Full wwPDB NMR Structure Validation Report (i)

Mar 4, 2026 – 08:36 PM UTC

PDB ID	:	1TU2 / pdb_00001tu2
Title	:	THE COMPLEX OF NOSTOC CYTOCHROME F AND PLASTOCYANIN DETERMIN WITH PARAMAGNETIC NMR. BASED ON THE STRUCTURES OF CYTOCHROME F AND PLASTOCYANIN, 10 STRUCTURES
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Deposited on	:	2004-06-24

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:

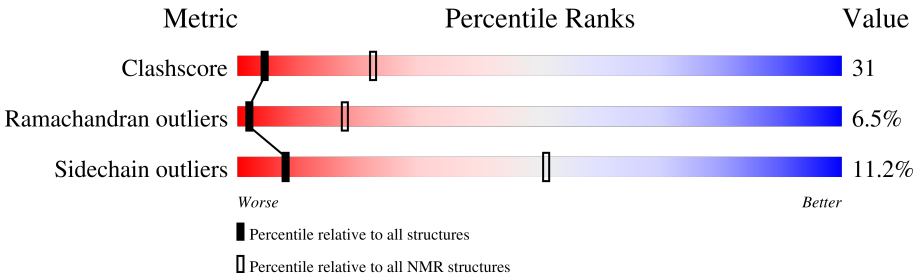
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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	105	19% 45% 29% 8%
2	B	254	78% 16% . .

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models). The authors have identified model 3 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:105, B:1-B:1 (106)	0.11	10
2	B:2-B:254 (253)	0.00	1

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 3 clusters. No single-model clusters were found.

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

3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5437 atoms, of which 2690 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Plastocyanin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	105	1566	499	784	129	151	3	0

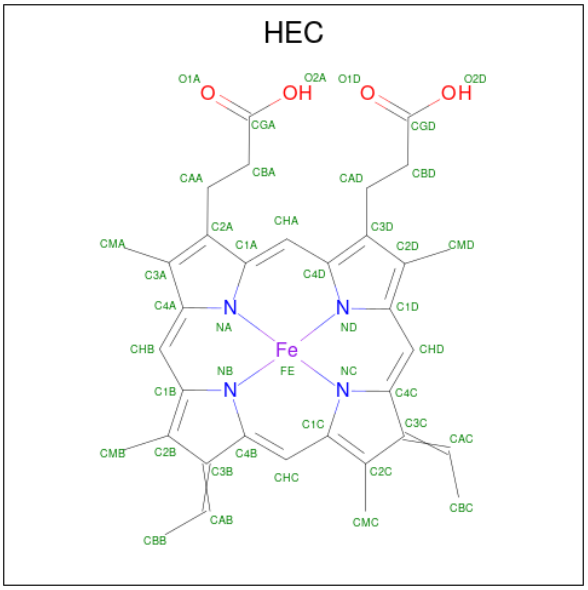
- Molecule 2 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	254	3795	1211	1874	320	387	3	0

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	
			Total	Cu
3	A	1	1	1

- Molecule 4 is HEME C (CCD ID: 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

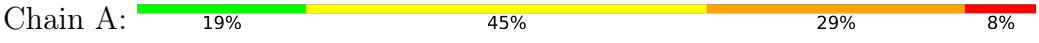
4 Residue-property plots

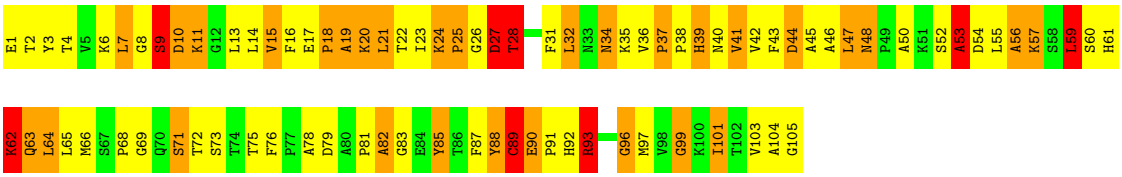
4.1 Average score per residue in the NMR ensemble

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

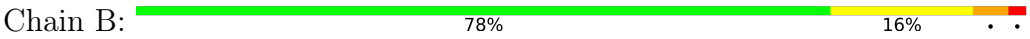
Chain A:

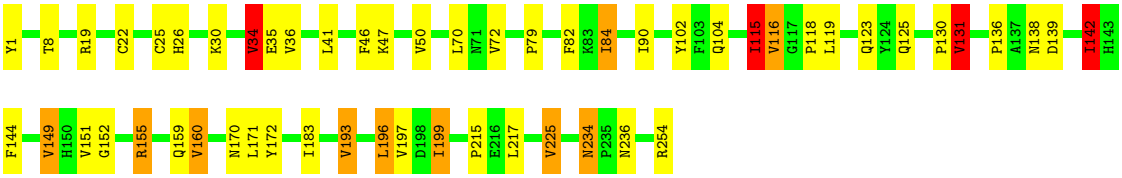




• Molecule 2: Apocytochrome f

Chain B:





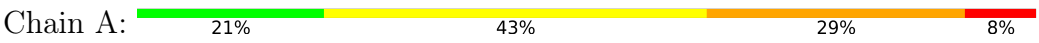
4.2 Scores per residue for each member of the ensemble

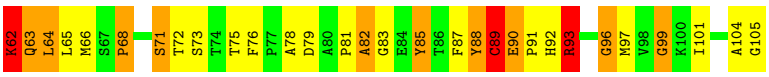
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

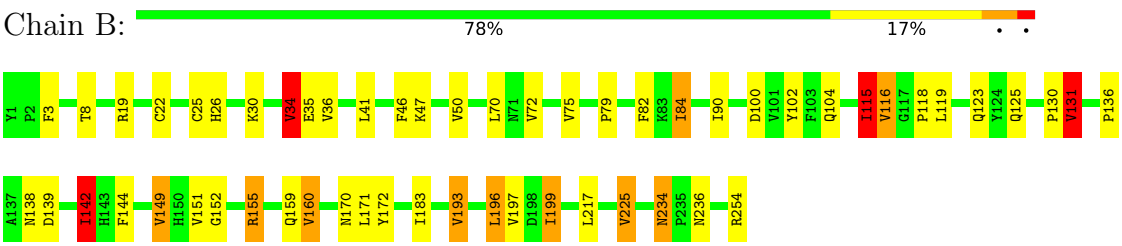
• Molecule 1: Plastocyanin

Chain A:



