Full wwPDB NMR Structure Validation Report (i)

Feb 19, 2022 – 09:13 PM EST

PDB ID	:	1TKW
Title	:	The transient complex of poplar plastocyanin with turnip cytochrome f determined with paramagnetic NMR
Authors	:	Lange, C.; Cornvik, T.; Diaz-Moreno, I.; Ubbink, M.
Deposited on	:	2004-06-09

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

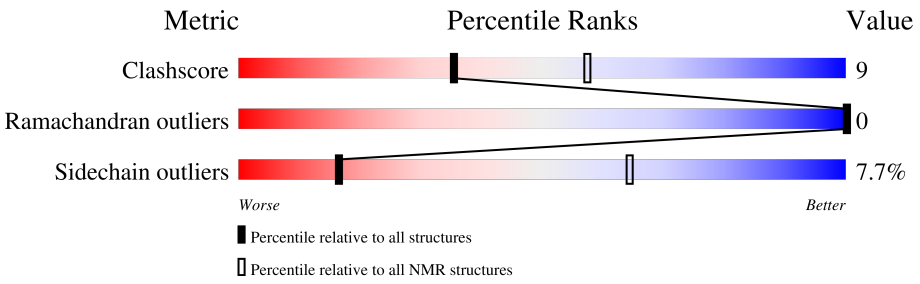
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	99	79% 20% •
2	B	252	84% 14% ••

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:1-A:99 (99)	0.02	3
2	B:1-B:250 (250)	0.02	6

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 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5396 atoms, of which 2690 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Plastocyanin A.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	99	1442	466	704	116	153	3	0

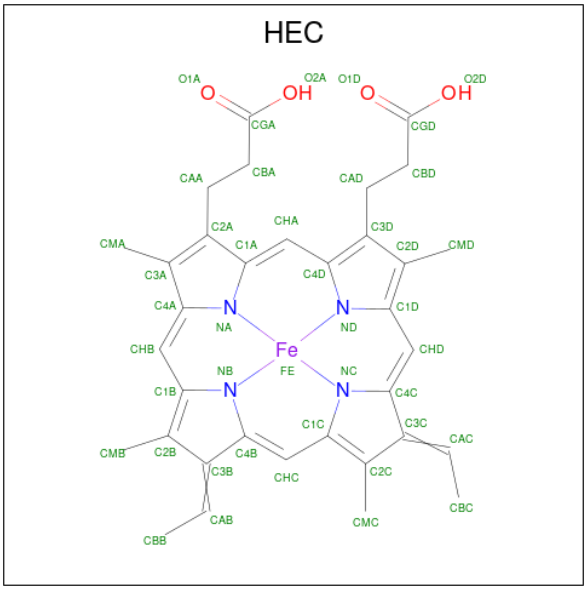
- Molecule 2 is a protein called Cytochrome f.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	250	3878	1226	1954	330	364	4	0

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	
			Total	Cu
3	A	1	1	1

- Molecule 4 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

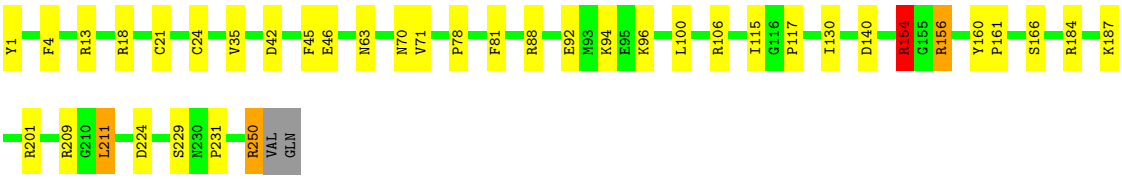
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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: Plastocyanin A

Chain A: 79% 20% •

• Molecule 2: Cytochrome f

Chain B: 84% 14% ••



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

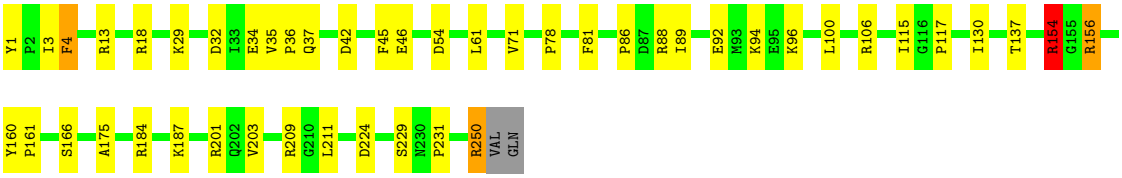
4.2.1 Score per residue for model 1

• Molecule 1: Plastocyanin A

Chain A: 77% 22% •

• Molecule 2: Cytochrome f

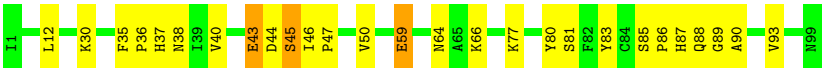
Chain B: 81% 17% ••



4.2.2 Score per residue for model 2

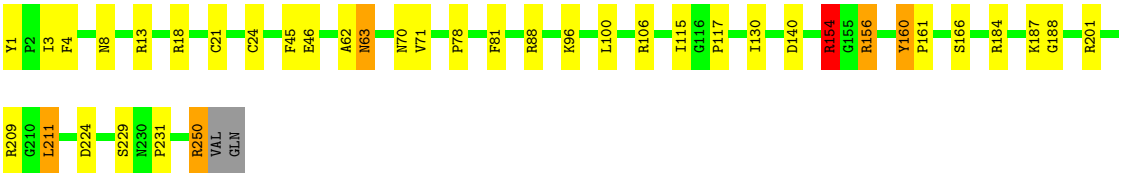
- Molecule 1: Plastocyanin A

Chain A:



- Molecule 2: Cytochrome f

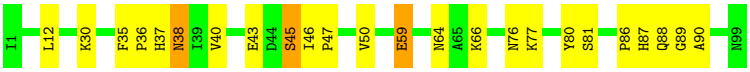
Chain B:



4.2.3 Score per residue for model 3

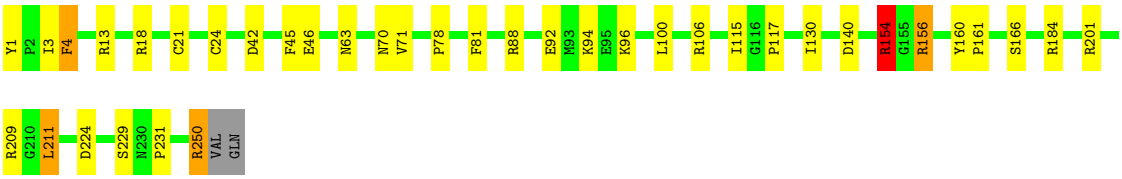
- Molecule 1: Plastocyanin A

Chain A:



- Molecule 2: Cytochrome f

Chain B:



4.2.4 Score per residue for model 4

- Molecule 1: Plastocyanin A

Chain A: 76% 22% •

I1 K30 F35 P36 H37 D42 E43 D44 S45 I46 P47 V50 S58 E59 E60 N64 A65 K66 K77 Y80 S81 C84 S85 P86 H87 Q88 G89 A90 N99

• Molecule 2: Cytochrome f

Chain B: 83% 15% ••

Y1 F4 R13 R18 D32 D42 F45 E46 D54 N70 V71 P78 F81 R88 I89 S90 P91 E92 M93 K94 E95 K96 L100 R106 I115 G116 P117 I130 T137 R154 G155 R156 G157 Q158 I159 Y160 P161 A175 R184 K187

R201 Q202 V203 R209 G210 L211 D224 S229 N230 P231 R250 VAL GLN

4.2.5 Score per residue for model 5

• Molecule 1: Plastocyanin A

Chain A: 78% 20% •

I1 L12 K30 F35 P36 H37 N38 I39 V40 S45 I46 P47 V50 E59 E60 N64 A65 K66 K77 Y80 S81 P86 H87 Q88 G89 A90 N99

• Molecule 2: Cytochrome f

Chain B: 83% 15% ••

Y1 P2 I3 F4 N8 R13 R18 C21 C24 D42 F45 E46 N63 N70 V71 P78 F81 R88 E92 M93 K94 E95 K96 L100 R106 I115 G116 P117 I130 D140 R154 G155 R156 Y160 P161 S166 R184

