Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2JQR
Title	:	Solution model of crosslinked complex of cytochrome c and adrenodoxin
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Deposited on	:	2007-06-07

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:

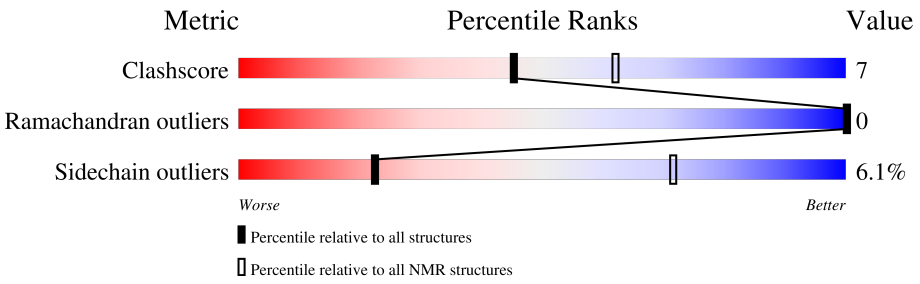
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	108	70% 27% • •
2	B	105	82% 15% • •

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 1 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:-4-A:103 (108)	0.00	1
2	B:6-B:108 (103)	0.00	5

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. No single-model clusters were found.

Cluster number	Models
1	1, 3, 5, 7
2	4, 10
3	2, 9
4	6, 8

3 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3339 atoms, of which 1653 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	108	1693	533	846	151	158	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	CYS	VAL	engineered mutation	UNP P00044
A	102	THR	CYS	engineered mutation	UNP P00044

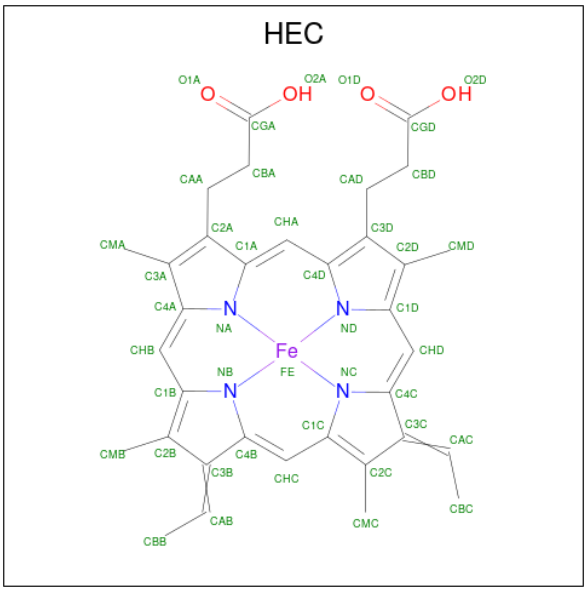
- Molecule 2 is a protein called Adrenodoxin, mitochondrial.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	103	1567	489	775	134	161	8	0

There are 2 discrepancies between the modelled and reference sequences:

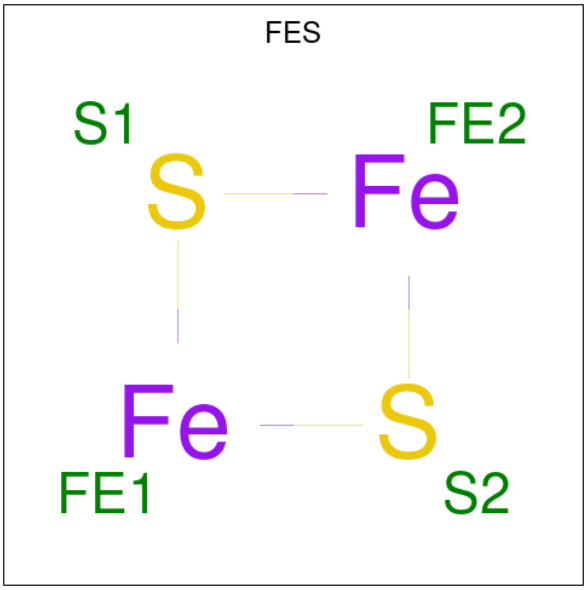
Chain	Residue	Modelled	Actual	Comment	Reference
B	80	CYS	LEU	engineered mutation	UNP P00257
B	95	SER	CYS	engineered mutation	UNP P00257

- Molecule 3 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
3	A	1	75	34	1	32	4	4

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms		
			Total	Fe	S
4	B	1	4	2	2

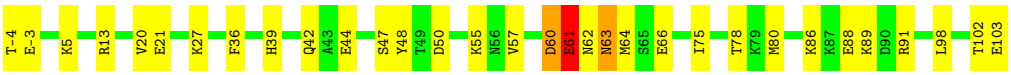
4 Residue-property plots (i)

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 c iso-1

Chain A:



• Molecule 2: Adrenodoxin, mitochondrial

Chain B:

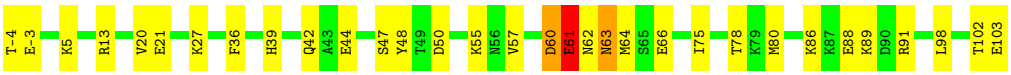
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Cytochrome c iso-1

Chain A:



• Molecule 2: Adrenodoxin, mitochondrial

Chain B:

4.2.2 Score per residue for model 2

- Molecule 1: Cytochrome c iso-1

Chain A: 69% 29%

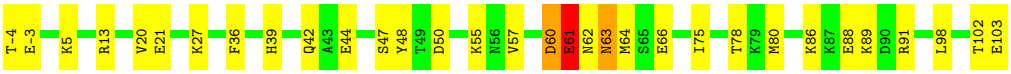
- Molecule 2: Adrenodoxin, mitochondrial

Chain B: 81% 16%

4.2.3 Score per residue for model 3

- Molecule 1: Cytochrome c iso-1

Chain A: 70% 27%



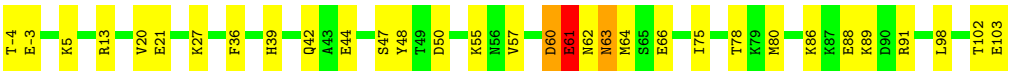
- Molecule 2: Adrenodoxin, mitochondrial

Chain B: 82% 15%

4.2.4 Score per residue for model 4

- Molecule 1: Cytochrome c iso-1

Chain A: 70% 27%



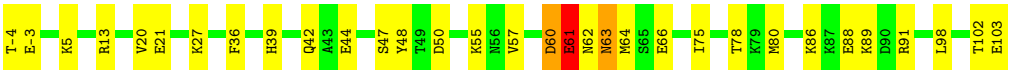
- Molecule 2: Adrenodoxin, mitochondrial

Chain B: 82% 15%

4.2.5 Score per residue for model 5

- Molecule 1: Cytochrome c iso-1

Chain A: 70% 27%



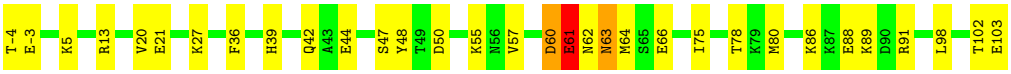
- Molecule 2: Adrenodoxin, mitochondrial

Chain B: 82% 15%

4.2.6 Score per residue for model 6

- Molecule 1: Cytochrome c iso-1

Chain A: 70% 27%



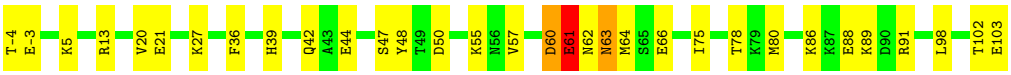
- Molecule 2: Adrenodoxin, mitochondrial

Chain B: 82% 15%

4.2.7 Score per residue for model 7

- Molecule 1: Cytochrome c iso-1

Chain A: 70% 27%



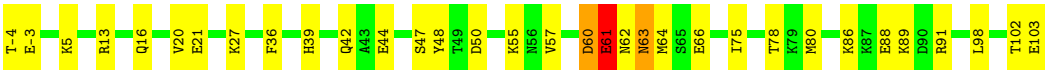
- Molecule 2: Adrenodoxin, mitochondrial

Chain B: 82% 15%

4.2.8 Score per residue for model 8

- Molecule 1: Cytochrome c iso-1

Chain A: 69% 28% • •



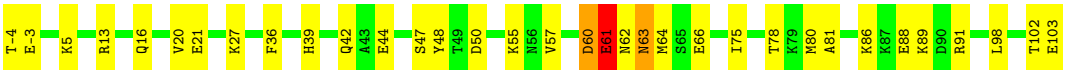
- Molecule 2: Adrenodoxin, mitochondrial

Chain B: 81% 16% • •

4.2.9 Score per residue for model 9

- Molecule 1: Cytochrome c iso-1

Chain A: 69% 29% • •



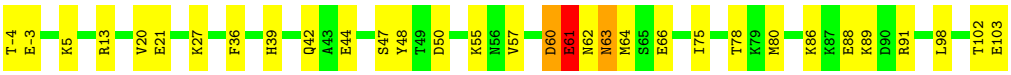
- Molecule 2: Adrenodoxin, mitochondrial

Chain B: 81% 16% • •

4.2.10 Score per residue for model 10

- Molecule 1: Cytochrome c iso-1

Chain A: 70% 27% • •



- Molecule 2: Adrenodoxin, mitochondrial

Chain B: 82% 15% • •

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular dynamics*.

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

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

Software name	Classification	Version
X-PLOR NIH	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.46±0.00	9±0/865 (1.0± 0.0%)	1.97±0.00	21±0/1156 (1.8± 0.0%)
2	B	0.60±0.00	0±0/800 (0.0± 0.0%)	0.77±0.00	0±0/1078 (0.0± 0.0%)
All	All	1.13	90/16650 (0.5%)	1.52	210/22340 (0.9%)

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
1	A	21	GLU	CD-OE2	6.95	1.33	1.25	1	10
1	A	88	GLU	CD-OE2	6.88	1.33	1.25	1	10
1	A	66	GLU	CD-OE2	6.37	1.32	1.25	1	10
1	A	47	SER	CA-CB	6.18	1.62	1.52	1	10
1	A	88	GLU	CD-OE1	-6.02	1.19	1.25	1	10
1	A	61	GLU	CD-OE1	5.94	1.32	1.25	1	10
1	A	-3	GLU	CD-OE1	5.89	1.32	1.25	1	10
1	A	103	GLU	CD-OE1	5.88	1.32	1.25	1	10
1	A	44	GLU	CD-OE2	5.57	1.31	1.25	1	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	91	ARG	NE-CZ-NH1	7.71	124.15	120.30	1	10
1	A	50	ASP	O-C-N	7.39	134.52	122.70	1	10
1	A	48	TYR	CB-CG-CD1	-7.07	116.76	121.00	1	10
1	A	66	GLU	CA-CB-CG	6.94	128.68	113.40	1	10
1	A	20	VAL	CA-CB-CG1	6.84	121.17	110.90	1	10
1	A	50	ASP	CB-CG-OD2	6.39	124.05	118.30	1	10
1	A	60	ASP	CB-CG-OD1	6.12	123.81	118.30	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	44	GLU	CA-CB-CG	6.01	126.61	113.40	1	10
1	A	61	GLU	O-C-N	-5.86	113.32	122.70	1	10
1	A	42	GLN	CB-CG-CD	5.82	126.72	111.60	1	10
1	A	13	ARG	NE-CZ-NH2	-5.80	117.40	120.30	1	10
1	A	21	GLU	OE1-CD-OE2	5.67	130.11	123.30	1	10
1	A	-3	GLU	OE1-CD-OE2	5.56	129.98	123.30	1	10
1	A	63	ASN	CA-C-N	-5.47	105.18	117.20	1	10
1	A	61	GLU	CG-CD-OE1	-5.33	107.64	118.30	1	10
1	A	27	LYS	CB-CA-C	5.28	120.95	110.40	1	10
1	A	44	GLU	N-CA-CB	5.27	120.08	110.60	1	10
1	A	61	GLU	CG-CD-OE2	5.26	128.83	118.30	1	10
1	A	64	MET	CA-CB-CG	-5.24	104.39	113.30	1	10
1	A	44	GLU	OE1-CD-OE2	5.10	129.43	123.30	1	10
1	A	80	MET	O-C-N	5.05	130.79	122.70	1	10

There are no chirality outliers.

There are no planarity outliers.

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	847	846	846	15±1
2	B	792	775	774	8±1
3	A	43	32	30	1±0
All	All	16860	16530	16500	225

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:LEU:O	1:A:102:THR:HG22	1.00	1.54	1	10
1:A:36:PHE:CD2	1:A:102:THR:HG21	0.72	2.20	1	10
1:A:55:LYS:HG3	1:A:57:VAL:CG2	0.62	2.24	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:PHE:HD2	1:A:102:THR:HG21	0.59	1.57	1	10
1:A:81:ALA:CB	2:B:51:ALA:HA	0.59	2.27	9	2
1:A:55:LYS:HG3	1:A:57:VAL:HG23	0.58	1.73	1	10
1:A:16:GLN:NE2	2:B:52:CYS:HB2	0.57	2.15	2	2
1:A:98:LEU:O	1:A:102:THR:CG2	0.54	2.45	1	10
1:A:-4:THR:HG21	1:A:61:GLU:OE2	0.53	2.04	1	10
2:B:52:CYS:O	2:B:77:MET:HG3	0.52	2.05	3	10
2:B:26:GLY:C	2:B:95:SER:OG	0.52	2.48	1	10
1:A:60:ASP:OD1	1:A:62:ASN:N	0.49	2.44	1	10
1:A:39:HIS:HA	1:A:57:VAL:O	0.48	2.09	1	10
2:B:26:GLY:C	2:B:95:SER:HG	0.48	2.12	5	5
2:B:32:VAL:O	2:B:36:ASN:ND2	0.46	2.49	1	10
1:A:86:LYS:N	1:A:86:LYS:HD3	0.45	2.27	1	10
1:A:60:ASP:OD1	1:A:60:ASP:C	0.44	2.56	1	10
1:A:55:LYS:CG	1:A:57:VAL:CG2	0.44	2.94	1	10
2:B:77:MET:HB3	2:B:90:LEU:HD11	0.42	1.91	6	10
1:A:36:PHE:CE2	1:A:102:THR:HG21	0.42	2.49	1	10
2:B:13:ASN:HB3	2:B:15:ASP:OD1	0.42	2.15	1	10
1:A:16:GLN:NE2	2:B:51:ALA:O	0.42	2.51	8	1
1:A:75:ILE:O	1:A:78:THR:HG22	0.42	2.15	1	10
2:B:56:HIS:CE1	2:B:108:PRO:HG3	0.42	2.50	2	10
2:B:26:GLY:O	2:B:95:SER:OG	0.41	2.39	4	4
3:A:104:HEC:HMC1	3:A:104:HEC:HBC3	0.41	1.91	1	10
1:A:16:GLN:NE2	2:B:52:CYS:CB	0.40	2.84	2	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	106/108 (98%)	103±0 (97±0%)	3±0 (3±0%)	0±0 (0±0%)	100	100
2	B	101/105 (96%)	101±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	2070/2130 (97%)	2040 (99%)	30 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	89/89 (100%)	85±0 (96±0%)	4±0 (4±0%)	31	80
2	B	90/92 (98%)	83±0 (92±0%)	7±0 (8±0%)	16	64
All	All	1790/1810 (99%)	1680 (94%)	110 (6%)	22	71

All 11 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	5	LYS	10
1	A	61	GLU	10
1	A	63	ASN	10
1	A	89	LYS	10
2	B	6	LYS	10
2	B	14	ARG	10
2	B	19	LEU	10
2	B	24	LYS	10
2	B	25	ILE	10
2	B	77	MET	10
2	B	80	CYS	10

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	HEC	A	104	1	32,50,50	1.99±0.00	9±0 (28±0%)
4	FES	B	109	2	0,4,4	0.00±0.00	-

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	HEC	A	104	1	24,82,82	1.90±0.00	7±0 (29±0%)
4	FES	B	109	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
3	HEC	A	104	1	-	0±0,10,54,54	-
4	FES	B	109	2	-	-	0±0,1,1,1

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
3	A	104	HEC	C3C-C2C	5.17	1.35	1.40	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	104	HEC	C2B-C3B	4.47	1.36	1.40	1	10
3	A	104	HEC	CMD-C2D	4.07	1.60	1.51	1	10
3	A	104	HEC	CMA-C3A	2.72	1.58	1.51	1	10
3	A	104	HEC	C2A-C1A	2.72	1.48	1.42	1	10
3	A	104	HEC	CMB-C2B	2.58	1.57	1.51	1	10
3	A	104	HEC	CAD-C3D	2.35	1.55	1.52	1	10
3	A	104	HEC	C1D-CHD	2.14	1.35	1.41	1	10
3	A	104	HEC	C1C-CHC	2.04	1.46	1.41	1	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	104	HEC	CMB-C2B-C1B	4.69	121.26	128.46	1	10
3	A	104	HEC	C2B-C3B-C4B	3.34	102.75	106.35	1	10
3	A	104	HEC	O1A-CGA-CBA	2.92	113.69	123.08	1	10
3	A	104	HEC	C4C-C3C-C2C	2.44	108.99	106.35	1	10
3	A	104	HEC	CMC-C2C-C3C	2.36	128.60	125.82	1	10
3	A	104	HEC	O2A-CGA-CBA	2.05	120.61	114.03	1	10
3	A	104	HEC	CBA-CAA-C2A	2.05	109.16	112.60	1	10

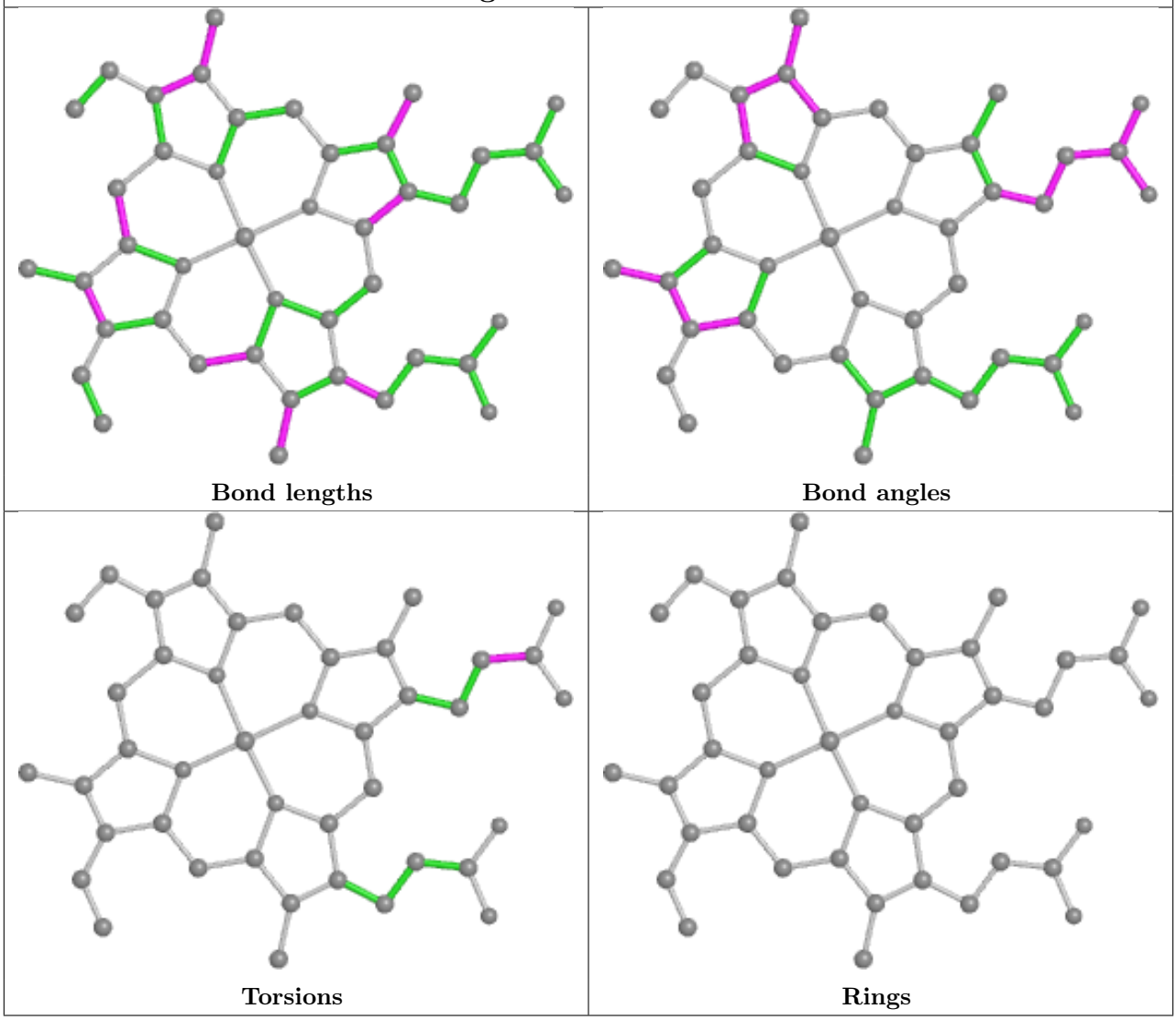
There are no chirality outliers.

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 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 104



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