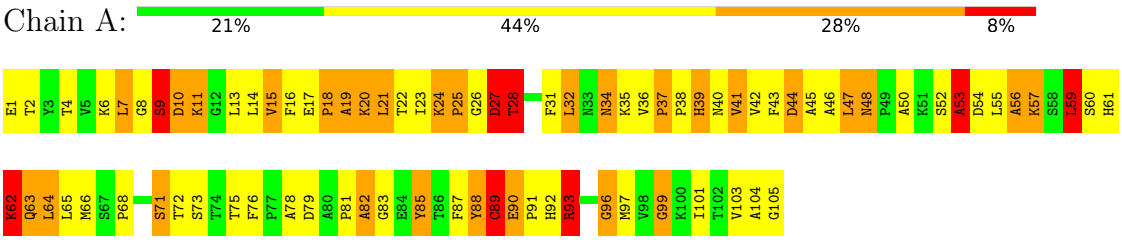


• Molecule 2: Apocytochrome f

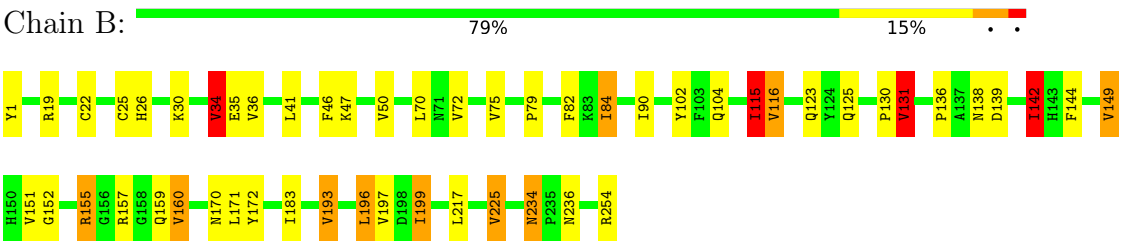


4.2.2 Score per residue for model 2

• Molecule 1: Plastocyanin

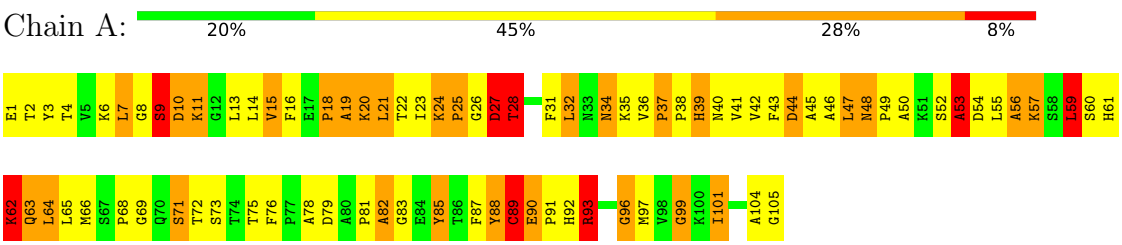


• Molecule 2: Apocytochrome f



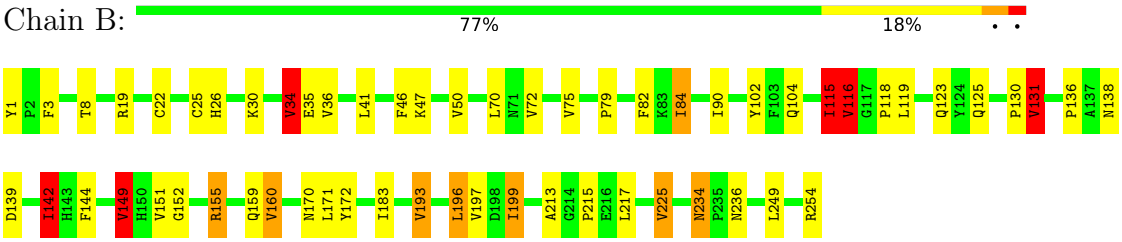
4.2.3 Score per residue for model 3

• Molecule 1: Plastocyanin



• Molecule 2: Apocytochrome f

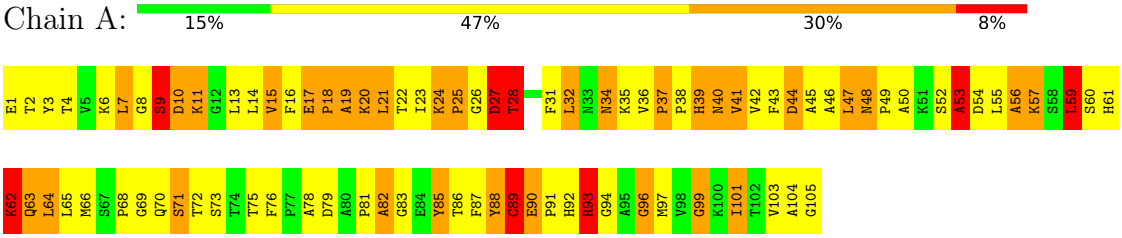
Chain B:



4.2.4 Score per residue for model 4

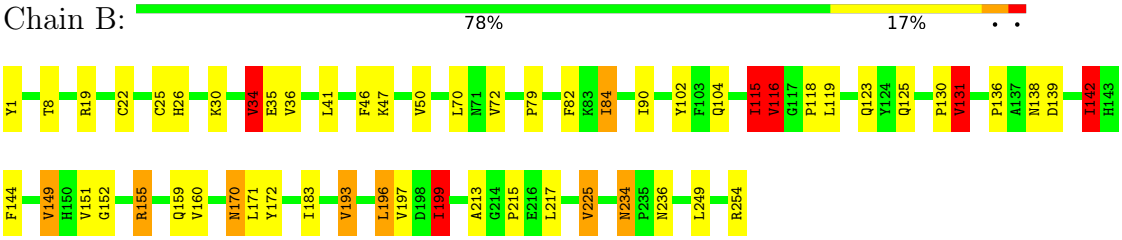
• Molecule 1: Plastocyanin

Chain A:



• Molecule 2: Apocytochrome f

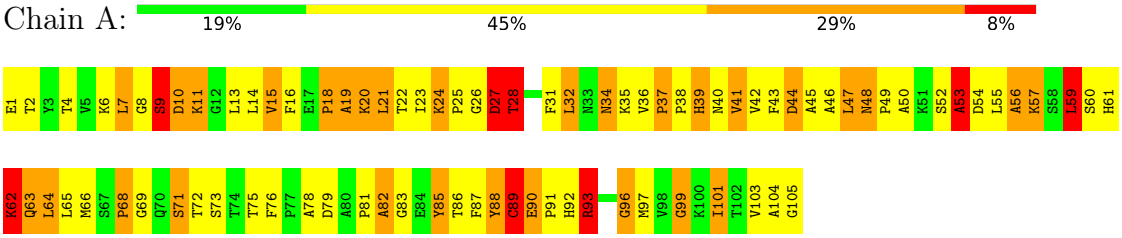
Chain B:



4.2.5 Score per residue for model 5

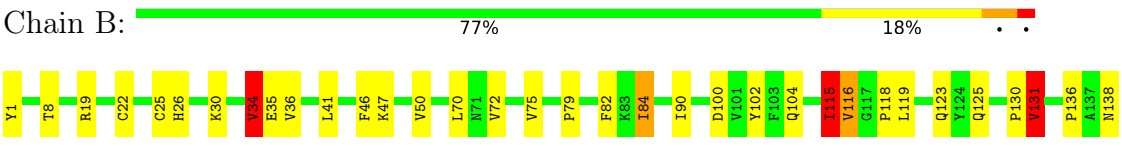
• Molecule 1: Plastocyanin

Chain A:



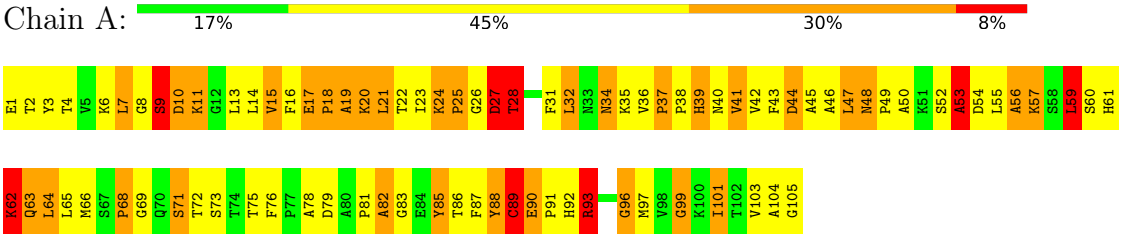
• Molecule 2: Apocytochrome f

Chain B:

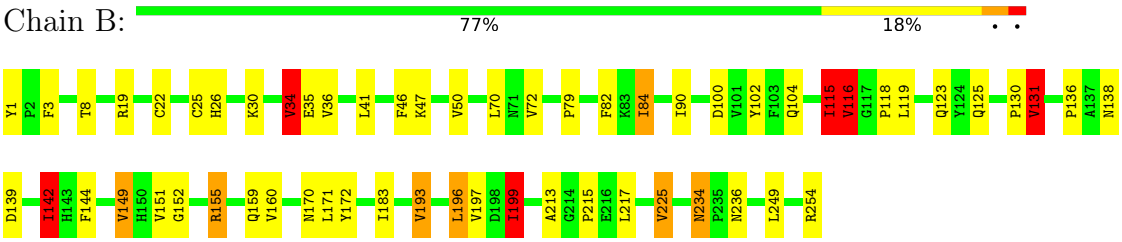


4.2.6 Score per residue for model 6

• Molecule 1: Plastocyanin

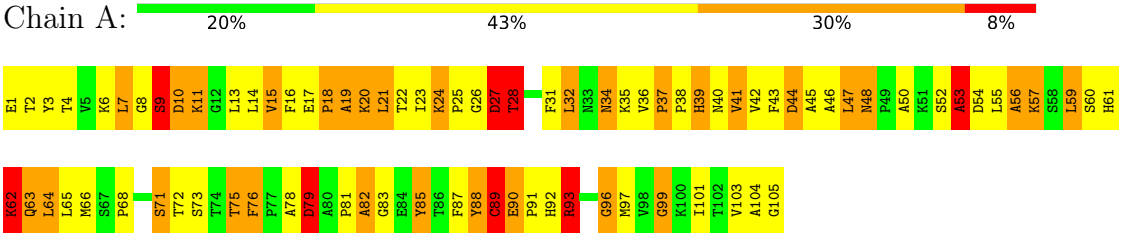


• Molecule 2: Apocytochrome f

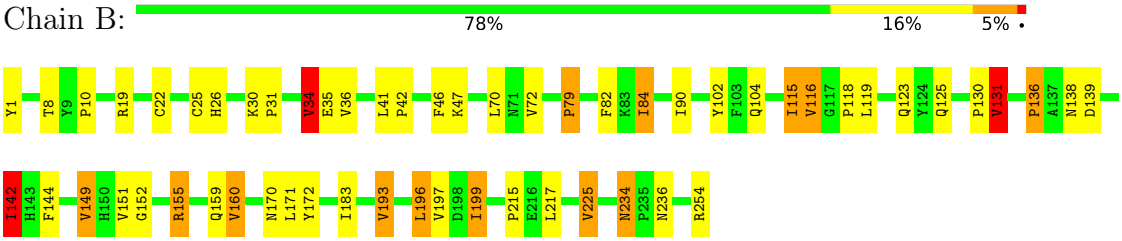


4.2.7 Score per residue for model 7

• Molecule 1: Plastocyanin



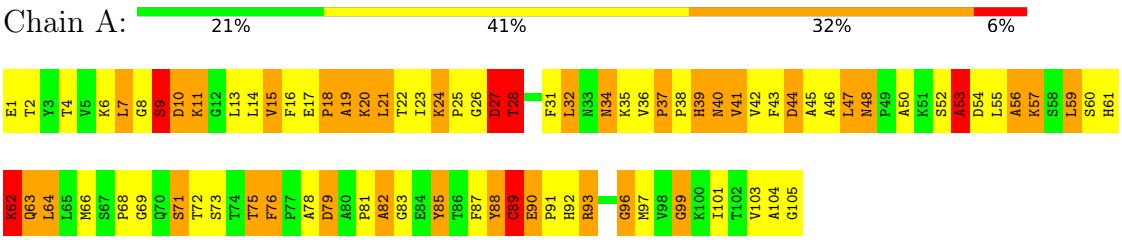
• Molecule 2: Apocytochrome f



4.2.8 Score per residue for model 8

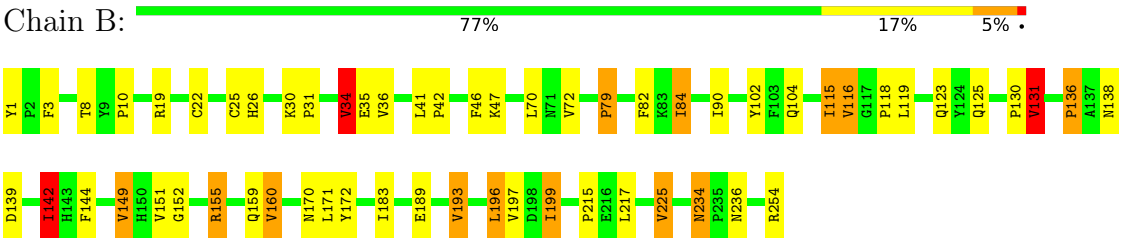
• Molecule 1: Plastocyanin

Chain A:



• Molecule 2: Apocytochrome f

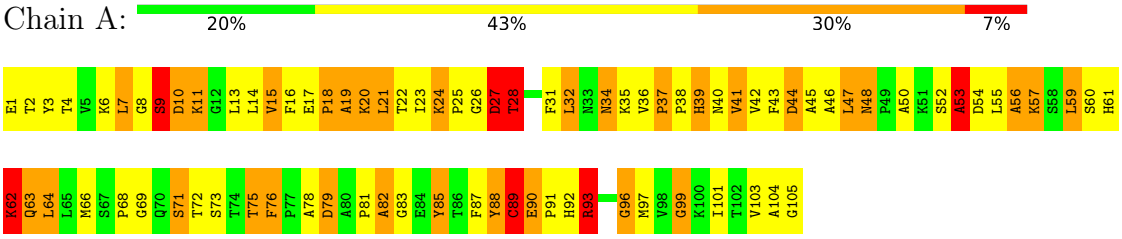
Chain B:



4.2.9 Score per residue for model 9

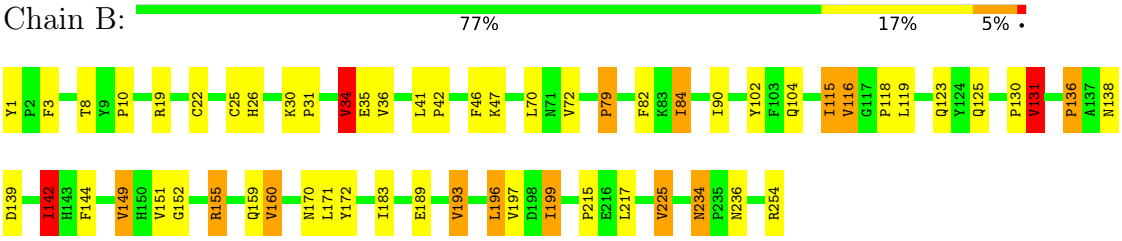
• Molecule 1: Plastocyanin

Chain A:



• Molecule 2: Apocytochrome f

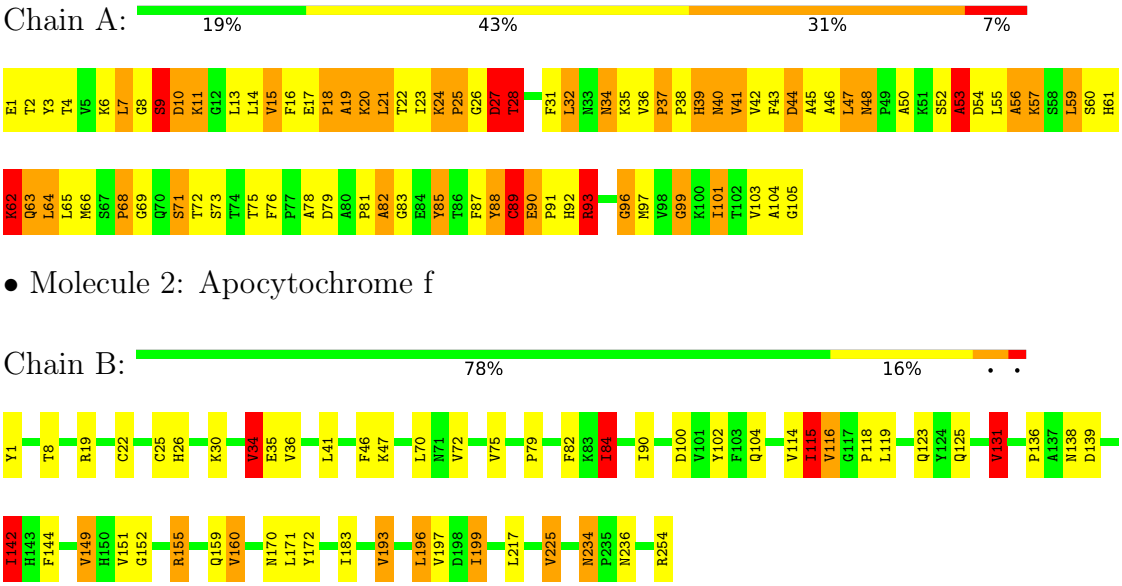
Chain B:



4.2.10 Score per residue for model 10

• Molecule 1: Plastocyanin

Chain A:



• Molecule 2: Apocytochrome f

Chain B:

5 Refinement protocol and experimental data overview

The models were refined using the following method: *DYNAMICS*.

Of the 5000 calculated structures, 10 were deposited, based on the following criterion: *REFER TO PUBLICATION*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851

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	2.09±0.01	22±1/801 (2.7± 0.1%)	1.76±0.02	19±1/1088 (1.8± 0.1%)
2	B	1.27±0.02	10±2/1963 (0.5± 0.1%)	1.62±0.07	34±7/2677 (1.3± 0.2%)
All	All	1.55	316/27640 (1.1%)	1.66	534/37650 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.0±0.0
2	B	0.9±1.4	3.0±0.0
All	All	9	40