Y190 R201 R209 G210 L211 E212 L213 D224 S229 N230 P231 R250 VAL GLN

4.2.6 Score per residue for model 6 (medoid)

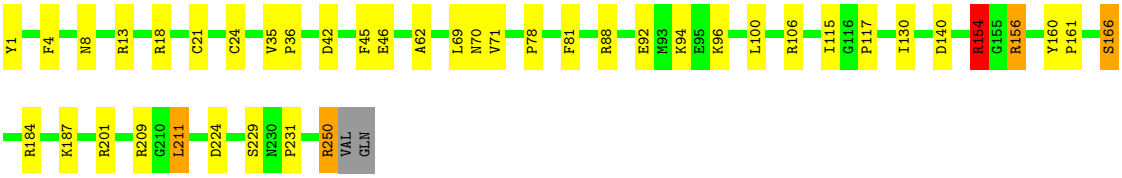
• Molecule 1: Plastocyanin A

Chain A: 78% 19% •

I1 K30 F35 P36 H37 E43 D44 S45 I46 P47 V50 S56 E59 N64 A65 K66 K77 Y80 S81 C84 S85 P86 H87 Q88 G89 A90 N99

• Molecule 2: Cytochrome f

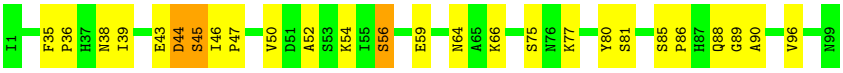
Chain B: 83% 15% ••



4.2.7 Score per residue for model 7

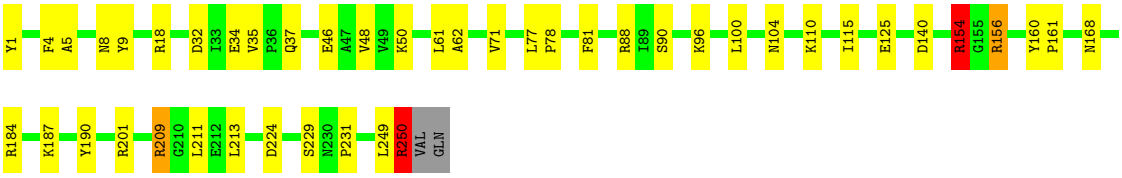
- Molecule 1: Plastocyanin A

Chain A: 74% 23% •



- Molecule 2: Cytochrome f

Chain B: 81% 16% •••



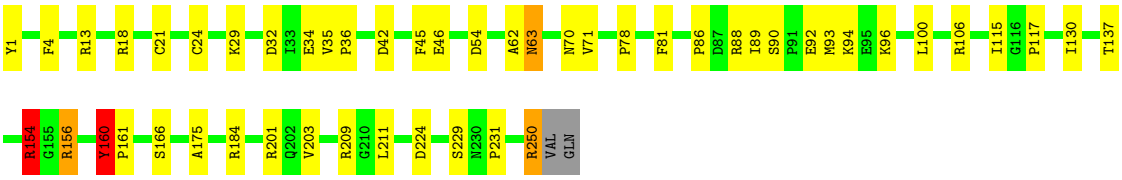
4.2.8 Score per residue for model 8

- Molecule 1: Plastocyanin A

Chain A: 78% 19% •

- Molecule 2: Cytochrome f

Chain B: 79% 18% •••



4.2.9 Score per residue for model 9

- Molecule 1: Plastocyanin A

Chain A: 81% 18%

I1 K30 F35 P36 E43 D44 S45 I46 P47 V50 E59 N64 A65 K66 K77 S81 S85 P86 H87 Q88 G89 A90 N99

• Molecule 2: Cytochrome f

Chain B: 83% 14%

Y1 P2 I3 F4 N8 R13 R18 V35 P36 D42 F45 E46 V71 P78 F81 R88 E92 M93 K94 E95 K96 L100 R106 I115 G116 P117 I130 D140 R154 G155 R156 Y160 P161 S166 A175 R184 Y190

R201 Q202 V203 R209 G210 L211 E212 L213 D224 S229 N230 P231 R250 VAL GLN

4.2.10 Score per residue for model 10

• Molecule 1: Plastocyanin A

Chain A: 73% 22% 5%

I1 L12 K30 F35 P36 H37 N38 I39 V40 E43 D44 S45 I46 P47 V50 M57 S58 E59 E60 N64 A65 K66 K77 Y80 S81 S85 P86 H87 Q88 G89 A90 N99

• Molecule 2: Cytochrome f

Chain B: 83% 15%

Y1 F4 R13 R18 C21 C24 V35 P36 D42 F45 E46 A62 N70 V71 P78 F81 R88 E92 M93 K94 E95 K96 L100 R106 I115 G116 P117 I130 T137 D140 R154 G155 R156 Y160 P161 S166

A175 R184 K187 R201 Q202 V203 L211 D224 S229 N230 P231 R250 VAL GLN

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Rigid body docking using intermolecular pseudocontact shifts restraints, chemical shift perturbation restraints and electrostatic restraints.*.

Of the 104 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations.*

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

Software name	Classification	Version
X-PLOR	structure solution	XPLOR-NIH 2.9.1
X-PLOR	refinement	XPLOR-NIH 2.9.1

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, CU

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	1.13±0.01	0±0/753 (0.0± 0.0%)	0.89±0.08	0±0/1017 (0.0± 0.0%)
2	B	1.09±0.01	1±1/1964 (0.1± 0.0%)	0.89±0.05	0±0/2669 (0.0± 0.0%)
All	All	1.10	12/27170 (0.0%)	0.89	1/36860 (0.0%)

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
2	B	0.0±0.0	9.7±0.6
All	All	0	97

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	B	21	CYS	CB-SG	-7.21	1.70	1.82	2	6
2	B	24	CYS	CB-SG	-6.31	1.71	1.82	10	6

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	160	TYR	CB-CG-CD2	-5.13	117.92	121.00	8	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)
2	B	18	ARG	Sidechain	10
2	B	88	ARG	Sidechain	10
2	B	154	ARG	Sidechain	10
2	B	156	ARG	Sidechain	10
2	B	184	ARG	Sidechain	10
2	B	201	ARG	Sidechain	10
2	B	250	ARG	Sidechain	10
2	B	13	ARG	Sidechain	9
2	B	106	ARG	Sidechain	9
2	B	209	ARG	Sidechain	9

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	738	704	704	27±8
2	B	1924	1954	1955	35±8
4	B	43	32	30	4±2
All	All	27060	26900	26890	465

