC	C4C-NC	2.09	1.35	1.39	7	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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	70	HEC	CHB-C1B-NB	4.87	129.66	124.42	13	35
2	A	69	HEC	CHD-C1D-ND	4.79	130.29	124.37	17	35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	71	HEC	CHD-C1D-ND	4.65	130.12	124.37	7	35
2	A	71	HEC	CHB-C4A-NA	4.64	129.51	124.45	7	35
2	A	69	HEC	CHA-C4D-ND	4.56	129.34	124.42	33	35
2	A	71	HEC	CHB-C1B-NB	4.50	129.26	124.42	13	35
2	A	70	HEC	CHD-C1D-ND	4.27	129.65	124.37	30	35
2	A	70	HEC	CHA-C4D-ND	4.22	128.97	124.42	11	35
2	A	71	HEC	CHA-C1A-NA	4.21	129.04	124.45	10	35
2	A	70	HEC	CHA-C1A-NA	4.16	128.98	124.45	21	35
2	A	70	HEC	CHB-C4A-NA	4.16	128.98	124.45	24	35
2	A	69	HEC	CHB-C4A-NA	4.13	128.95	124.45	2	35
2	A	69	HEC	CHB-C1B-NB	4.09	128.82	124.42	3	35
2	A	71	HEC	CHA-C4D-ND	4.07	128.81	124.42	35	29
2	A	70	HEC	C1D-ND-C4D	4.05	110.00	105.21	29	35
2	A	71	HEC	CAD-C3D-C4D	4.02	131.70	124.70	19	11
2	A	69	HEC	C4B-NB-C1B	4.02	109.97	105.21	33	35
2	A	71	HEC	C1D-ND-C4D	4.00	109.94	105.21	23	35
2	A	69	HEC	CAD-C3D-C4D	3.99	131.65	124.70	32	1
2	A	70	HEC	CHC-C4B-NB	3.98	129.29	124.37	6	35
2	A	69	HEC	CBD-CAD-C3D	3.93	123.40	112.53	32	9
2	A	69	HEC	C1D-ND-C4D	3.87	109.78	105.21	27	35
2	A	70	HEC	C4B-NB-C1B	3.81	109.72	105.21	33	35
2	A	71	HEC	C4B-NB-C1B	3.72	109.62	105.21	20	35
2	A	71	HEC	CHC-C4B-NB	3.71	128.96	124.37	11	35
2	A	69	HEC	CHA-C1A-NA	3.69	128.47	124.45	21	35
2	A	71	HEC	CAD-C3D-C2D	3.26	121.75	127.87	19	9
2	A	69	HEC	CAD-C3D-C2D	3.18	121.91	127.87	32	1
2	A	71	HEC	C3D-C4D-ND	3.15	107.31	110.35	23	26
2	A	71	HEC	C2A-C1A-NA	3.09	107.34	110.32	2	33
2	A	70	HEC	CHC-C1C-NC	3.07	129.42	123.86	29	34
2	A	71	HEC	CHC-C1C-NC	3.00	129.31	123.86	5	35
2	A	71	HEC	O1D-CGD-CBD	2.95	113.72	123.09	2	5
2	A	71	HEC	CBD-CAD-C3D	2.89	120.52	112.53	19	5
2	A	70	HEC	C3D-C4D-ND	2.88	107.57	110.35	28	35
2	A	70	HEC	C2A-C1A-NA	2.86	107.57	110.32	14	34
2	A	69	HEC	C2A-C1A-NA	2.85	107.58	110.32	24	22
2	A	69	HEC	CHC-C4B-NB	2.80	127.83	124.37	10	34
2	A	70	HEC	CHD-C4C-NC	2.77	128.88	123.86	2	34
2	A	69	HEC	CAB-C3B-C4B	2.77	128.39	124.79	25	1
2	A	69	HEC	O1D-CGD-CBD	2.76	114.33	123.09	17	7
2	A	69	HEC	CAD-CBD-CGD	2.71	106.49	113.67	28	7
2	A	71	HEC	CHD-C4C-NC	2.70	128.76	123.86	32	35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	70	HEC	CBC-CAC-C3C	2.69	119.70	112.42	33	1
2	A	69	HEC	CHC-C1C-NC	2.68	128.73	123.86	9	35