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	116	VAL	CA-CB	18.32	1.74	1.55	2	9
2	B	131	VAL	CA-CB	18.28	1.78	1.54	3	10
2	B	115	ILE	CA-CB	15.70	1.78	1.54	2	8
2	B	193	VAL	CA-CB	14.47	1.71	1.54	6	10
2	B	84	ILE	CA-CB	11.47	1.66	1.54	6	10
2	B	199	ILE	CA-CB	10.57	1.66	1.53	6	10
2	B	34	VAL	CA-CB	8.82	1.66	1.54	8	3
2	B	160	VAL	CA-CB	8.78	1.67	1.54	8	4
1	A	39	HIS	CD2-NE2	-8.59	1.28	1.37	7	10
2	B	149	VAL	CA-CB	8.55	1.66	1.54	8	8
1	A	99	GLY	N-CA	8.47	1.54	1.45	8	10
1	A	92	HIS	CD2-NE2	-7.95	1.29	1.37	9	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	142	ILE	CA-CB	7.82	1.65	1.54	6	7
2	B	225	VAL	CA-CB	7.17	1.67	1.55	8	3
2	B	26	HIS	CE1-NE2	-7.14	1.25	1.32	3	10
1	A	28	THR	N-CA	6.40	1.54	1.46	2	10
1	A	46	ALA	CA-C	6.25	1.57	1.52	10	10
2	B	116	VAL	CB-CG1	-6.20	1.32	1.52	1	1
1	A	73	SER	N-CA	6.17	1.53	1.46	4	10
1	A	59	LEU	CA-C	6.03	1.60	1.52	8	10
1	A	57	LYS	N-CA	5.94	1.53	1.46	10	10
1	A	37	PRO	CA-C	5.68	1.57	1.52	5	10
1	A	75	THR	N-CA	5.63	1.53	1.45	5	10
1	A	4	THR	N-CA	5.59	1.53	1.46	4	10
1	A	89	CYS	N-CA	5.55	1.53	1.46	3	10
1	A	72	THR	N-CA	5.49	1.52	1.45	4	10
1	A	96	GLY	N-CA	5.42	1.53	1.45	6	10
1	A	62	LYS	N-CA	5.38	1.53	1.46	8	10
1	A	9	SER	N-CA	5.36	1.53	1.46	7	10
2	B	115	ILE	CB-CG1	-5.33	1.42	1.53	2	1
1	A	89	CYS	CA-C	5.19	1.59	1.52	1	10
1	A	53	ALA	N-CA	5.18	1.52	1.46	3	10
1	A	39	HIS	CE1-NE2	-5.17	1.27	1.32	7	3
1	A	3	TYR	N-CA	5.12	1.51	1.45	9	7
1	A	69	GLY	N-CA	5.08	1.52	1.45	3	7
1	A	45	ALA	CA-C	5.07	1.60	1.52	4	10
2	B	225	VAL	CB-CG2	5.07	1.69	1.52	9	3
1	A	26	GLY	N-CA	5.07	1.52	1.45	7	10
2	B	157	ARG	NE-CZ	-5.05	1.27	1.33	2	1
1	A	94	GLY	N-CA	5.00	1.52	1.45	4	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	B	115	ILE	N-CA-CB	-20.29	86.43	112.60	10	10
2	B	116	VAL	CB-CA-C	-17.29	87.76	111.80	10	10
2	B	115	ILE	CA-CB-CG2	-14.59	85.69	110.50	2	6
2	B	225	VAL	CB-CA-C	-14.04	88.22	110.69	8	10
1	A	88	TYR	N-CA-C	13.87	132.66	108.52	4	10
2	B	116	VAL	CA-CB-CG1	-12.82	88.60	110.40	10	4
2	B	34	VAL	CB-CA-C	-12.49	90.81	111.29	7	10
2	B	131	VAL	CA-CB-CG1	-12.45	89.24	110.40	3	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	116	VAL	CA-CB-CG2	-11.71	90.48	110.40	1	5
2	B	193	VAL	N-CA-CB	11.23	123.80	111.00	8	10
2	B	115	ILE	CA-CB-CG1	-11.12	91.50	110.40	3	5
1	A	45	ALA	N-CA-C	-9.88	101.17	113.02	7	10
1	A	41	VAL	N-CA-C	9.40	121.48	107.75	6	10
2	B	115	ILE	CB-CA-C	9.39	124.06	111.19	2	5
2	B	116	VAL	N-CA-CB	9.35	124.79	111.05	1	6
2	B	193	VAL	CG1-CB-CG2	9.22	131.09	110.80	7	7
2	B	193	VAL	CA-CB-CG1	-9.04	95.03	110.40	6	4
2	B	131	VAL	CG1-CB-CG2	8.98	130.55	110.80	8	7
2	B	149	VAL	CG1-CB-CG2	8.47	129.44	110.80	9	7
2	B	142	ILE	CA-CB-CG1	8.03	124.05	110.40	9	6
2	B	84	ILE	CB-CA-C	8.02	124.39	111.32	6	4
2	B	142	ILE	CB-CA-C	7.98	123.57	111.68	6	6
2	B	199	ILE	CB-CA-C	7.88	121.78	111.53	6	5
2	B	131	VAL	CA-CB-CG2	-7.83	97.08	110.40	6	7
1	A	17	GLU	CB-CA-C	-7.53	98.25	108.87	6	7
2	B	160	VAL	CG1-CB-CG2	7.52	127.34	110.80	9	3
2	B	130	PRO	CB-CA-C	7.45	120.76	111.23	9	3
2	B	149	VAL	N-CA-CB	7.44	123.51	111.23	8	6
1	A	32	LEU	N-CA-C	7.36	120.79	108.20	6	10
1	A	88	TYR	CA-C-O	-7.33	113.53	122.41	7	10
2	B	84	ILE	CG1-CB-CG2	7.04	131.82	110.70	10	10
2	B	131	VAL	N-CA-CB	7.01	122.94	111.58	5	8
2	B	90	ILE	CA-C-O	-6.97	115.22	119.12	1	10
2	B	199	ILE	CG1-CB-CG2	6.89	131.37	110.70	10	10
2	B	116	VAL	CG1-CB-CG2	6.87	125.90	110.80	9	4
2	B	199	ILE	CA-CB-CG2	-6.82	98.90	110.50	6	2
2	B	225	VAL	N-CA-CB	6.69	124.31	111.93	7	10
2	B	149	VAL	CA-CB-CG2	6.68	121.76	110.40	8	3
2	B	199	ILE	CA-CB-CG1	6.67	121.74	110.40	7	3
2	B	193	VAL	CA-CB-CG2	6.65	121.70	110.40	8	5
1	A	15	VAL	N-CA-C	6.55	118.60	109.29	7	10
2	B	199	ILE	N-CA-CB	6.40	119.71	111.83	1	10
2	B	160	VAL	CA-CB-CG2	6.35	121.20	110.40	9	3
2	B	115	ILE	CB-CG1-CD1	-6.34	100.49	113.80	10	5
2	B	34	VAL	N-CA-CB	6.33	121.67	111.23	6	5
1	A	44	ASP	N-CA-C	6.29	124.20	110.80	10	10
2	B	84	ILE	CA-CB-CG2	-6.29	99.81	110.50	6	2
2	B	84	ILE	CA-CB-CG1	6.27	121.05	110.40	7	3
1	A	71	SER	N-CA-C	6.26	119.75	109.85	3	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	47	LEU	N-CA-C	6.26	119.00	109.62	1	10
2	B	34	VAL	CG1-CB-CG2	6.22	124.49	110.80	8	3
1	A	34	ASN	N-CA-C	6.18	118.95	111.40	7	10
2	B	142	ILE	CG1-CB-CG2	6.17	129.20	110.70	10	8
1	A	31	PHE	CA-CB-CG	-6.12	107.68	113.80	4	10
2	B	115	ILE	CG1-CB-CG2	5.93	128.49	110.70	1	4
2	B	160	VAL	CB-CA-C	5.86	119.52	110.50	3	5
2	B	84	ILE	CB-CG1-CD1	-5.84	101.54	113.80	1	7
2	B	42	PRO	CB-CA-C	5.64	120.86	111.56	8	3
2	B	142	ILE	CB-CG1-CD1	-5.58	102.07	113.80	1	4
2	B	199	ILE	CB-CG1-CD1	-5.57	102.11	113.80	1	4
2	B	152	GLY	CA-C-O	-5.55	116.61	120.94	1	10
2	B	136	PRO	CB-CA-C	5.54	121.76	112.62	7	3
1	A	73	SER	N-CA-C	5.46	118.39	109.59	7	10
1	A	19	ALA	N-CA-C	5.42	122.34	110.80	7	10
2	B	79	PRO	CB-CA-C	5.40	119.38	111.22	8	3
2	B	215	PRO	CB-CA-C	5.38	120.44	111.56	7	3
1	A	27	ASP	N-CA-C	5.37	122.23	110.80	6	10
1	A	4	THR	N-CA-C	5.36	117.26	108.52	5	10
2	B	10	PRO	CB-CA-C	5.34	120.54	112.21	8	3
2	B	31	PRO	CB-CA-C	5.32	118.24	110.63	8	3
1	A	39	HIS	CA-CB-CG	-5.32	108.48	113.80	6	3
2	B	84	ILE	N-CA-CB	5.29	119.02	110.13	7	3
1	A	76	PHE	CA-CB-CG	-5.26	108.54	113.80	4	10
2	B	125	GLN	N-CA-C	-5.24	105.47	111.07	1	10
1	A	92	HIS	CA-CB-CG	-5.21	108.58	113.80	3	7
2	B	30	LYS	CA-C-O	-5.18	115.74	120.50	1	10
1	A	79	ASP	CA-CB-CG	-5.17	107.43	112.60	7	3
1	A	78	ALA	N-CA-C	-5.14	107.17	113.50	8	10
2	B	26	HIS	CA-CB-CG	-5.12	108.68	113.80	8	7
2	B	225	VAL	CG1-CB-CG2	5.06	121.93	110.80	9	3
1	A	15	VAL	N-CA-CB	-5.06	106.58	112.34	9	3

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	B	84	ILE	CB	3
2	B	142	ILE	CB	3
2	B	199	ILE	CB	3

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	93	ARG	Sidechain	10
2	B	19	ARG	Sidechain	10
2	B	155	ARG	Sidechain	10
2	B	254	ARG	Sidechain	10

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	782	784	784	129±9
2	B	1921	1874	1877	68±13
4	B	43	32	32	4±0
All	All	27470	26900	26930	1697