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:253:HEC:CMA	4:B:253:HEC:C3A	1.63	1.75	2	2
1:A:90:ALA:HB2	2:B:4:PHE:CZ	1.01	1.91	2	7
1:A:89:GLY:O	2:B:161:PRO:HD2	1.00	1.56	5	1
1:A:89:GLY:HA3	4:B:253:HEC:HMD1	0.95	1.31	2	1
1:A:90:ALA:O	2:B:4:PHE:HZ	0.93	1.45	4	1
1:A:85:SER:O	2:B:62:ALA:HB3	0.90	1.65	6	2
2:B:1:TYR:CE1	2:B:117:PRO:HG3	0.88	2.04	3	9
1:A:43:GLU:HB2	2:B:187:LYS:HB3	0.88	1.43	2	1
1:A:89:GLY:HA3	4:B:253:HEC:HBD2	0.86	1.45	1	4
1:A:90:ALA:CB	2:B:4:PHE:CZ	0.85	2.58	2	6
1:A:89:GLY:HA2	2:B:160:TYR:CZ	0.84	2.08	6	5
1:A:89:GLY:HA2	2:B:160:TYR:CE1	0.83	2.08	4	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:GLY:O	2:B:160:TYR:HB3	0.83	1.73	8	3
1:A:88:GLN:HB3	2:B:62:ALA:HB1	0.81	1.49	10	2
1:A:43:GLU:CB	2:B:187:LYS:HB3	0.81	2.04	2	1
1:A:43:GLU:HB2	2:B:187:LYS:CB	0.81	2.06	2	2
1:A:88:GLN:OE1	1:A:93:VAL:HG12	0.80	1.75	2	1
2:B:1:TYR:HD2	2:B:4:PHE:CZ	0.79	1.95	5	5
1:A:85:SER:O	2:B:62:ALA:CB	0.79	2.30	10	4
2:B:1:TYR:HB2	2:B:4:PHE:CE1	0.79	2.13	3	3
1:A:59:GLU:CB	2:B:63:ASN:CB	0.78	2.61	5	1
1:A:90:ALA:O	2:B:4:PHE:CZ	0.78	2.36	4	1
1:A:89:GLY:HA3	4:B:253:HEC:CMD	0.77	2.07	2	1
2:B:160:TYR:OH	2:B:166:SER:HA	0.77	1.78	10	3
1:A:89:GLY:O	2:B:160:TYR:CG	0.77	2.38	10	2
1:A:44:ASP:OD1	2:B:188:GLY:O	0.76	2.04	2	1
1:A:86:PRO:O	2:B:1:TYR:OH	0.76	2.03	10	5
1:A:59:GLU:HB3	2:B:63:ASN:CG	0.76	2.01	2	2
2:B:156:ARG:HD2	4:B:253:HEC:O2D	0.75	1.81	1	10
1:A:59:GLU:HB3	2:B:63:ASN:HB3	0.75	1.54	5	2
1:A:85:SER:O	2:B:62:ALA:HB1	0.75	1.81	8	1
1:A:89:GLY:HA2	2:B:160:TYR:CG	0.75	2.17	5	1
1:A:44:ASP:CA	2:B:187:LYS:HB2	0.73	2.12	10	1
1:A:43:GLU:C	2:B:187:LYS:HG2	0.72	2.05	10	1
1:A:85:SER:OG	1:A:86:PRO:HD3	0.72	1.85	1	6
2:B:1:TYR:CD2	2:B:4:PHE:CZ	0.72	2.77	3	5
1:A:90:ALA:HB2	2:B:4:PHE:CE1	0.70	2.22	5	3
1:A:59:GLU:HB3	2:B:63:ASN:CB	0.70	2.15	5	2
1:A:44:ASP:CB	2:B:187:LYS:HB2	0.69	2.17	10	1
2:B:211:LEU:HD21	2:B:231:PRO:HG3	0.69	1.64	7	6
1:A:89:GLY:CA	4:B:253:HEC:HBD2	0.68	2.18	1	3
1:A:90:ALA:HA	2:B:4:PHE:CZ	0.68	2.24	9	3
1:A:59:GLU:HB2	2:B:63:ASN:CG	0.67	2.10	5	1
1:A:89:GLY:HA3	4:B:253:HEC:O1D	0.67	1.89	4	2
1:A:44:ASP:OD1	2:B:209:ARG:NH1	0.66	2.29	7	1
1:A:89:GLY:N	4:B:253:HEC:O1D	0.65	2.29	6	1
1:A:89:GLY:HA3	4:B:253:HEC:CBD	0.65	2.20	4	1
1:A:59:GLU:HG2	2:B:63:ASN:HB2	0.64	1.70	5	2
2:B:4:PHE:CD1	2:B:4:PHE:N	0.64	2.65	3	5
2:B:78:PRO:HG2	2:B:81:PHE:CD1	0.63	2.29	3	10
1:A:45:SER:HB3	1:A:81:SER:HB2	0.63	1.69	7	10
1:A:87:HIS:HD2	2:B:1:TYR:CE2	0.63	2.11	9	4
1:A:59:GLU:CB	2:B:63:ASN:CG	0.63	2.68	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:160:TYR:CE1	2:B:166:SER:HB3	0.62	2.28	3	6
1:A:90:ALA:HB1	2:B:4:PHE:CZ	0.61	2.31	6	2
1:A:90:ALA:CA	2:B:4:PHE:CZ	0.61	2.83	9	3
1:A:90:ALA:CB	2:B:4:PHE:CE1	0.61	2.84	3	4
1:A:89:GLY:CA	4:B:253:HEC:CMD	0.60	2.79	2	1
1:A:59:GLU:HG2	2:B:63:ASN:OD1	0.60	1.96	3	1
1:A:59:GLU:CG	2:B:63:ASN:HB2	0.60	2.27	5	1
2:B:160:TYR:HE1	2:B:166:SER:CB	0.60	2.09	10	4
2:B:1:TYR:HD2	2:B:4:PHE:HZ	0.60	1.39	3	1
1:A:88:GLN:CB	2:B:62:ALA:HB1	0.60	2.25	10	1
1:A:43:GLU:HG3	2:B:187:LYS:HG2	0.60	1.74	6	2
1:A:90:ALA:HB1	2:B:4:PHE:HZ	0.59	1.56	6	1
2:B:3:ILE:HG23	2:B:4:PHE:CD1	0.59	2.33	1	5
1:A:85:SER:O	2:B:62:ALA:HB2	0.59	1.97	2	2
2:B:160:TYR:CD1	2:B:160:TYR:N	0.59	2.70	2	4
1:A:89:GLY:CA	2:B:160:TYR:CD1	0.59	2.85	5	1
1:A:90:ALA:HB2	2:B:4:PHE:CE2	0.59	2.31	2	1
2:B:160:TYR:HB3	2:B:161:PRO:HD2	0.58	1.74	8	9
1:A:44:ASP:HA	2:B:187:LYS:HB2	0.58	1.73	10	1
2:B:160:TYR:HE1	2:B:166:SER:HB3	0.58	1.58	2	5
1:A:89:GLY:CA	4:B:253:HEC:HMD1	0.58	2.18	2	1
2:B:45:PHE:CZ	2:B:130:ILE:HB	0.57	2.35	8	9
1:A:89:GLY:O	2:B:160:TYR:CD1	0.57	2.58	4	3
1:A:35:PHE:HB2	1:A:36:PRO:HA	0.57	1.76	1	10
1:A:43:GLU:CB	2:B:187:LYS:CB	0.57	2.75	2	1
2:B:1:TYR:CD2	2:B:4:PHE:HZ	0.57	2.16	3	1
1:A:89:GLY:HA3	4:B:253:HEC:CGD	0.56	2.30	4	1
2:B:160:TYR:CE1	2:B:166:SER:CB	0.56	2.88	6	5
1:A:89:GLY:O	2:B:160:TYR:CB	0.56	2.53	2	2
2:B:100:LEU:HD22	2:B:115:ILE:HD11	0.55	1.77	2	10
1:A:89:GLY:HA2	2:B:160:TYR:CD1	0.55	2.36	3	3
1:A:89:GLY:O	2:B:160:TYR:HA	0.55	2.01	2	1
1:A:38:ASN:HD21	1:A:40:VAL:CG2	0.55	2.14	8	4
1:A:90:ALA:HA	2:B:4:PHE:CE2	0.55	2.37	9	2
1:A:89:GLY:CA	2:B:160:TYR:CE1	0.55	2.89	4	4
1:A:59:GLU:CG	2:B:63:ASN:CB	0.55	2.84	5	1
2:B:229:SER:O	2:B:231:PRO:HD3	0.55	2.02	1	10
1:A:89:GLY:HA2	2:B:160:TYR:HE1	0.54	1.61	4	1
1:A:43:GLU:O	2:B:187:LYS:HG2	0.54	2.02	10	1
1:A:47:PRO:HG2	1:A:50:VAL:HG21	0.54	1.79	7	10
1:A:89:GLY:HA3	2:B:160:TYR:CD1	0.54	2.37	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ILE:HB	1:A:47:PRO:HD2	0.54	1.80	7	10
1:A:87:HIS:CD2	2:B:1:TYR:CE2	0.54	2.96	3	1
1:A:86:PRO:O	2:B:1:TYR:CE2	0.53	2.61	3	2
2:B:211:LEU:CD2	2:B:231:PRO:HG3	0.53	2.32	7	1
1:A:59:GLU:HB3	2:B:63:ASN:ND2	0.53	2.17	2	2
1:A:43:GLU:HB2	2:B:187:LYS:HG2	0.53	1.78	1	1
1:A:12:LEU:HD12	2:B:4:PHE:CE1	0.53	2.39	2	2
2:B:1:TYR:HB2	2:B:4:PHE:CZ	0.53	2.38	3	4
1:A:89:GLY:CA	4:B:253:HEC:O1D	0.52	2.57	6	2
1:A:89:GLY:CA	2:B:160:TYR:CG	0.52	2.92	5	1
1:A:89:GLY:O	2:B:160:TYR:CD2	0.52	2.62	10	1
2:B:3:ILE:HG23	2:B:4:PHE:CE1	0.52	2.40	2	1
2:B:1:TYR:CZ	2:B:117:PRO:HG3	0.51	2.40	1	1
1:A:44:ASP:CA	2:B:187:LYS:CB	0.51	2.88	10	1
1:A:43:GLU:CG	2:B:209:ARG:HH12	0.50	2.19	7	1
1:A:83:TYR:CB	1:A:88:GLN:OE1	0.50	2.59	2	1
1:A:59:GLU:CB	2:B:63:ASN:HB3	0.50	2.28	5	1
1:A:89:GLY:HA2	2:B:160:TYR:CD2	0.50	2.41	5	1
2:B:154:ARG:O	2:B:154:ARG:HG2	0.50	2.06	4	10
2:B:1:TYR:CE2	4:B:253:HEC:HBD1	0.49	2.41	10	2
1:A:59:GLU:HG2	2:B:63:ASN:CB	0.49	2.37	5	1
2:B:175:ALA:HB3	2:B:203:VAL:HG21	0.49	1.84	1	5
1:A:44:ASP:HB3	2:B:187:LYS:CB	0.49	2.37	10	1
1:A:12:LEU:CD1	2:B:3:ILE:HG21	0.49	2.38	3	2
2:B:4:PHE:CE2	2:B:161:PRO:HD3	0.49	2.43	4	1
2:B:249:LEU:O	2:B:250:ARG:HG3	0.49	2.08	7	1
1:A:59:GLU:CB	2:B:63:ASN:ND2	0.49	2.76	3	1
1:A:35:PHE:HA	1:A:37:HIS:CD2	0.48	2.43	2	7
1:A:88:GLN:OE1	1:A:93:VAL:CG1	0.48	2.57	2	1
1:A:12:LEU:HD12	2:B:4:PHE:HE1	0.48	1.68	2	1
1:A:88:GLN:HE21	2:B:62:ALA:HB1	0.48	1.68	7	1
1:A:44:ASP:OD1	2:B:187:LYS:HB3	0.47	2.09	7	1
1:A:44:ASP:CB	2:B:187:LYS:CB	0.47	2.90	10	1
2:B:90:SER:OG	2:B:93:MET:HB2	0.47	2.09	4	2
2:B:35:VAL:HG13	2:B:36:PRO:HD2	0.47	1.87	9	5
2:B:125:GLU:O	2:B:125:GLU:HG3	0.47	2.09	7	1
1:A:43:GLU:CG	2:B:187:LYS:HG2	0.46	2.39	6	1
1:A:90:ALA:O	2:B:161:PRO:CG	0.46	2.64	2	1
1:A:43:GLU:HB2	2:B:187:LYS:HB2	0.46	1.88	4	1
1:A:38:ASN:ND2	1:A:40:VAL:HG23	0.46	2.25	5	1
2:B:29:LYS:HB3	2:B:154:ARG:NH2	0.46	2.26	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:4:PHE:N	2:B:4:PHE:HD1	0.46	2.08	3	1
2:B:1:TYR:HB2	2:B:4:PHE:CE2	0.45	2.46	2	1
2:B:1:TYR:CE1	4:B:253:HEC:HAA2	0.45	2.46	9	1
1:A:59:GLU:OE1	1:A:60:GLU:HG3	0.45	2.11	10	1
2:B:104:ASN:ND2	2:B:110:LYS:HA	0.45	2.26	7	1
2:B:1:TYR:CE1	2:B:117:PRO:CG	0.45	2.97	9	3
1:A:89:GLY:C	4:B:253:HEC:HMD2	0.45	2.32	2	1
1:A:47:PRO:HG3	1:A:80:TYR:CZ	0.44	2.47	8	7
1:A:89:GLY:HA2	2:B:160:TYR:CE2	0.44	2.47	1	1
1:A:86:PRO:O	2:B:1:TYR:HE2	0.44	1.95	5	1
1:A:38:ASN:ND2	1:A:40:VAL:CG2	0.44	2.81	5	2
1:A:83:TYR:HB2	1:A:88:GLN:OE1	0.44	2.12	2	1
1:A:44:ASP:CG	2:B:188:GLY:O	0.44	2.55	2	1
1:A:89:GLY:O	4:B:253:HEC:HMD2	0.44	2.12	2	1
2:B:100:LEU:HB3	2:B:115:ILE:HD11	0.44	1.88	7	2
2:B:1:TYR:CD2	2:B:4:PHE:CE2	0.44	3.06	2	1
1:A:43:GLU:H	1:A:43:GLU:HG2	0.44	1.34	4	2
1:A:86:PRO:O	2:B:1:TYR:CZ	0.43	2.70	3	2
2:B:86:PRO:HA	2:B:89:ILE:HD12	0.43	1.90	8	2
1:A:38:ASN:HD21	1:A:40:VAL:HG22	0.43	1.73	8	1
1:A:89:GLY:O	2:B:160:TYR:CA	0.43	2.66	2	1
1:A:59:GLU:CB	2:B:63:ASN:HB2	0.43	2.43	8	1
1:A:85:SER:OG	1:A:86:PRO:CD	0.43	2.65	9	2
1:A:39:ILE:HD12	1:A:39:ILE:N	0.43	2.28	7	1
2:B:190:TYR:CD2	2:B:213:LEU:HD11	0.43	2.48	7	1
2:B:160:TYR:CB	2:B:161:PRO:HD2	0.42	2.43	8	3
2:B:34:GLU:HB2	2:B:48:VAL:HG13	0.42	1.89	7	1
1:A:52:ALA:O	1:A:56:SER:OG	0.42	2.31	7	1
1:A:12:LEU:HD11	2:B:3:ILE:HG21	0.42	1.91	5	1
2:B:160:TYR:N	2:B:160:TYR:CD1	0.42	2.87	9	1
1:A:47:PRO:CG	1:A:80:TYR:CZ	0.42	3.02	5	7
1:A:76:ASN:O	1:A:80:TYR:OH	0.41	2.27	8	2
1:A:41:PHE:HB2	1:A:56:SER:OG	0.41	2.15	1	1
1:A:84:CYS:SG	1:A:86:PRO:HD2	0.41	2.54	4	2
2:B:1:TYR:HD2	2:B:4:PHE:CE2	0.41	2.33	2	1
2:B:70:ASN:HB2	4:B:253:HEC:CGA	0.41	2.46	5	7
1:A:89:GLY:O	2:B:161:PRO:CD	0.41	2.48	5	1
2:B:5:ALA:HA	2:B:9:TYR:HD2	0.41	1.75	7	1
1:A:12:LEU:HD12	2:B:3:ILE:HG21	0.41	1.92	3	1
2:B:69:LEU:HD12	2:B:69:LEU:N	0.41	2.31	6	1
2:B:32:ASP:HB3	2:B:50:LYS:HB2	0.41	1.93	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:160:TYR:CE1	4:B:253:HEC:HMD1	0.41	2.51	7	1
1:A:88:GLN:HB3	2:B:62:ALA:CB	0.41	2.34	10	1
1:A:80:TYR:HB2	1:A:96:VAL:HG13	0.41	1.92	7	1
2:B:4:PHE:CZ	2:B:161:PRO:HG3	0.40	2.51	4	1
2:B:190:TYR:CG	2:B:213:LEU:HD11	0.40	2.52	9	2
2:B:77:LEU:HB3	2:B:78:PRO:HD2	0.40	1.92	7	1
2:B:160:TYR:CD1	4:B:253:HEC:HMD2	0.40	2.51	7	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	97/99 (98%)	97±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
2	B	248/252 (98%)	238±1 (96±0%)	10±1 (4±0%)	0±0 (0±0%)	100	100
All	All	3450/3510 (98%)	3352 (97%)	98 (3%)	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	82/82 (100%)	73±1 (89±1%)	9±1 (11±1%)	10	54
2	B	211/213 (99%)	197±2 (94±1%)	14±2 (6±1%)	21	70
All	All	2930/2950 (99%)	2704 (92%)	226 (8%)	16	64

All 46 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	45	SER	10
1	A	66	LYS	10
1	A	77	LYS	10
2	B	46	GLU	10
2	B	71	VAL	10
2	B	96	LYS	10
2	B	154	ARG	10
2	B	224	ASP	10
2	B	250	ARG	10
1	A	30	LYS	9
2	B	211	LEU	9
1	A	64	ASN	9
2	B	42	ASP	8
2	B	92	GLU	8
2	B	94	LYS	8
1	A	59	GLU	8
1	A	88	GLN	7
2	B	140	ASP	7
1	A	43	GLU	5
2	B	8	ASN	5
2	B	137	THR	4
1	A	38	ASN	4
1	A	42	ASP	3
1	A	60	GLU	3
2	B	4	PHE	3
2	B	32	ASP	3
2	B	54	ASP	3
2	B	160	TYR	3
1	A	22	SER	2
1	A	54	LYS	2
2	B	34	GLU	2
2	B	37	GLN	2
2	B	61	LEU	2
2	B	63	ASN	2
1	A	56	SER	2
2	B	166	SER	2
1	A	44	ASP	2
1	A	58	SER	1
2	B	158	GLN	1
2	B	187	LYS	1
1	A	75	SER	1
2	B	35	VAL	1
2	B	90	SER	1

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Mol	Chain	Res	Type	Models (Total)
2	B	168	ASN	1
1	A	85	SER	1
1	A	57	MET	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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
4	HEC	B	253	2	26,50,50	2.93±1.09	10±5 (40±17%)

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
4	HEC	B	253	2	18,82,82	1.89±0.21	6±2 (30±9%)

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
4	HEC	B	253	2	-	0±0,6,54,54	-

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
4	B	253	HEC	CMA-C3A	14.08	1.85	1.51	10	6
4	B	253	HEC	C2B-C3B	11.20	1.52	1.40	10	8
4	B	253	HEC	C3C-C4C	9.36	1.60	1.43	10	10
4	B	253	HEC	C3A-C4A	6.63	1.57	1.42	2	6
4	B	253	HEC	CMB-C2B	5.63	1.65	1.51	10	2
4	B	253	HEC	CBC-CAC	5.24	1.69	1.49	2	7
4	B	253	HEC	CBB-CAB	4.77	1.67	1.49	2	5
4	B	253	HEC	CMD-C2D	4.25	1.60	1.51	4	6
4	B	253	HEC	CAA-C2A	4.16	1.44	1.52	10	6
4	B	253	HEC	C4B-C3B	4.05	1.50	1.43	8	7
4	B	253	HEC	C3C-C2C	4.00	1.44	1.40	8	7
4	B	253	HEC	CAD-C3D	3.74	1.46	1.52	10	5
4	B	253	HEC	C1B-NB	3.44	1.43	1.36	10	6
4	B	253	HEC	C2A-C3A	3.18	1.28	1.37	2	6
4	B	253	HEC	C1C-NC	3.03	1.42	1.36	7	6
4	B	253	HEC	C1D-ND	2.87	1.42	1.36	7	1
4	B	253	HEC	C4D-CHA	2.73	1.33	1.41	3	6
4	B	253	HEC	CMC-C2C	2.66	1.57	1.51	4	3
4	B	253	HEC	C2A-C1A	2.12	1.47	1.42	10	2

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
4	B	253	HEC	C1D-C2D-C3D	5.13	103.42	107.00	10	7
4	B	253	HEC	CMB-C2B-C3B	5.05	131.76	125.82	7	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	B	253	HEC	CMB-C2B-C1B	4.50	121.55	128.46	7	9
4	B	253	HEC	CMA-C3A-C2A	4.13	132.73	124.94	10	5
4	B	253	HEC	CBD-CAD-C3D	3.36	106.30	112.49	10	7
4	B	253	HEC	C2B-C3B-C4B	3.12	102.98	106.35	4	3
4	B	253	HEC	CAD-CBD-CGD	3.06	107.53	112.67	7	4
4	B	253	HEC	C4C-C3C-C2C	2.93	103.19	106.35	4	4
4	B	253	HEC	CMD-C2D-C1D	2.48	124.65	128.46	3	2
4	B	253	HEC	CMD-C2D-C3D	2.43	129.52	124.94	8	1
4	B	253	HEC	CAA-C2A-C3A	2.38	120.41	127.25	2	2
4	B	253	HEC	C3B-C4B-NB	2.32	115.32	110.94	4	1
4	B	253	HEC	CAD-C3D-C2D	2.25	120.78	127.25	10	1
4	B	253	HEC	CMC-C2C-C1C	2.09	125.25	128.46	4	1
4	B	253	HEC	CBA-CAA-C2A	2.05	108.71	112.48	2	2

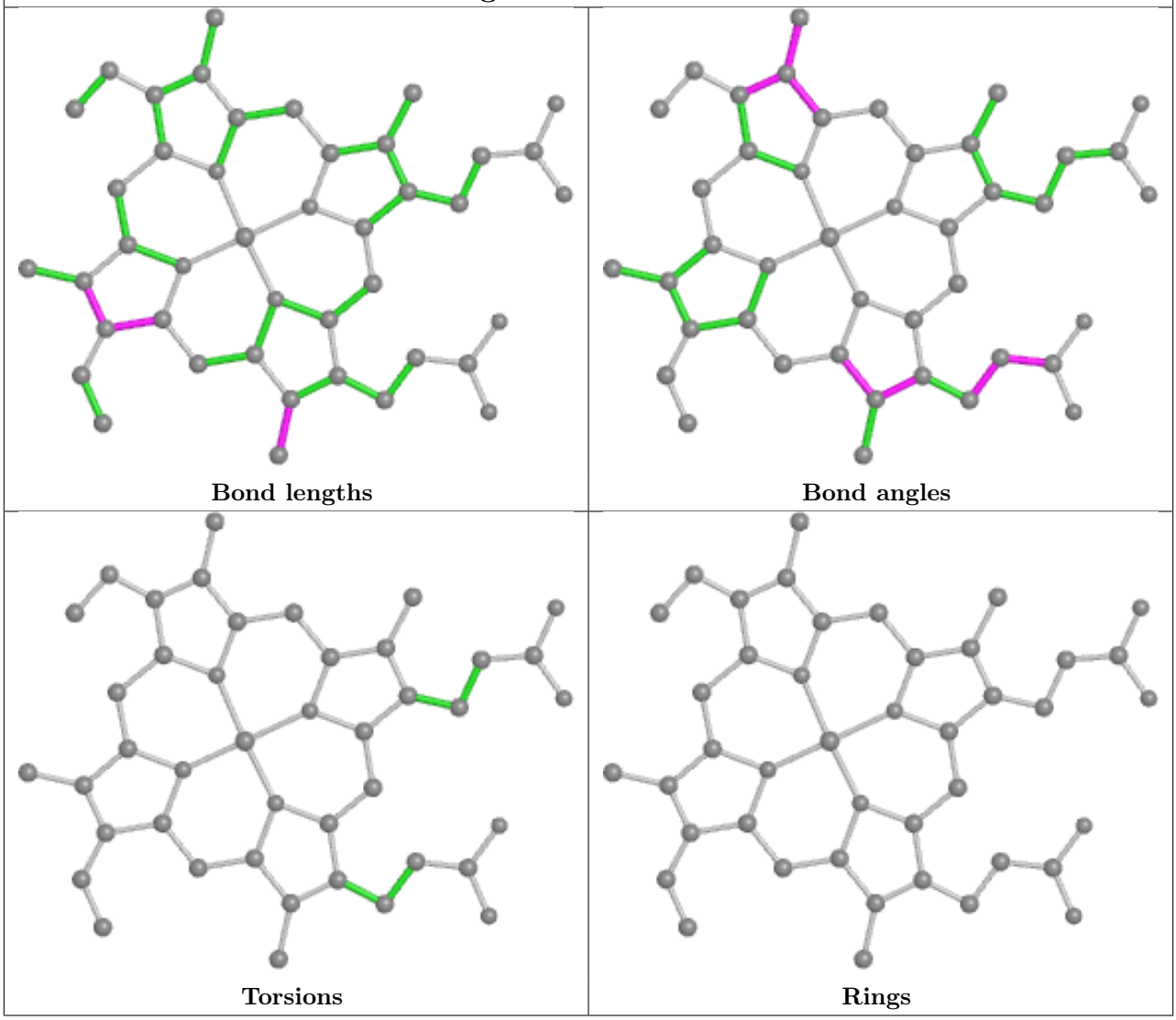
There are no chirality outliers.

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 B 253



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