2	A	71	HEC	O1A-CGA-CBA	2.59	114.86	123.09	15	8
2	A	69	HEC	CHD-C4C-NC	2.55	128.49	123.86	25	31
2	A	71	HEC	CMC-C2C-C3C	2.53	131.00	125.62	4	4
2	A	70	HEC	C4A-NA-C1A	2.53	109.94	105.82	14	28
2	A	71	HEC	O2D-CGD-CBD	2.48	121.83	114.00	15	2
2	A	71	HEC	C4A-NA-C1A	2.47	109.85	105.82	7	35
2	A	69	HEC	C3B-C4B-NB	2.43	107.51	110.17	16	17
2	A	69	HEC	O2D-CGD-CBD	2.39	121.55	114.00	4	2
2	A	69	HEC	C4C-NC-C1C	2.38	109.70	105.82	6	30
2	A	70	HEC	C4A-CHB-C1B	2.36	120.99	126.02	30	18
2	A	71	HEC	CBA-CAA-C2A	2.36	119.06	112.53	1	1
2	A	69	HEC	C4C-CHD-C1D	2.34	120.74	126.25	6	4
2	A	71	HEC	C4A-CHB-C1B	2.29	121.14	126.02	15	8
2	A	70	HEC	C3B-C4B-NB	2.29	107.66	110.17	33	2
2	A	71	HEC	CAD-CBD-CGD	2.29	107.59	113.67	35	1
2	A	69	HEC	C4A-NA-C1A	2.28	109.54	105.82	27	18
2	A	69	HEC	C4A-CHB-C1B	2.28	121.17	126.02	6	3
2	A	71	HEC	CMD-C2D-C1D	2.28	128.60	125.03	25	6
2	A	70	HEC	CAC-C3C-C2C	2.26	130.47	126.89	33	1
2	A	69	HEC	CMA-C3A-C4A	2.26	128.71	124.73	4	2
2	A	70	HEC	C4C-NC-C1C	2.26	109.50	105.82	13	15
2	A	69	HEC	C3D-C4D-ND	2.25	108.18	110.35	24	11
2	A	69	HEC	C3C-C4C-NC	2.23	107.68	110.15	30	6
2	A	69	HEC	O1A-CGA-CBA	2.22	116.04	123.09	4	4
2	A	71	HEC	CHC-C1C-C2C	2.22	120.97	127.43	4	9
2	A	69	HEC	C1A-CHA-C4D	2.21	121.31	126.02	34	15
2	A	69	HEC	CHA-C4D-C3D	2.21	121.56	124.77	33	4
2	A	71	HEC	C4C-NC-C1C	2.20	109.40	105.82	13	2
2	A	71	HEC	CAA-C2A-C3A	2.19	123.77	127.87	19	3
2	A	69	HEC	C2D-C1D-ND	2.18	107.33	109.84	27	2
2	A	71	HEC	O2D-CGD-O1D	2.18	128.94	123.33	23	1
2	A	71	HEC	C3C-C4C-NC	2.17	107.75	110.15	5	2
2	A	69	HEC	CHD-C1D-C2D	2.16	120.81	126.95	17	1
2	A	70	HEC	O1A-CGA-CBA	2.15	116.28	123.09	7	5
2	A	70	HEC	O2D-CGD-CBD	2.13	120.73	114.00	26	2
2	A	70	HEC	C1A-CHA-C4D	2.13	121.49	126.02	33	1
2	A	70	HEC	O1D-CGD-CBD	2.12	116.37	123.09	28	2
2	A	70	HEC	C1C-CHC-C4B	2.11	121.28	126.25	33	1
2	A	70	HEC	CAD-C3D-C4D	2.10	128.36	124.70	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	71	HEC	C4C-CHD-C1D	2.09	121.33	126.25	21	3
2	A	70	HEC	CHB-C1B-C2B	2.08	121.74	125.03	13	1
2	A	70	HEC	CHD-C1D-C2D	2.08	121.03	126.95	33	1
2	A	71	HEC	CMA-C3A-C4A	2.08	128.39	124.73	8	2
2	A	70	HEC	CMD-C2D-C1D	2.07	128.27	125.03	4	1
2	A	69	HEC	CMD-C2D-C1D	2.06	128.25	125.03	27	1
2	A	70	HEC	C3C-C4C-NC	2.03	107.89	110.15	7	2
2	A	70	HEC	C4C-CHD-C1D	2.03	121.46	126.25	19	1
2	A	71	HEC	CAC-C3C-C4C	2.03	127.71	124.91	21	1
2	A	69	HEC	CAA-C2A-C3A	2.02	124.08	127.87	24	1
2	A	71	HEC	CHD-C1D-C2D	2.02	121.20	126.95	7	1