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 31.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:115:ILE:CA	2:B:115:ILE:CB	1.58	1.75	1	2
2:B:131:VAL:CA	2:B:131:VAL:CB	1.56	1.78	3	4
1:A:64:LEU:HD23	2:B:118:PRO:CG	1.51	1.33	5	7
1:A:37:PRO:HD2	2:B:102:TYR:CZ	1.50	1.41	3	7
1:A:66:MET:HE3	2:B:119:LEU:CD2	1.46	1.36	1	4
1:A:64:LEU:HD21	2:B:1:TYR:CE1	1.45	1.43	3	9
1:A:66:MET:CE	2:B:118:PRO:O	1.42	1.66	5	4
1:A:37:PRO:HD2	2:B:102:TYR:CE2	1.38	1.52	7	9
1:A:64:LEU:CD2	2:B:118:PRO:HG3	1.37	1.46	5	6
1:A:66:MET:CE	2:B:119:LEU:CD2	1.31	2.06	1	1
1:A:36:VAL:HG12	2:B:104:GLN:NE2	1.28	1.40	3	8
1:A:37:PRO:HD2	2:B:102:TYR:CE1	1.28	1.62	8	3
1:A:37:PRO:HG2	2:B:102:TYR:CE2	1.27	1.64	6	2
1:A:66:MET:CE	2:B:119:LEU:HA	1.27	1.57	8	4
1:A:37:PRO:CD	2:B:102:TYR:CE2	1.24	2.21	6	9
1:A:66:MET:HE1	2:B:118:PRO:O	1.23	1.29	8	1
1:A:66:MET:HE2	2:B:118:PRO:O	1.21	1.02	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:PRO:CG	2:B:102:TYR:CE2	1.20	2.23	6	4
1:A:64:LEU:CD2	2:B:1:TYR:CE1	1.19	2.25	3	8
1:A:66:MET:CE	2:B:119:LEU:HD23	1.19	1.60	1	4
1:A:37:PRO:HG2	2:B:102:TYR:CZ	1.17	1.75	6	4
1:A:36:VAL:CG1	2:B:104:GLN:HE22	1.17	1.53	3	8
1:A:37:PRO:HD2	2:B:102:TYR:CD2	1.15	1.75	1	2
1:A:66:MET:HE2	2:B:118:PRO:C	1.10	1.71	5	3
1:A:37:PRO:CD	2:B:102:TYR:CZ	1.10	2.34	3	7
1:A:66:MET:HG3	2:B:118:PRO:O	1.07	1.49	6	2
2:B:46:PHE:CE1	2:B:131:VAL:HG22	1.06	1.85	4	10
1:A:64:LEU:HD21	2:B:1:TYR:CZ	1.06	1.85	2	4
2:B:115:ILE:CA	2:B:115:ILE:CG2	1.06	2.33	2	2
1:A:36:VAL:HG12	2:B:104:GLN:HE22	1.05	0.98	4	7
1:A:64:LEU:HD21	2:B:1:TYR:HE1	1.02	1.13	8	2
1:A:66:MET:HE3	2:B:119:LEU:HA	1.02	1.24	10	5
1:A:66:MET:HE3	2:B:119:LEU:HD21	1.01	1.06	1	2
1:A:43:PHE:HB2	1:A:59:LEU:HD12	1.00	1.33	6	10
1:A:64:LEU:HD23	2:B:118:PRO:HG3	0.99	1.23	3	5
1:A:66:MET:CG	2:B:118:PRO:O	0.99	2.10	6	2
2:B:46:PHE:CZ	2:B:131:VAL:CG2	0.99	2.45	4	10
2:B:131:VAL:CA	2:B:131:VAL:CG1	0.99	2.39	3	4
1:A:43:PHE:CB	1:A:59:LEU:HD12	0.98	1.89	4	10
1:A:37:PRO:CD	2:B:102:TYR:CE1	0.97	2.48	8	3
1:A:66:MET:CE	2:B:119:LEU:CA	0.96	2.44	8	4
1:A:37:PRO:HD2	2:B:102:TYR:HE2	0.96	1.19	7	3
1:A:37:PRO:CD	2:B:102:TYR:CD2	0.96	2.49	1	3
2:B:46:PHE:CZ	2:B:131:VAL:HG21	0.96	1.96	6	4
1:A:36:VAL:HA	2:B:104:GLN:HE22	0.95	1.20	6	4
1:A:36:VAL:CG1	2:B:104:GLN:NE2	0.94	2.30	8	3
2:B:79:PRO:HG2	2:B:82:PHE:CD1	0.94	1.98	6	10
2:B:115:ILE:CB	2:B:115:ILE:N	0.94	2.31	2	2
2:B:46:PHE:CE1	2:B:131:VAL:CG2	0.93	2.52	6	6
1:A:64:LEU:HD21	2:B:1:TYR:CD1	0.91	1.99	6	3
1:A:64:LEU:CD2	2:B:118:PRO:CG	0.91	2.25	5	5
1:A:64:LEU:HD11	2:B:1:TYR:OH	0.91	1.64	8	2
1:A:66:MET:CE	2:B:119:LEU:HD21	0.91	1.82	1	1
1:A:66:MET:HE3	2:B:119:LEU:HD23	0.91	1.41	7	6
2:B:115:ILE:CA	2:B:115:ILE:CG1	0.90	2.48	2	2
1:A:64:LEU:HD23	2:B:118:PRO:HG2	0.90	1.40	7	4
2:B:131:VAL:CA	2:B:131:VAL:CG2	0.90	2.49	5	4
1:A:37:PRO:CG	2:B:102:TYR:CD2	0.88	2.55	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:196:LEU:C	2:B:196:LEU:HD22	0.88	1.93	6	10
1:A:66:MET:HE2	2:B:119:LEU:HD23	0.87	1.43	1	1
1:A:36:VAL:HA	2:B:104:GLN:NE2	0.86	1.85	6	3
1:A:37:PRO:HG2	2:B:102:TYR:CD2	0.85	2.07	6	1
1:A:36:VAL:HG11	2:B:104:GLN:HE22	0.85	1.31	8	1
1:A:64:LEU:CD2	2:B:1:TYR:HE1	0.84	1.73	3	3
1:A:91:PRO:O	2:B:3:PHE:CE2	0.84	2.30	6	4
1:A:66:MET:HB3	2:B:119:LEU:CD2	0.83	2.04	6	1
2:B:115:ILE:CG2	2:B:115:ILE:C	0.83	2.52	1	2
1:A:66:MET:SD	2:B:118:PRO:O	0.82	2.37	6	2
1:A:68:PRO:HG3	2:B:100:ASP:O	0.81	1.76	6	1
1:A:37:PRO:HD2	2:B:102:TYR:OH	0.79	1.77	2	3
1:A:66:MET:HB3	2:B:119:LEU:HD23	0.79	1.53	6	2
1:A:36:VAL:HA	2:B:102:TYR:CE2	0.77	2.14	8	1
1:A:66:MET:CB	2:B:119:LEU:HD23	0.77	2.10	6	1
2:B:46:PHE:CZ	2:B:131:VAL:HG22	0.75	2.15	10	10
1:A:64:LEU:HD21	2:B:1:TYR:OH	0.75	1.82	2	1
1:A:64:LEU:CD2	2:B:1:TYR:OH	0.75	2.35	2	1
2:B:79:PRO:HG2	2:B:82:PHE:CE1	0.75	2.17	4	10
1:A:37:PRO:CG	2:B:102:TYR:CZ	0.74	2.61	6	4
2:B:131:VAL:CB	2:B:131:VAL:HA	0.74	2.07	5	2
1:A:21:LEU:C	1:A:21:LEU:CD2	0.74	2.61	4	10
1:A:64:LEU:HD21	2:B:118:PRO:HG3	0.73	1.60	9	3
2:B:159:GLN:N	2:B:159:GLN:CD	0.73	2.46	4	10
1:A:57:LYS:HE2	2:B:189:GLU:OE1	0.73	1.83	8	2
1:A:37:PRO:O	2:B:102:TYR:OH	0.73	2.07	8	5
2:B:131:VAL:CG1	2:B:131:VAL:N	0.72	2.52	6	4
1:A:64:LEU:HD22	2:B:1:TYR:CE1	0.72	2.20	5	2
1:A:64:LEU:CD2	2:B:1:TYR:CZ	0.72	2.71	2	3
1:A:47:LEU:HD12	1:A:47:LEU:N	0.71	2.01	4	5
2:B:196:LEU:C	2:B:196:LEU:CD2	0.71	2.63	6	10
1:A:43:PHE:CB	1:A:59:LEU:CD1	0.71	2.69	6	10
1:A:59:LEU:HG	1:A:60:SER:H	0.70	1.46	4	10
1:A:64:LEU:HD12	1:A:64:LEU:N	0.70	2.01	4	9
1:A:21:LEU:HD22	1:A:23:ILE:HG23	0.70	1.63	6	10
1:A:64:LEU:HD12	1:A:64:LEU:H	0.69	1.47	4	8
1:A:64:LEU:CD1	2:B:1:TYR:OH	0.69	2.38	8	3
1:A:47:LEU:N	1:A:47:LEU:CD1	0.69	2.55	4	5
2:B:131:VAL:CG2	2:B:131:VAL:C	0.69	2.66	5	4
1:A:66:MET:CE	2:B:118:PRO:C	0.69	2.66	8	1
1:A:66:MET:HE1	2:B:119:LEU:HA	0.68	1.61	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LEU:HD13	1:A:39:HIS:HB2	0.68	1.66	7	10
1:A:39:HIS:HB3	1:A:89:CYS:SG	0.68	2.29	9	10
1:A:68:PRO:CG	2:B:100:ASP:OD2	0.68	2.42	1	1
1:A:68:PRO:CG	2:B:100:ASP:O	0.67	2.42	6	1
1:A:15:VAL:HG22	1:A:16:PHE:N	0.67	2.03	6	10
1:A:37:PRO:HG2	2:B:102:TYR:CE1	0.67	2.25	6	6
1:A:15:VAL:CG2	1:A:16:PHE:N	0.67	2.58	6	10
1:A:66:MET:HE1	2:B:118:PRO:C	0.66	2.13	8	1
1:A:1:GLU:N	1:A:1:GLU:CD	0.65	2.55	7	10
2:B:171:LEU:HD23	2:B:171:LEU:C	0.65	2.17	4	10
1:A:20:LYS:O	1:A:20:LYS:NZ	0.65	2.30	6	10
1:A:47:LEU:CD1	1:A:47:LEU:N	0.65	2.60	3	5
2:B:34:VAL:HG13	2:B:50:VAL:HG22	0.64	1.69	6	6
1:A:47:LEU:N	1:A:47:LEU:HD12	0.64	2.05	3	5
1:A:66:MET:HE2	2:B:119:LEU:CA	0.64	2.22	8	1
2:B:139:ASP:CG	2:B:142:ILE:CG2	0.64	2.71	6	6
1:A:64:LEU:HD11	2:B:1:TYR:CZ	0.64	2.28	8	3
1:A:48:ASN:OD1	1:A:50:ALA:N	0.64	2.31	6	10
1:A:64:LEU:N	1:A:64:LEU:CD1	0.64	2.61	4	9
1:A:40:ASN:HD21	1:A:65:LEU:N	0.63	1.90	3	7
1:A:61:HIS:CG	1:A:62:LYS:H	0.63	2.12	4	10
1:A:38:PRO:HG3	1:A:66:MET:SD	0.62	2.34	6	10
1:A:24:LYS:N	1:A:24:LYS:HD3	0.62	2.10	4	10
1:A:53:ALA:O	1:A:59:LEU:HD21	0.62	1.95	8	10
2:B:139:ASP:CG	2:B:142:ILE:HG23	0.62	2.20	5	10
1:A:61:HIS:CG	1:A:62:LYS:N	0.61	2.69	3	10
2:B:22:CYS:SG	4:B:255:HEC:CAB	0.61	2.88	7	10
2:B:171:LEU:HD23	2:B:172:TYR:N	0.61	2.10	4	10
1:A:68:PRO:HB2	2:B:100:ASP:OD2	0.61	1.95	10	1
2:B:136:PRO:HG2	2:B:144:PHE:CZ	0.61	2.31	8	10
1:A:40:ASN:HD21	1:A:64:LEU:N	0.60	1.93	8	2
2:B:131:VAL:CB	2:B:131:VAL:C	0.60	2.72	3	1
1:A:64:LEU:H	1:A:64:LEU:HD12	0.60	1.57	9	2
1:A:66:MET:HE2	2:B:118:PRO:N	0.60	2.11	5	1
1:A:66:MET:HE3	2:B:119:LEU:CG	0.60	2.26	6	1
1:A:66:MET:CG	2:B:119:LEU:HD23	0.60	2.27	6	1
1:A:1:GLU:N	1:A:27:ASP:CG	0.60	2.60	4	10
1:A:64:LEU:N	1:A:64:LEU:HD12	0.59	2.11	8	1
1:A:61:HIS:O	1:A:62:LYS:HB3	0.59	1.97	4	10
1:A:66:MET:HE3	2:B:118:PRO:O	0.59	1.86	5	1
2:B:234:ASN:C	2:B:234:ASN:OD1	0.59	2.45	4	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:PRO:HG2	2:B:100:ASP:OD2	0.59	1.96	1	3
2:B:41:LEU:N	2:B:41:LEU:HD22	0.59	2.11	4	10
1:A:40:ASN:ND2	1:A:63:GLN:C	0.59	2.61	8	4
1:A:59:LEU:CG	1:A:60:SER:H	0.59	2.11	4	10
1:A:32:LEU:C	1:A:32:LEU:HD23	0.58	2.23	6	10
1:A:40:ASN:HD21	1:A:63:GLN:C	0.57	2.06	8	3
2:B:196:LEU:HD13	2:B:196:LEU:N	0.57	2.15	6	10
2:B:236:ASN:OD1	2:B:236:ASN:C	0.57	2.48	8	10
1:A:43:PHE:HB2	1:A:59:LEU:CD1	0.57	2.22	6	10
1:A:39:HIS:CB	1:A:89:CYS:SG	0.57	2.93	9	10
1:A:1:GLU:N	1:A:27:ASP:OD2	0.56	2.38	8	10
1:A:40:ASN:ND2	1:A:64:LEU:N	0.56	2.53	8	3
1:A:61:HIS:O	1:A:62:LYS:CB	0.56	2.53	6	10
1:A:91:PRO:O	2:B:3:PHE:CD2	0.56	2.58	3	5
1:A:1:GLU:CD	1:A:1:GLU:H1	0.56	2.09	3	7
1:A:40:ASN:ND2	1:A:65:LEU:HG	0.56	2.16	3	7
2:B:115:ILE:C	2:B:115:ILE:HG23	0.56	2.26	2	2
1:A:21:LEU:HD13	1:A:23:ILE:CG2	0.55	2.31	6	10
1:A:34:ASN:OD1	1:A:35:LYS:N	0.55	2.39	7	10
1:A:64:LEU:CD1	1:A:64:LEU:N	0.55	2.69	8	1
2:B:115:ILE:C	2:B:115:ILE:HG22	0.55	2.27	1	2
1:A:37:PRO:CG	2:B:102:TYR:CE1	0.55	2.90	3	2
1:A:91:PRO:O	2:B:3:PHE:HE2	0.55	1.84	6	1
1:A:48:ASN:HD21	1:A:50:ALA:C	0.55	2.10	6	7
1:A:28:THR:HG22	1:A:28:THR:O	0.54	2.02	6	10
2:B:102:TYR:O	2:B:102:TYR:CG	0.54	2.59	8	10
1:A:66:MET:HE2	2:B:118:PRO:CA	0.54	2.30	5	1
1:A:40:ASN:CB	1:A:62:LYS:HA	0.54	2.33	9	9
2:B:199:ILE:HG13	2:B:199:ILE:O	0.54	2.03	6	2
1:A:13:LEU:HG	1:A:14:LEU:N	0.54	2.18	4	10
2:B:8:THR:O	2:B:8:THR:OG1	0.54	2.25	4	9
2:B:142:ILE:HD11	2:B:249:LEU:HD22	0.54	1.80	6	4
1:A:21:LEU:C	1:A:21:LEU:HD23	0.54	2.26	6	10
1:A:59:LEU:CG	1:A:60:SER:N	0.54	2.70	6	10
1:A:55:LEU:C	1:A:55:LEU:HD12	0.54	2.28	4	10
1:A:62:LYS:O	1:A:63:GLN:CB	0.53	2.56	8	10
1:A:66:MET:CE	2:B:119:LEU:HG	0.53	2.34	6	1
1:A:82:ALA:N	1:A:105:GLY:HA2	0.53	2.19	6	10
1:A:11:LYS:CE	1:A:11:LYS:O	0.53	2.56	4	8
1:A:40:ASN:ND2	1:A:65:LEU:N	0.53	2.57	4	7
1:A:42:VAL:HG22	1:A:88:TYR:CB	0.53	2.34	4	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:136:PRO:CG	2:B:144:PHE:CZ	0.53	2.91	6	7
2:B:196:LEU:HD22	2:B:196:LEU:O	0.53	2.04	6	7
2:B:34:VAL:CG2	2:B:151:VAL:HG11	0.53	2.34	6	4
2:B:115:ILE:CA	2:B:115:ILE:HG13	0.52	2.31	2	2
2:B:35:GLU:N	2:B:35:GLU:OE1	0.52	2.42	7	10
1:A:40:ASN:HD21	1:A:64:LEU:C	0.52	2.11	4	6
1:A:15:VAL:CG2	1:A:16:PHE:H	0.52	2.18	6	10
1:A:11:LYS:O	1:A:11:LYS:NZ	0.52	2.43	4	10
1:A:18:PRO:O	1:A:20:LYS:N	0.52	2.43	3	10
1:A:48:ASN:OD1	1:A:48:ASN:C	0.52	2.53	6	7
2:B:159:GLN:N	2:B:159:GLN:OE1	0.52	2.43	6	10
1:A:66:MET:HE3	2:B:119:LEU:HG	0.52	1.81	6	1
1:A:16:PHE:CE1	1:A:97:MET:HG2	0.52	2.40	7	10
1:A:88:TYR:O	1:A:90:GLU:N	0.52	2.43	5	10
1:A:21:LEU:HD23	1:A:22:THR:N	0.51	2.20	4	10
1:A:57:LYS:CE	2:B:189:GLU:OE1	0.51	2.57	8	2
1:A:14:LEU:HD21	1:A:36:VAL:CG2	0.51	2.36	4	10
1:A:59:LEU:HG	1:A:60:SER:N	0.51	2.19	6	5
1:A:11:LYS:O	1:A:11:LYS:CE	0.51	2.58	2	2
2:B:130:PRO:C	2:B:131:VAL:HG12	0.51	2.31	5	6
1:A:62:LYS:NZ	1:A:63:GLN:HB2	0.51	2.21	8	10
1:A:64:LEU:CD2	2:B:1:TYR:CD1	0.50	2.83	6	1
1:A:66:MET:HE2	2:B:119:LEU:HA	0.50	1.83	9	1
1:A:6:LYS:O	1:A:8:GLY:N	0.50	2.45	8	10