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

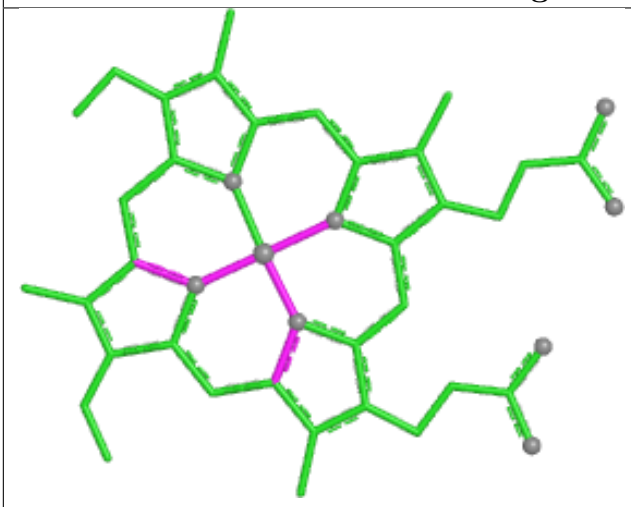
Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	69	HEC	NA	35
2	A	70	HEC	NA	35
2	A	71	HEC	NA	35

There are no torsion outliers.

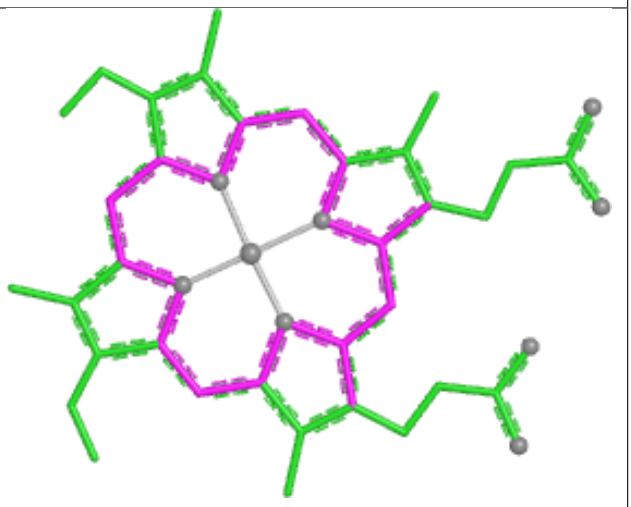
There are no ring outliers.

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 then 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.