1:A:42:VAL:CG2	1:A:88:TYR:HB2	0.50	2.36	6	10
1:A:16:PHE:CE1	1:A:97:MET:CG	0.50	2.95	7	10
2:B:70:LEU:HD12	2:B:70:LEU:N	0.50	2.22	4	10
1:A:1:GLU:H2	1:A:27:ASP:CG	0.50	2.15	3	10
1:A:43:PHE:H	1:A:60:SER:CB	0.50	2.20	9	10
1:A:20:LYS:O	1:A:20:LYS:HG3	0.50	2.07	4	10
1:A:21:LEU:C	1:A:21:LEU:HD22	0.50	2.30	6	10
1:A:64:LEU:HD23	2:B:118:PRO:CB	0.50	2.33	9	1
1:A:43:PHE:HB3	1:A:59:LEU:CD1	0.49	2.38	8	10
1:A:48:ASN:OD1	1:A:49:PRO:N	0.49	2.45	6	5
2:B:46:PHE:HZ	2:B:131:VAL:HG21	0.49	1.61	4	2
1:A:66:MET:HE2	2:B:119:LEU:CD2	0.48	2.10	1	1
1:A:55:LEU:HG	1:A:59:LEU:CD2	0.48	2.39	9	7
1:A:40:ASN:HB2	1:A:62:LYS:HA	0.48	1.85	8	4
1:A:9:SER:O	1:A:11:LYS:N	0.48	2.47	3	10
1:A:87:PHE:CE2	1:A:99:GLY:HA3	0.48	2.44	6	10
2:B:25:CYS:SG	4:B:255:HEC:HBC3	0.48	2.49	10	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:75:VAL:HG23	2:B:115:ILE:HD11	0.48	1.85	1	5
1:A:64:LEU:HD22	2:B:1:TYR:HE1	0.48	1.62	3	1
1:A:57:LYS:C	1:A:59:LEU:N	0.47	2.71	4	10
2:B:34:VAL:HG22	2:B:151:VAL:HG11	0.47	1.86	7	8
1:A:8:GLY:O	1:A:10:ASP:N	0.47	2.48	7	10
1:A:59:LEU:HD12	1:A:60:SER:N	0.47	2.25	9	10
2:B:171:LEU:C	2:B:171:LEU:CD2	0.47	2.87	4	10
1:A:13:LEU:HG	1:A:14:LEU:H	0.47	1.69	4	7
1:A:39:HIS:HA	1:A:89:CYS:SG	0.46	2.50	1	10
2:B:131:VAL:N	2:B:131:VAL:HG12	0.46	2.25	6	2
2:B:41:LEU:N	2:B:41:LEU:CD2	0.46	2.78	4	4
1:A:83:GLY:HA3	1:A:85:TYR:CE1	0.46	2.46	7	10
1:A:87:PHE:CD1	1:A:87:PHE:N	0.46	2.83	6	7
1:A:87:PHE:N	1:A:87:PHE:CD1	0.46	2.84	4	3
1:A:32:LEU:CB	1:A:71:SER:OG	0.46	2.64	4	10
1:A:43:PHE:CD2	1:A:59:LEU:HB2	0.46	2.46	6	6
2:B:115:ILE:HG23	2:B:116:VAL:N	0.46	2.24	6	3
1:A:21:LEU:CD2	1:A:23:ILE:HG23	0.45	2.39	6	8
1:A:13:LEU:CG	1:A:14:LEU:N	0.45	2.79	4	7
1:A:36:VAL:HG12	2:B:104:GLN:HE21	0.45	1.59	2	1
1:A:42:VAL:CG2	1:A:88:TYR:CB	0.45	2.95	4	10
1:A:7:LEU:C	1:A:97:MET:HE2	0.45	2.37	6	10
1:A:68:PRO:HG3	2:B:100:ASP:OD2	0.45	2.11	1	1
1:A:85:TYR:CD1	1:A:85:TYR:N	0.45	2.84	2	10
1:A:89:CYS:HB2	1:A:97:MET:HG2	0.45	1.89	8	10
2:B:131:VAL:C	2:B:131:VAL:HG23	0.45	2.36	5	2
1:A:41:VAL:HG23	1:A:41:VAL:O	0.45	2.11	7	9
1:A:24:LYS:HB3	1:A:25:PRO:HD2	0.44	1.89	6	6
1:A:101:ILE:O	1:A:101:ILE:HG22	0.44	2.12	6	4
1:A:64:LEU:HD13	2:B:1:TYR:OH	0.44	2.12	3	1
2:B:102:TYR:O	2:B:102:TYR:CD2	0.44	2.71	7	8
2:B:213:ALA:C	2:B:215:PRO:HD2	0.44	2.38	4	4
1:A:21:LEU:CD1	1:A:23:ILE:CG2	0.44	2.96	6	9
1:A:42:VAL:HG22	1:A:88:TYR:HB2	0.44	1.90	6	2
2:B:149:VAL:O	2:B:149:VAL:CG2	0.44	2.65	3	3
1:A:53:ALA:O	1:A:54:ASP:C	0.43	2.61	4	10
1:A:21:LEU:HD22	1:A:23:ILE:CG2	0.43	2.40	4	3
1:A:21:LEU:HD13	1:A:23:ILE:HG23	0.43	1.89	7	7
1:A:88:TYR:CE2	1:A:93:ARG:HG3	0.43	2.48	4	5
1:A:88:TYR:CE2	1:A:93:ARG:NE	0.43	2.87	6	2
1:A:79:ASP:OD1	1:A:79:ASP:N	0.43	2.52	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:LYS:O	1:A:36:VAL:C	0.43	2.62	7	10
2:B:196:LEU:N	2:B:196:LEU:CD1	0.43	2.82	6	2
1:A:101:ILE:HG22	1:A:101:ILE:O	0.43	2.12	4	1
1:A:55:LEU:HD12	1:A:56:ALA:CB	0.43	2.44	5	10
1:A:23:ILE:HD11	1:A:103:VAL:CG2	0.43	2.44	9	8
4:B:255:HEC:HMC1	4:B:255:HEC:CBC	0.43	2.44	1	10
1:A:66:MET:HG3	2:B:119:LEU:HA	0.43	1.91	6	1
2:B:102:TYR:CD2	2:B:102:TYR:O	0.42	2.72	6	2
1:A:86:THR:HG23	1:A:99:GLY:O	0.42	2.14	4	3
1:A:93:ARG:O	1:A:93:ARG:CD	0.42	2.68	6	4
1:A:39:HIS:CA	1:A:89:CYS:SG	0.42	3.08	9	10
1:A:81:PRO:O	1:A:83:GLY:N	0.42	2.53	7	10
1:A:66:MET:HE1	2:B:119:LEU:HD23	0.42	1.91	8	1
1:A:37:PRO:HG2	2:B:102:TYR:CD1	0.42	2.50	1	1
1:A:43:PHE:HB2	1:A:60:SER:CA	0.42	2.45	9	8
1:A:64:LEU:HD22	2:B:1:TYR:OH	0.42	2.11	2	1
1:A:40:ASN:OD1	1:A:64:LEU:N	0.42	2.53	7	2
1:A:55:LEU:CG	1:A:59:LEU:HD22	0.42	2.45	9	3
1:A:23:ILE:CD1	1:A:103:VAL:CG2	0.42	2.98	7	4
1:A:52:SER:O	1:A:53:ALA:C	0.42	2.63	2	10
1:A:64:LEU:CD1	2:B:1:TYR:CZ	0.42	3.03	3	1
1:A:13:LEU:CG	1:A:14:LEU:H	0.42	2.27	6	2
1:A:66:MET:CE	2:B:118:PRO:N	0.42	2.82	5	1
1:A:90:GLU:CB	1:A:91:PRO:CD	0.42	2.98	7	10
1:A:75:THR:HG22	1:A:76:PHE:N	0.42	2.30	8	3
2:B:131:VAL:N	2:B:131:VAL:HG13	0.41	2.29	3	1
2:B:25:CYS:SG	4:B:255:HEC:CBC	0.41	3.08	10	10
1:A:42:VAL:CG1	1:A:62:LYS:HB3	0.41	2.46	8	2
1:A:40:ASN:HD21	1:A:64:LEU:CA	0.41	2.28	10	1
1:A:14:LEU:C	1:A:97:MET:HE3	0.41	2.41	6	5
2:B:136:PRO:HG3	2:B:144:PHE:CZ	0.41	2.51	6	2
1:A:66:MET:HG3	2:B:119:LEU:HD23	0.41	1.91	6	1
1:A:59:LEU:CD1	1:A:60:SER:N	0.41	2.84	4	4
1:A:41:VAL:HG12	1:A:88:TYR:C	0.41	2.41	9	4
1:A:93:ARG:CD	1:A:93:ARG:C	0.41	2.94	4	2
1:A:89:CYS:CB	1:A:97:MET:HG2	0.41	2.46	9	2
2:B:84:ILE:HG22	2:B:114:VAL:HG11	0.40	1.93	10	1
2:B:136:PRO:HG2	2:B:144:PHE:CE2	0.40	2.50	8	3
1:A:23:ILE:CD1	1:A:103:VAL:HG22	0.40	2.47	8	1
1:A:70:GLN:CG	1:A:71:SER:N	0.40	2.84	4	1
2:B:170:ASN:ND2	2:B:170:ASN:C	0.40	2.78	4	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	103/105 (98%)	50±0 (49±0%)	30±0 (29±0%)	23±0 (22±0%)	0 2
2	B	252/254 (99%)	229±0 (91±0%)	23±0 (9±0%)	0±0 (0±0%)	100 100
All	All	3550/3590 (99%)	2790 (79%)	530 (15%)	230 (6%)	2 18