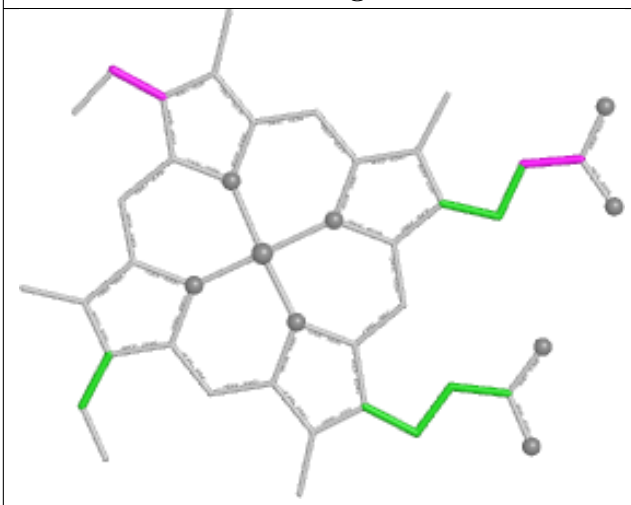
Ligand HEC A 70



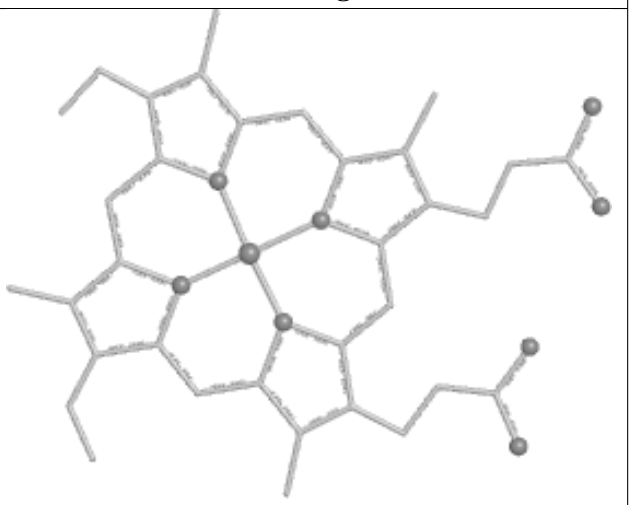
Bond lengths



Bond angles

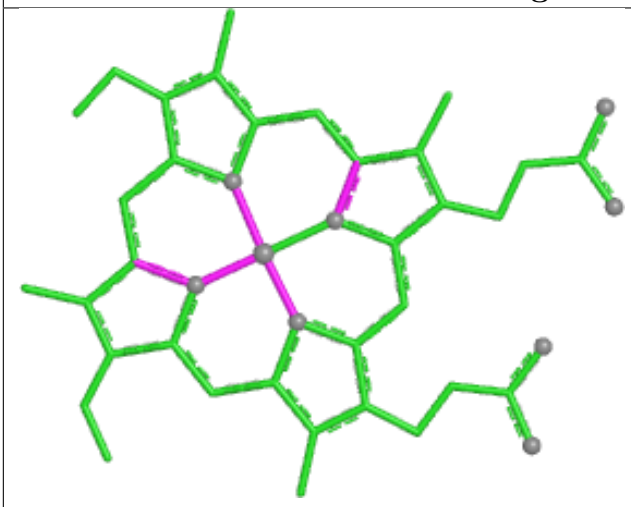


Torsions

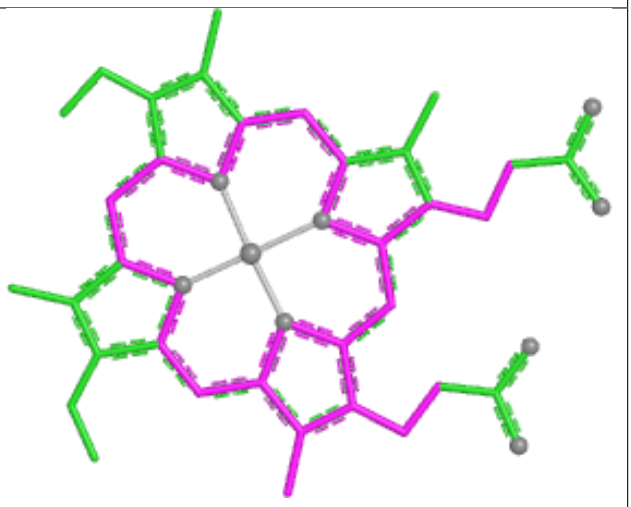


Rings

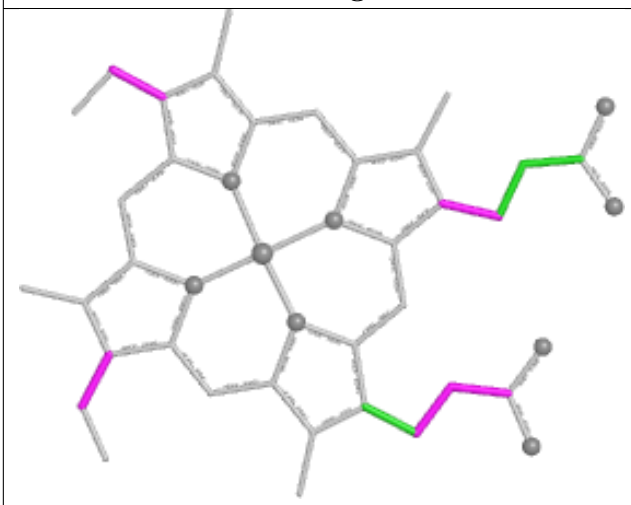
Ligand HEC A 71



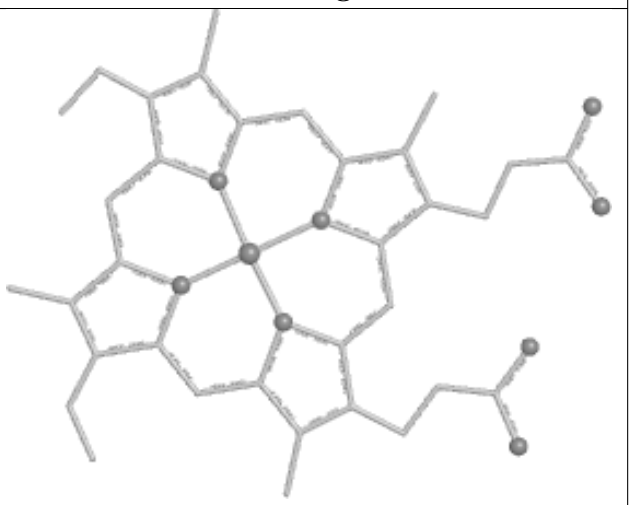
Bond lengths



Bond angles

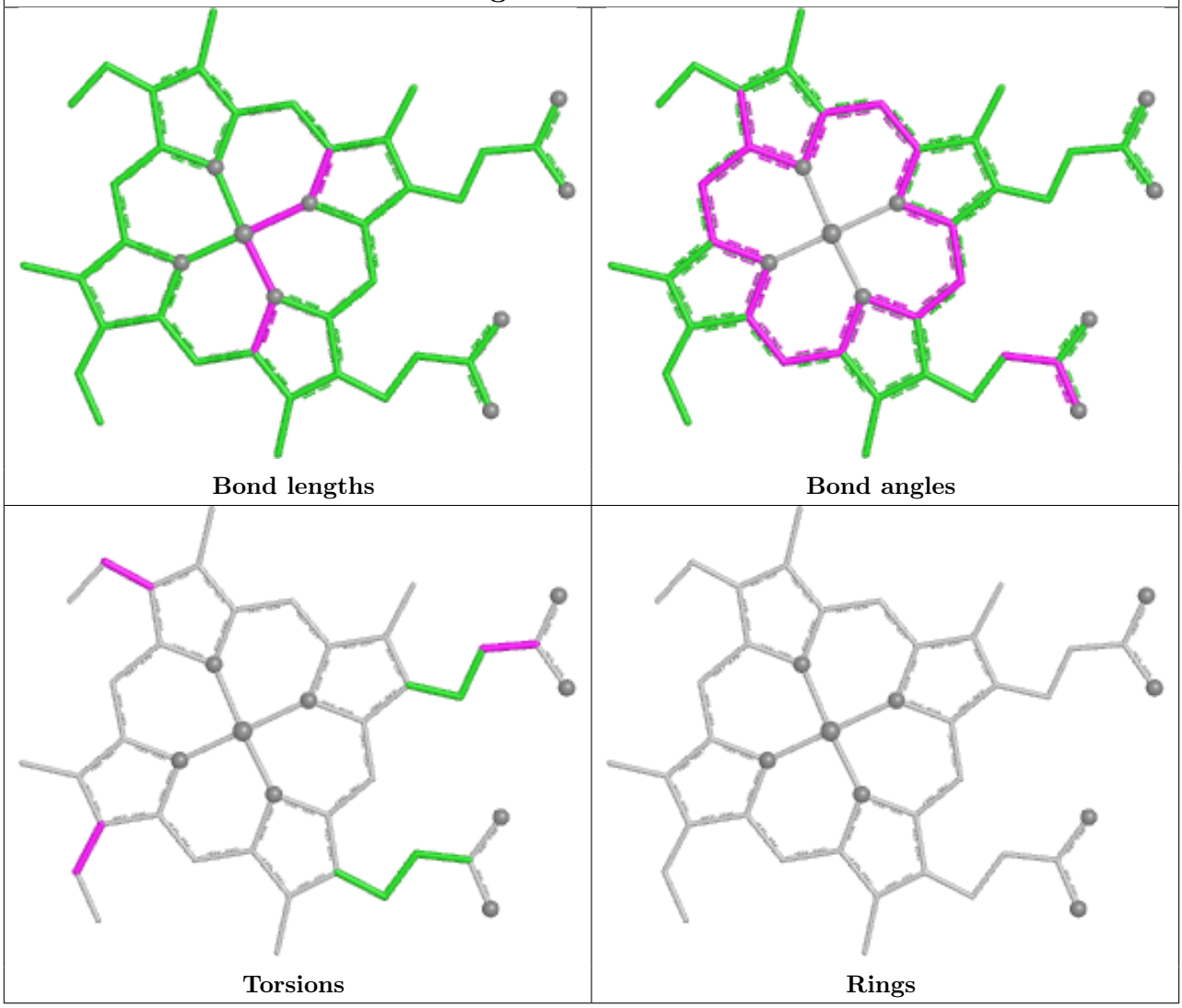


Torsions



Rings

Ligand HEC A 69



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