All 23 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	2	THR	10
1	A	7	LEU	10
1	A	9	SER	10
1	A	10	ASP	10
1	A	18	PRO	10
1	A	19	ALA	10
1	A	25	PRO	10
1	A	27	ASP	10
1	A	28	THR	10
1	A	44	ASP	10
1	A	53	ALA	10
1	A	56	ALA	10
1	A	62	LYS	10
1	A	63	GLN	10
1	A	64	LEU	10
1	A	68	PRO	10
1	A	82	ALA	10
1	A	85	TYR	10
1	A	89	CYS	10
1	A	90	GLU	10
1	A	93	ARG	10
1	A	96	GLY	10
1	A	104	ALA	10

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	85/85 (100%)	75±1 (88±1%)	10±1 (12±1%)	7 49
2	B	209/209 (100%)	186±0 (89±0%)	23±0 (11±0%)	8 51
All	All	2940/2940 (100%)	2610 (89%)	330 (11%)	8 51

All 35 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	11	LYS	10
1	A	20	LYS	10
1	A	21	LEU	10
1	A	24	LYS	10
1	A	48	ASN	10
1	A	62	LYS	10
1	A	79	ASP	10
1	A	101	ILE	10
2	B	34	VAL	10
2	B	36	VAL	10
2	B	47	LYS	10
2	B	72	VAL	10
2	B	84	ILE	10
2	B	115	ILE	10
2	B	116	VAL	10
2	B	123	GLN	10
2	B	131	VAL	10
2	B	138	ASN	10
2	B	142	ILE	10
2	B	149	VAL	10
2	B	155	ARG	10
2	B	160	VAL	10
2	B	170	ASN	10
2	B	183	ILE	10
2	B	193	VAL	10
2	B	196	LEU	10
2	B	197	VAL	10
2	B	199	ILE	10

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Mol	Chain	Res	Type	Models (Total)
2	B	217	LEU	10
2	B	225	VAL	10
2	B	234	ASN	10
1	A	93	ARG	9
1	A	59	LEU	6
1	A	40	ASN	3
1	A	17	GLU	2

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

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	255	2	46,50,50	2.92±0.00	23±0 (50±0%)

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

considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	HEC	B	255	2	58,82,82	1.82±0.00	10±0 (17±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEC	B	255	2	-	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
4	B	255	HEC	C1B-NB	6.64	1.27	1.39	1	10
4	B	255	HEC	CHB-C4A	6.61	1.51	1.38	1	10
4	B	255	HEC	CHA-C1A	6.59	1.51	1.38	1	10
4	B	255	HEC	C4B-NB	6.54	1.27	1.39	1	10
4	B	255	HEC	C4D-ND	6.48	1.27	1.39	1	10
4	B	255	HEC	C1D-ND	6.35	1.27	1.39	1	10
4	B	255	HEC	C1C-NC	3.15	1.33	1.39	1	10
4	B	255	HEC	C4C-NC	2.96	1.34	1.39	1	10
4	B	255	HEC	C1A-C2A	2.95	1.40	1.45	1	10
4	B	255	HEC	C4A-C3A	2.75	1.39	1.45	1	10
4	B	255	HEC	C1D-C2D	2.54	1.49	1.43	1	10
4	B	255	HEC	O2A-CGA	2.52	1.22	1.30	5	10
4	B	255	HEC	C4A-NA	2.49	1.34	1.39	1	10
4	B	255	HEC	CHA-C4D	2.49	1.33	1.39	1	10
4	B	255	HEC	O2D-CGD	2.48	1.22	1.30	7	10
4	B	255	HEC	C1C-C2C	2.43	1.48	1.43	1	10
4	B	255	HEC	CHB-C1B	2.34	1.34	1.39	1	10
4	B	255	HEC	CHD-C1D	2.33	1.34	1.39	1	10
4	B	255	HEC	C1A-NA	2.33	1.35	1.39	1	10
4	B	255	HEC	C3B-C4B	2.32	1.50	1.46	1	10
4	B	255	HEC	C1B-C2B	2.11	1.48	1.43	1	10
4	B	255	HEC	C3C-C2C	2.08	1.34	1.41	1	10
4	B	255	HEC	CHC-C1C	2.05	1.34	1.39	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
4	B	255	HEC	C4D-ND-C1D	6.35	116.17	105.82	1	10
4	B	255	HEC	C4B-NB-C1B	6.22	115.96	105.82	1	10
4	B	255	HEC	C3D-C4D-ND	3.88	105.85	110.15	1	10
4	B	255	HEC	C2D-C1D-ND	2.87	105.54	110.14	1	10
4	B	255	HEC	C1C-CHC-C4B	2.80	133.31	124.66	1	10
4	B	255	HEC	CMD-C2D-C1D	2.63	129.42	125.42	1	10
4	B	255	HEC	C2B-C1B-NB	2.58	106.01	110.14	1	10
4	B	255	HEC	CHA-C4D-ND	2.57	128.53	123.86	1	10
4	B	255	HEC	O2A-CGA-CBA	2.20	120.95	114.00	7	10
4	B	255	HEC	C1D-CHD-C4C	2.04	130.95	124.66	1	10

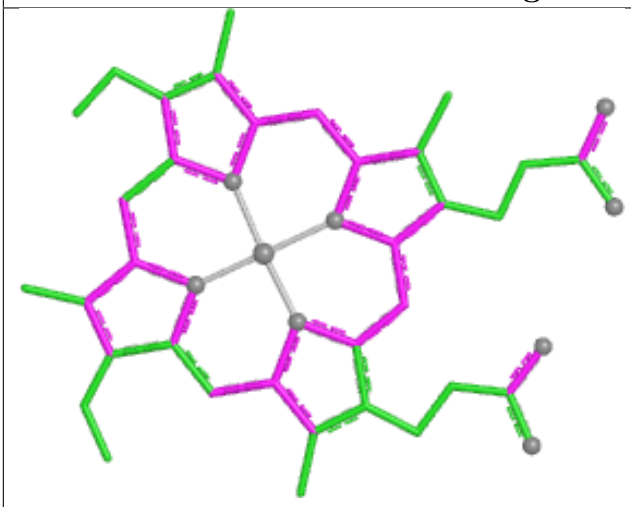
There are no chirality outliers.

There are no torsion outliers.

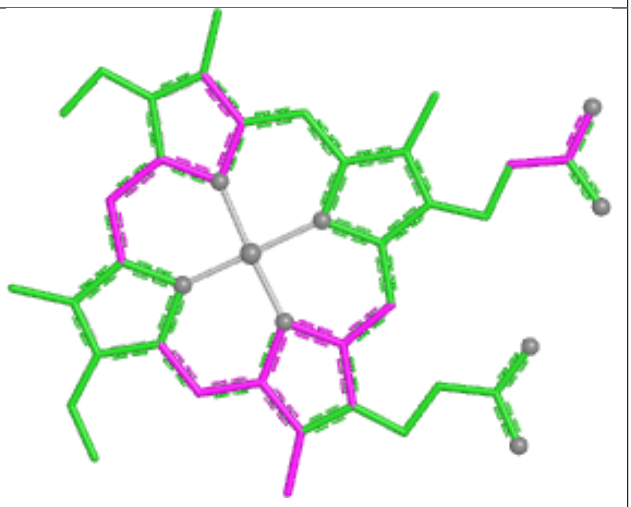
There are no ring outliers.

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.

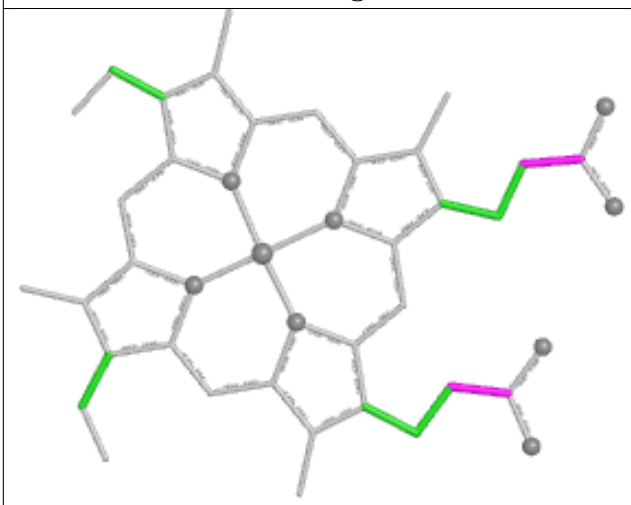
Ligand HEC B 255



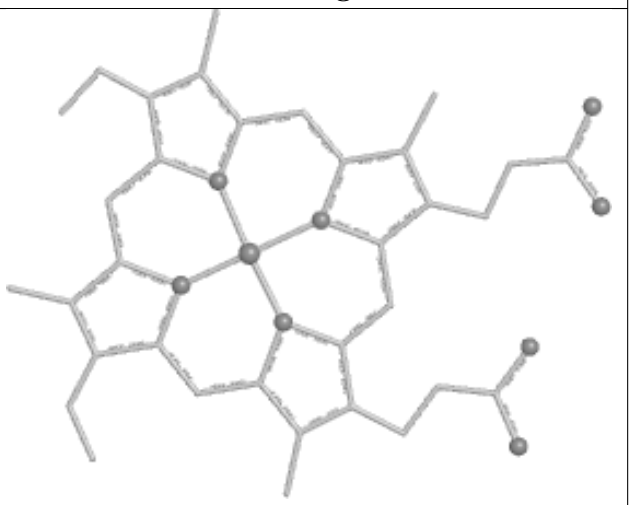
Bond lengths



Bond angles



Torsions



Rings

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided