Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 08:49 pm BST

PDB ID	:	1TU2
Title	:	THE COMPLEX OF NOSTOC CYTOCHROME F AND PLASTOCYANIN DETERMIN WITH PARAMAGNETIC NMR. BASED ON THE STRUCTURES OF CYTOCHROME F AND PLASTOCYANIN, 10 STRUCTURES
Authors	:	Diaz-Moreno, I.; Diaz-Quintana, A.; De la Rosa, M.A.; Ubbink, M.
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 following versions of software and data (see references (1)) were used in the production of this report:

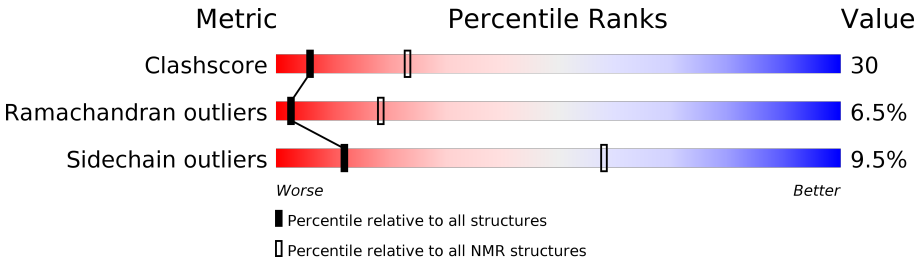
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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	105	31% 44% 22% ·
2	B	254	81% 15% · ·

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)	0.06	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

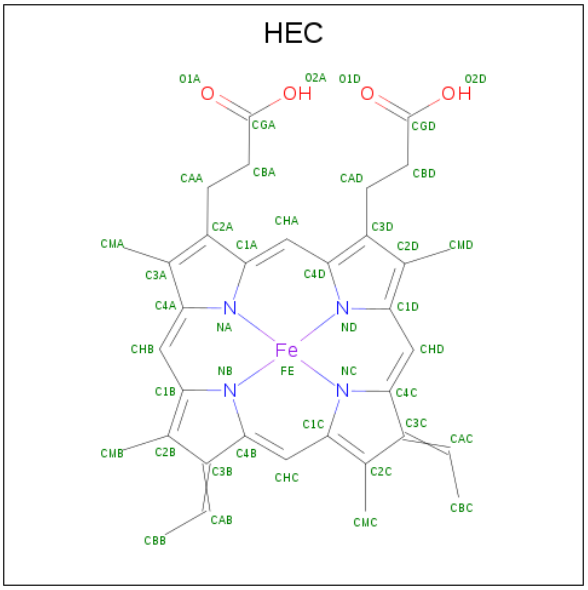
- Molecule 2 is a protein called Apocytochrome f.

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 (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

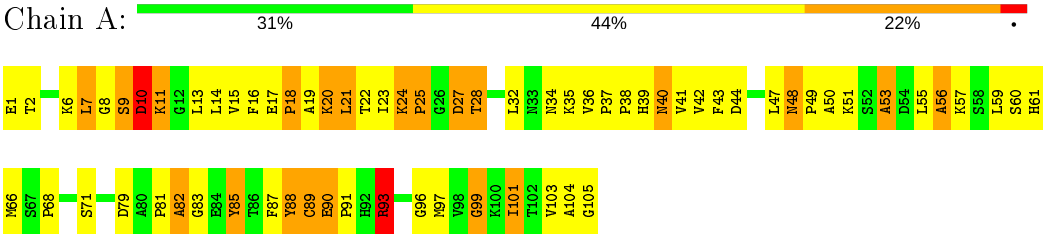
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

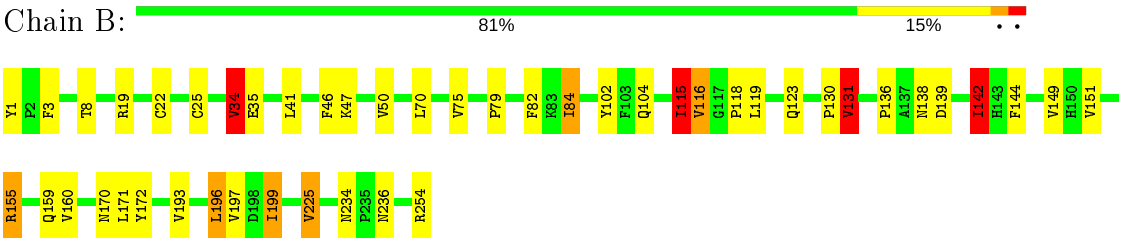
• Molecule 1: Plastocyanin

Chain A:



• Molecule 2: Apocytochrome f

Chain B:



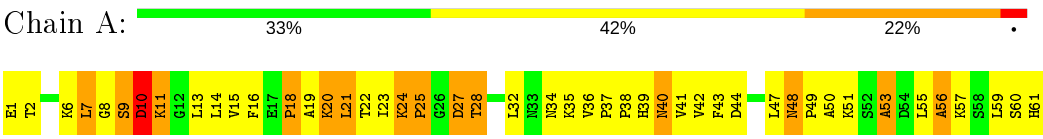
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

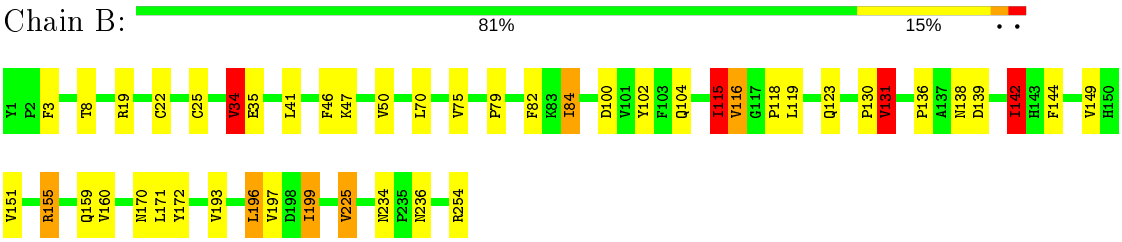
4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Plastocyanin

Chain A:

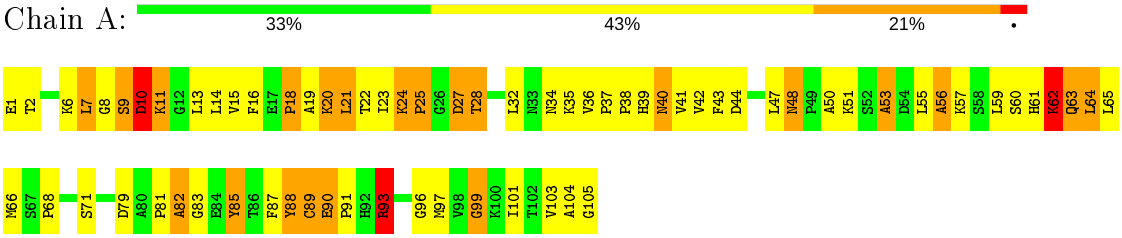


• Molecule 2: Apocytochrome f

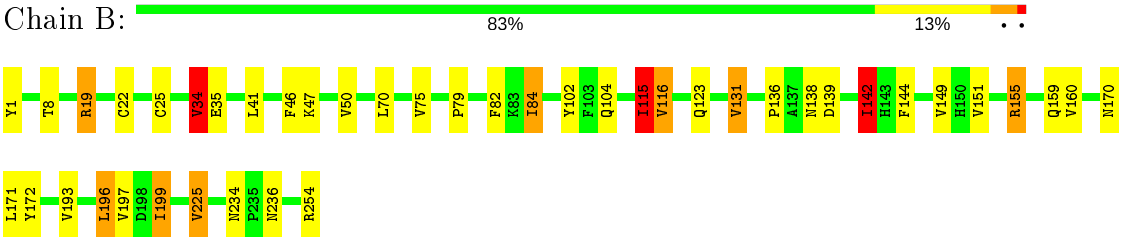


4.2.2 Score per residue for model 2

• Molecule 1: Plastocyanin

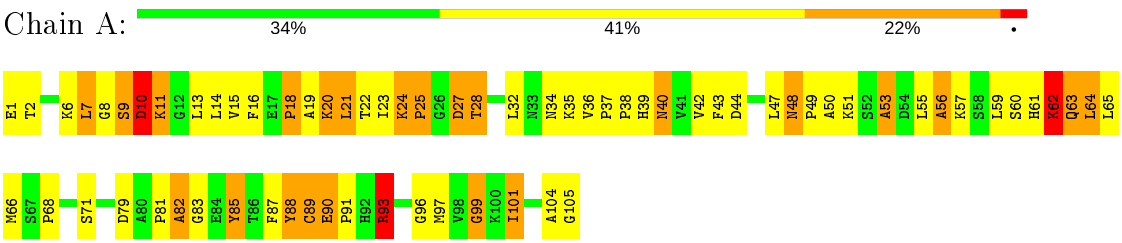


• Molecule 2: Apocytochrome f



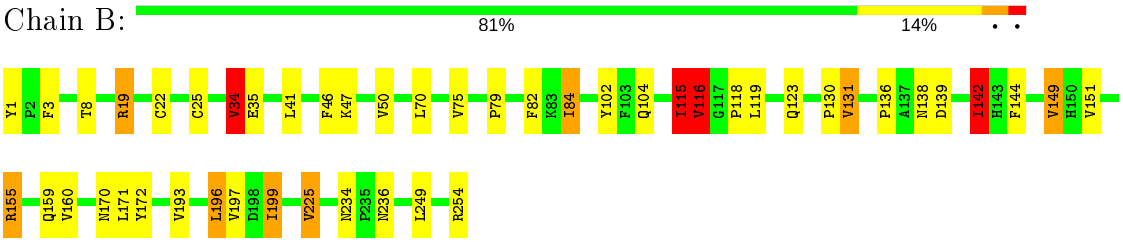
4.2.3 Score per residue for model 3

• Molecule 1: Plastocyanin



• Molecule 2: Apocytochrome f

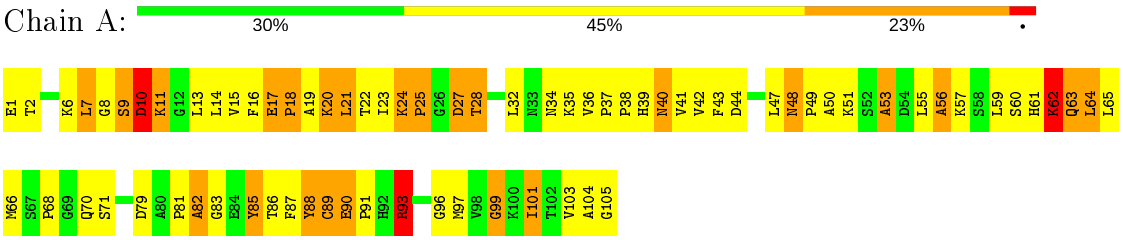
Chain B:



4.2.4 Score per residue for model 4

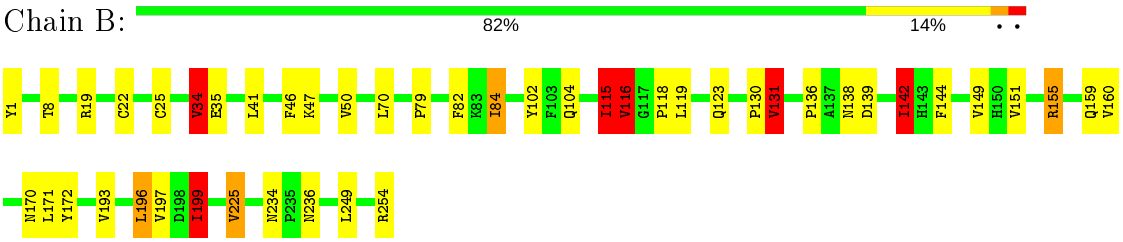
- Molecule 1: Plastocyanin

Chain A:



- Molecule 2: Apocytochrome f

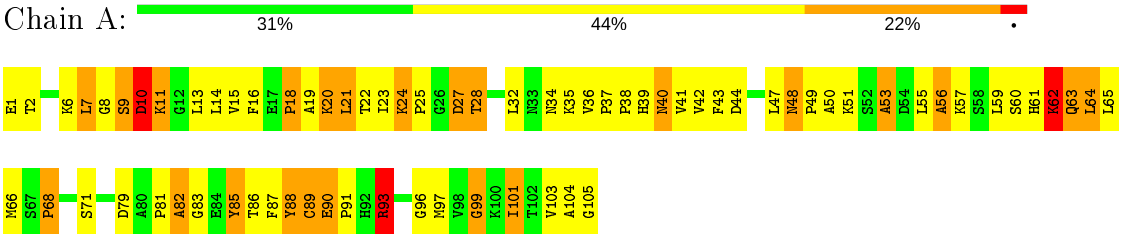
Chain B:



4.2.5 Score per residue for model 5

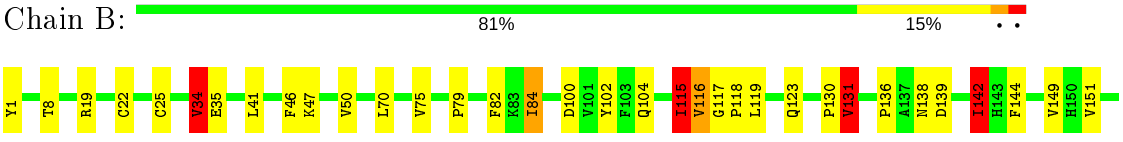
- Molecule 1: Plastocyanin

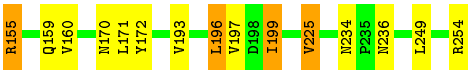
Chain A:



- Molecule 2: Apocytochrome f

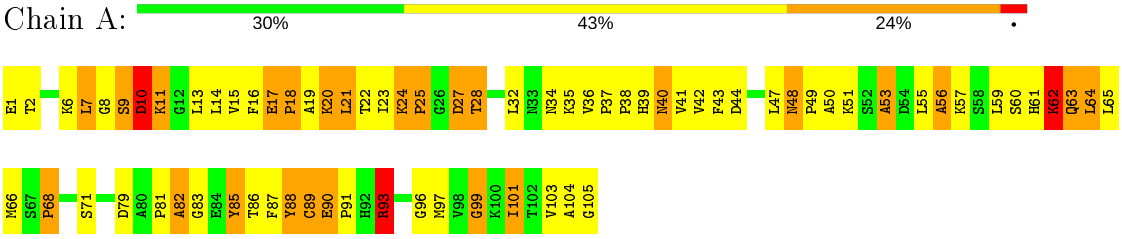
Chain B:



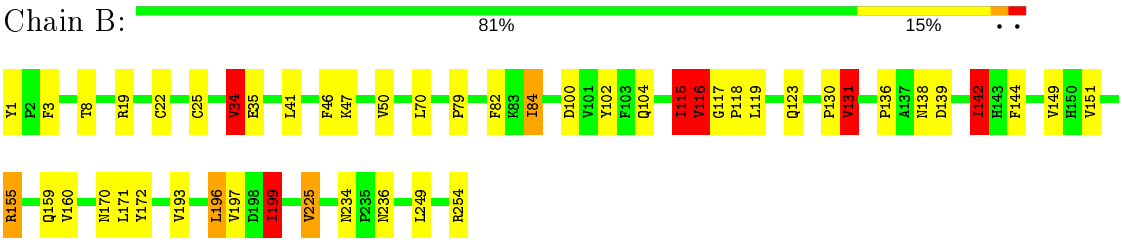


4.2.6 Score per residue for model 6

- Molecule 1: Plastocyanin

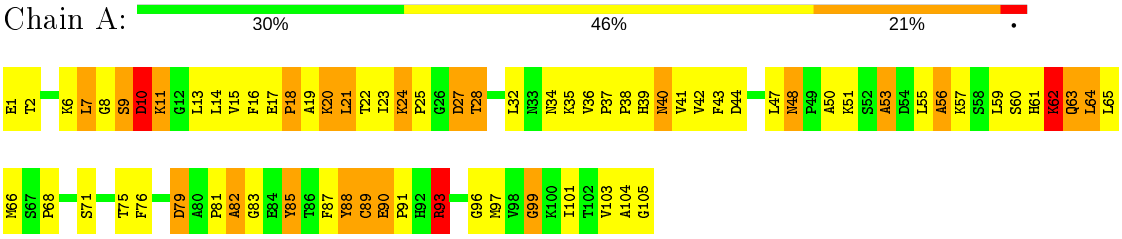


- Molecule 2: Apocytochrome f

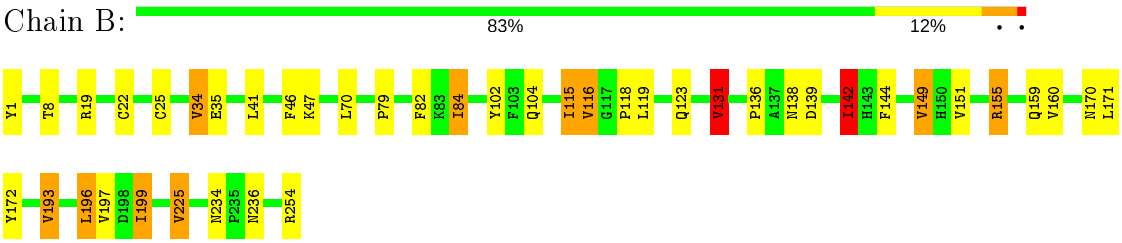


4.2.7 Score per residue for model 7

- Molecule 1: Plastocyanin



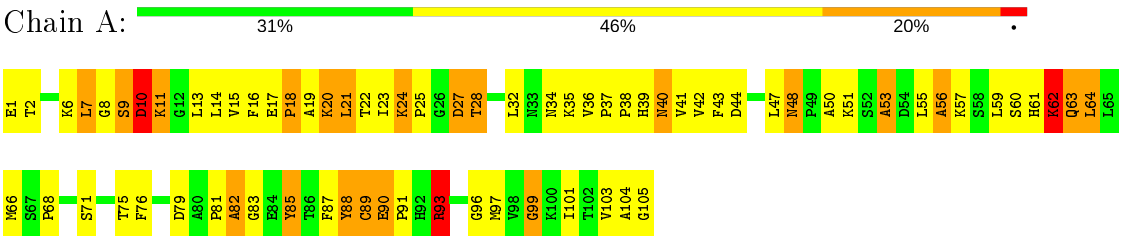
- Molecule 2: Apocytochrome f



4.2.8 Score per residue for model 8

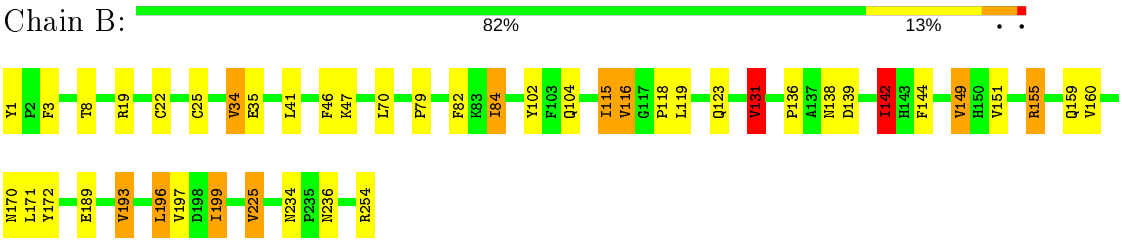
- Molecule 1: Plastocyanin

Chain A:



- Molecule 2: Apocytochrome f

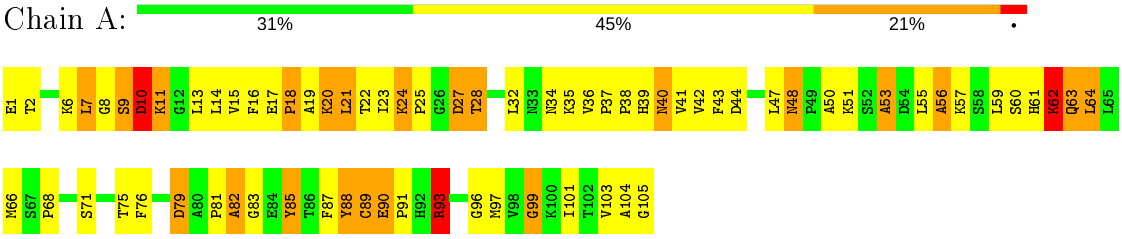
Chain B:



4.2.9 Score per residue for model 9

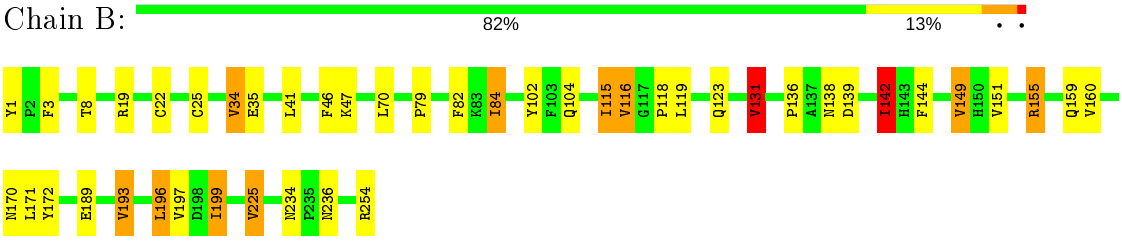
- Molecule 1: Plastocyanin

Chain A:



- Molecule 2: Apocytochrome f

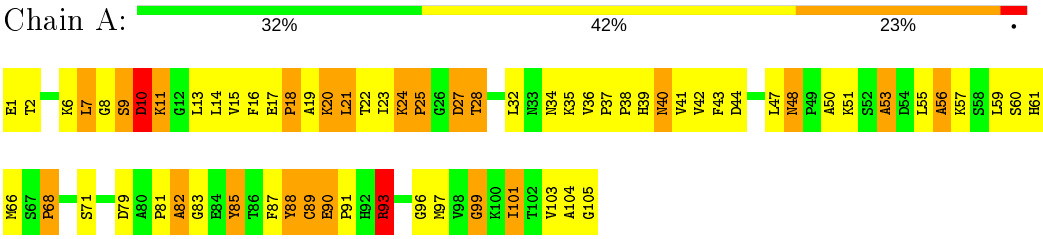
Chain B:



4.2.10 Score per residue for model 10

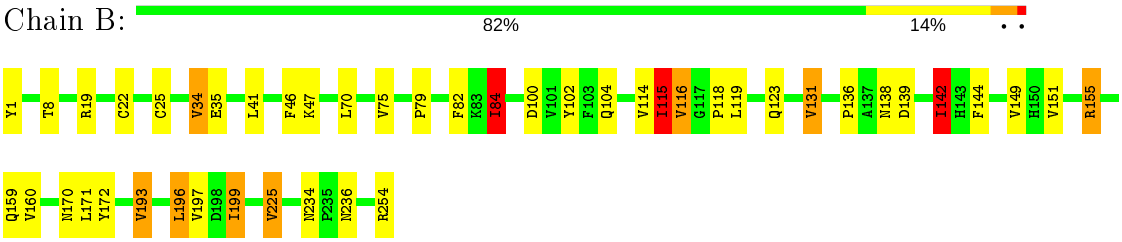
- Molecule 1: Plastocyanin

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. No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	782	784	784	122±9
2	B	1921	1874	1877	66±12
4	B	43	32	32	4±0
All	All	27470	26900	26930	1607

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 30.

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	1
2:B:115:ILE:CB	2:B:115:ILE:CA	1.57	1.78	2	1
2:B:131:VAL:CB	2:B:131:VAL:CA	1.56	1.78	3	3
2:B:131:VAL:CA	2:B:131:VAL:CB	1.56	1.78	4	1
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	2
1:A:66:MET:HE2	2:B:119:LEU:CD2	1.31	1.55	1	1
1:A:66:MET:HE1	2:B:118:PRO:O	1.29	1.20	8	2
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: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	5
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:O	1.15	1.37	6	2
1:A:37:PRO:CD	2:B:102:TYR:CZ	1.10	2.34	3	7
1:A:66:MET:HE2	2:B:118:PRO:C	1.10	1.66	5	2
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
1:A:66:MET:HE3	2:B:119:LEU:HA	1.06	1.23	10	4
2:B:115:ILE:CG2	2:B:115:ILE:CA	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:HD21	1.01	1.21	1	1
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	2
1:A:43:PHE:CB	1:A:59:LEU:HD12	0.98	1.89	4	10
2:B:131:VAL:CG1	2:B:131:VAL:CA	0.98	2.41	6	2
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:115:ILE:CB	2:B:115:ILE:N	0.94	2.31	2	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:79:PRO:HG2	2:B:82:PHE:CD1	0.94	1.98	6	10
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
2:B:115:ILE:CG1	2:B:115:ILE:CA	0.90	2.48	2	1
1:A:64:LEU:HD23	2:B:118:PRO:HG2	0.90	1.40	7	4
2:B:131:VAL:CG2	2:B:131:VAL:CA	0.90	2.49	5	2
2:B:131:VAL:CA	2:B:131:VAL:CG2	0.89	2.51	3	2
1:A:37:PRO:CG	2:B:102:TYR:CD2	0.88	2.55	6	2
2:B:115:ILE:CA	2:B:115:ILE:CG1	0.87	2.52	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
2:B:196:LEU:HD22	2:B:196:LEU:C	0.84	1.93	6	6
1:A:66:MET:HB3	2:B:119:LEU:CD2	0.83	2.04	6	1
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
2:B:115:ILE:C	2:B:115:ILE:CG2	0.78	2.52	1	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:196:LEU:C	2:B:196:LEU:HD22	0.76	2.01	5	4
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
2:B:131:VAL:CB	2:B:131:VAL:HA	0.74	2.07	5	2
1:A:37:PRO:CG	2:B:102:TYR:CZ	0.74	2.61	6	4
1:A:64:LEU:HD21	2:B:118:PRO:HG3	0.73	1.60	9	3
1:A:57:LYS:HE2	2:B:189:GLU:OE1	0.73	1.83	8	2
1:A:66:MET:HE1	2:B:118:PRO:C	0.73	2.03	8	1
1:A:37:PRO:O	2:B:102:TYR:OH	0.73	2.07	8	5
2:B:131:VAL:N	2:B:131:VAL:CG1	0.72	2.52	6	2
1:A:66:MET:HE2	2:B:119:LEU:HD23	0.72	0.77	1	2
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LEU:HD12	1:A:47:LEU:N	0.71	2.01	4	7
1:A:43:PHE:CB	1:A:59:LEU:CD1	0.71	2.69	6	10
1:A:47:LEU:N	1:A:47:LEU:HD12	0.71	2.01	6	3
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	6
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	6
1:A:64:LEU:CD1	2:B:1:TYR:OH	0.69	2.38	8	3
1:A:47:LEU:CD1	1:A:47:LEU:N	0.69	2.55	4	5
2:B:159:GLN:CD	2:B:159:GLN:N	0.68	2.46	4	3
2:B:159:GLN:N	2:B:159:GLN:CD	0.68	2.46	8	7
1:A:64:LEU:N	1:A:64:LEU:HD12	0.68	2.01	6	4
1:A:7:LEU:HD13	1:A:39:HIS:HB2	0.68	1.66	7	10
1:A:68:PRO:CG	2:B:100:ASP:OD2	0.68	2.42	1	1
1:A:21:LEU:CD2	1:A:21:LEU:C	0.68	2.61	6	5
1:A:39:HIS:HB3	1:A:89:CYS:SG	0.68	2.29	9	10
1:A:21:LEU:C	1:A:21:LEU:CD2	0.68	2.61	4	5
1:A:15:VAL:HG22	1:A:16:PHE:N	0.68	2.03	4	10
1:A:47:LEU:N	1:A:47:LEU:CD1	0.68	2.56	6	5
1:A:68:PRO:CG	2:B:100:ASP:O	0.67	2.42	6	1
2:B:196:LEU:C	2:B:196:LEU:CD2	0.67	2.63	6	6
1:A:37:PRO:HG2	2:B:102:TYR:CE1	0.67	2.25	6	6
2:B:131:VAL:CG1	2:B:131:VAL:N	0.67	2.56	3	2
1:A:15:VAL:CG2	1:A:16:PHE:N	0.67	2.58	6	10
1:A:64:LEU:H	1:A:64:LEU:HD12	0.66	1.47	6	4
1:A:66:MET:HE3	2:B:119:LEU:HD23	0.66	1.67	9	4
1:A:20:LYS:NZ	1:A:20:LYS:O	0.65	2.30	6	3
2:B:131:VAL:C	2:B:131:VAL:CG2	0.65	2.66	5	3
2:B:34:VAL:HG13	2:B:50:VAL:HG22	0.64	1.69	6	6
1:A:20:LYS:O	1:A:20:LYS:NZ	0.64	2.31	2	7
1:A:64:LEU:HD11	2:B:1:TYR:CZ	0.64	2.28	8	3
1:A:66:MET:CE	2:B:118:PRO:C	0.64	2.66	8	1
1:A:48:ASN:OD1	1:A:50:ALA:N	0.64	2.31	6	10
1:A:66:MET:HE2	2:B:119:LEU:CA	0.64	2.21	8	1
1:A:66:MET:HE1	2:B:119:LEU:HA	0.64	1.63	8	1
1:A:64:LEU:N	1:A:64:LEU:CD1	0.64	2.61	4	5
1:A:40:ASN:HD21	1:A:65:LEU:N	0.63	1.90	3	7
1:A:64:LEU:CD1	1:A:64:LEU:N	0.63	2.61	6	5
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:61:HIS:CG	1:A:62:LYS:N	0.62	2.68	4	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ALA:O	1:A:59:LEU:HD21	0.62	1.95	8	10
1:A:24:LYS:HD3	1:A:24:LYS:N	0.62	2.10	4	7
2:B:196:LEU:CD2	2:B:196:LEU:C	0.61	2.69	3	4
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:1:GLU:CD	1:A:1:GLU:N	0.60	2.55	7	7
1:A:40:ASN:HD21	1:A:64:LEU:N	0.60	1.93	8	2
2:B:171:LEU:C	2:B:171:LEU:HD23	0.60	2.17	4	6
2:B:171:LEU:HD23	2:B:171:LEU:C	0.60	2.17	6	4
1:A:66:MET:CG	2:B:119:LEU:HD23	0.60	2.27	6	1
1:A:1:GLU:N	1:A:1:GLU:CD	0.60	2.55	2	3
1:A:61:HIS:O	1:A:62:LYS:HB3	0.59	1.97	4	10
2:B:139:ASP:CG	2:B:142:ILE:CG2	0.59	2.71	6	5
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	7
2:B:41:LEU:HD22	2:B:41:LEU:N	0.59	2.11	6	3
2:B:131:VAL:CG2	2:B:131:VAL:C	0.59	2.71	6	1
1:A:59:LEU:CG	1:A:60:SER:H	0.59	2.11	4	10
2:B:196:LEU:N	2:B:196:LEU:HD13	0.57	2.15	6	3
2:B:139:ASP:CG	2:B:142:ILE:HG23	0.57	2.20	1	10
1:A:43:PHE:HB2	1:A:59:LEU:CD1	0.57	2.22	6	10
2:B:196:LEU:HD13	2:B:196:LEU:N	0.57	2.15	4	7
1:A:39:HIS:CB	1:A:89:CYS:SG	0.57	2.93	9	10
1:A:66:MET:HE2	2:B:119:LEU:HA	0.57	1.64	8	1
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:24:LYS:N	1:A:24:LYS:HD3	0.56	2.14	1	3
1:A:40:ASN:ND2	1:A:65:LEU:HG	0.56	2.16	3	7
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:66:MET:HE2	2:B:119:LEU:HG	0.55	1.77	6	1
1:A:1:GLU:N	1:A:27:ASP:CG	0.55	2.60	4	10
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
2:B:234:ASN:OD1	2:B:234:ASN:C	0.55	2.45	6	7
2:B:234:ASN:C	2:B:234:ASN:OD1	0.55	2.45	4	3
1:A:66:MET:HE1	2:B:119:LEU:HD23	0.55	1.79	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:102:TYR:O	2:B:102:TYR:CG	0.54	2.59	8	7
1:A:28:THR:O	1:A:28:THR:HG22	0.54	2.02	6	7
1:A:40:ASN:CB	1:A:62:LYS:HA	0.54	2.33	9	9
2:B:102:TYR:CG	2:B:102:TYR:O	0.54	2.59	9	3
2:B:199:ILE:O	2:B:199:ILE:HG13	0.54	2.03	6	1
2:B:8:THR:OG1	2:B:8:THR:O	0.54	2.25	4	5
1:A:13:LEU:HG	1:A:14:LEU:N	0.54	2.18	4	10
2:B:142:ILE:HD11	2:B:249:LEU:HD22	0.54	1.80	6	4
2:B:199:ILE:HG13	2:B:199:ILE:O	0.54	2.03	4	1
1:A:40:ASN:ND2	1:A:63:GLN:C	0.54	2.61	8	2
1:A:32:LEU:C	1:A:32:LEU:HD23	0.54	2.23	6	4
1:A:59:LEU:CG	1:A:60:SER:N	0.54	2.70	6	10
1:A:62:LYS:O	1:A:63:GLN:CB	0.53	2.56	8	10
1:A:66:MET:HE1	2:B:117:GLY:C	0.53	2.24	5	2
1:A:66:MET:HE3	2:B:119:LEU:CD2	0.53	1.87	1	2
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	6
1:A:28:THR:HG22	1:A:28:THR:O	0.53	2.03	3	3
1:A:42:VAL:HG22	1:A:88:TYR:CB	0.53	2.34	4	10
2:B:136:PRO:CG	2:B:144:PHE:CZ	0.53	2.91	6	7
1:A:40:ASN:ND2	1:A:65:LEU:N	0.53	2.57	4	7
1:A:40:ASN:HD21	1:A:63:GLN:C	0.53	2.06	8	1
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:HG13	2:B:115:ILE:CA	0.52	2.31	2	1
2:B:35:GLU:N	2:B:35:GLU:OE1	0.52	2.42	7	3
2:B:35:GLU:OE1	2:B:35:GLU:N	0.52	2.42	8	7
1:A:32:LEU:HD23	1:A:32:LEU:C	0.52	2.23	4	6
2:B:236:ASN:OD1	2:B:236:ASN:C	0.52	2.48	8	5
2:B:236:ASN:C	2:B:236:ASN:OD1	0.52	2.48	9	5
1:A:15:VAL:CG2	1:A:16:PHE:H	0.52	2.18	6	10
1:A:18:PRO:O	1:A:20:LYS:N	0.52	2.43	3	10
1:A:11:LYS:NZ	1:A:11:LYS:O	0.52	2.43	4	5
2:B:159:GLN:N	2:B:159:GLN:OE1	0.52	2.43	6	8
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:11:LYS:O	1:A:11:LYS:CE	0.52	2.58	3	4
1:A:66:MET:HE1	2:B:118:PRO:N	0.52	2.20	5	1
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	6
2:B:115:ILE:C	2:B:115:ILE:HG23	0.51	2.26	2	1
1:A:11:LYS:O	1:A:11:LYS:NZ	0.51	2.43	1	5
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: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
2:B:115:ILE:C	2:B:115:ILE:HG22	0.50	2.27	1	2
1:A:16:PHE:CE1	1:A:97:MET:CG	0.50	2.95	7	10
2:B:70:LEU:N	2:B:70:LEU:HD12	0.50	2.22	4	4
1:A:43:PHE:H	1:A:60:SER:CB	0.50	2.20	9	10
1:A:20:LYS:HG3	1:A:20:LYS:O	0.50	2.07	4	6
2:B:8:THR:O	2:B:8:THR:OG1	0.50	2.29	5	5
1:A:48:ASN:HD21	1:A:50:ALA:C	0.50	2.10	6	6
1:A:64:LEU:HD23	2:B:118:PRO:CB	0.50	2.33	9	1
1:A:55:LEU:C	1:A:55:LEU:HD12	0.49	2.28	6	5
1:A:21:LEU:HD23	1:A:21:LEU:C	0.49	2.26	6	3
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
1:A:21:LEU:C	1:A:21:LEU:HD23	0.49	2.26	4	7
2:B:46:PHE:HZ	2:B:131:VAL:HG21	0.49	1.61	4	2
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
2:B:75:VAL:HG23	2:B:115:ILE:HD11	0.48	1.85	1	5
2:B:25:CYS:SG	4:B:255:HEC:HBC3	0.48	2.49	10	10
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
1:A:64:LEU:HD22	2:B:1:TYR:HE1	0.48	1.62	3	1
2:B:159:GLN:OE1	2:B:159:GLN:N	0.47	2.47	1	2
1:A:40:ASN:HD21	1:A:64:LEU:C	0.47	2.11	4	3
1:A:1:GLU:H1	1:A:1:GLU:CD	0.47	2.13	1	4
1:A:48:ASN:OD1	1:A:48:ASN:C	0.47	2.53	6	2
2:B:115:ILE:HG23	2:B:115:ILE:C	0.47	2.28	1	1
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:70:LEU:HD12	2:B:70:LEU:N	0.47	2.25	5	6
2:B:115:ILE:CA	2:B:115:ILE:HG13	0.47	2.37	1	1
1:A:13:LEU:HG	1:A:14:LEU:H	0.47	1.69	4	7
1:A:21:LEU:HD22	1:A:21:LEU:C	0.47	2.30	6	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	3
2:B:41:LEU:CD2	2:B:41:LEU:N	0.46	2.78	6	1
1:A:83:GLY:HA3	1:A:85:TYR:CE1	0.46	2.46	7	10
1:A:1:GLU:CD	1:A:1:GLU:H1	0.46	2.14	10	2
1:A:87:PHE:CD1	1:A:87:PHE:N	0.46	2.83	6	6
1:A:48:ASN:C	1:A:48:ASN:OD1	0.46	2.53	4	2
1:A:41:VAL:HG23	1:A:41:VAL:O	0.46	2.11	7	1
2:B:130:PRO:C	2:B:131:VAL:HG12	0.46	2.31	5	5
1:A:20:LYS:O	1:A:20:LYS:HG3	0.46	2.10	3	4
1:A:21:LEU:C	1:A:21:LEU:HD22	0.46	2.31	4	3
1:A:55:LEU:HD12	1:A:55:LEU:C	0.46	2.31	5	5
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:68:PRO:HG3	2:B:100:ASP:OD2	0.45	2.11	1	1
1:A:85:TYR:N	1:A:85:TYR:CD1	0.45	2.84	2	5
1:A:89:CYS:HB2	1:A:97:MET:HG2	0.45	1.89	8	10
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:87:PHE:N	1:A:87:PHE:CD1	0.44	2.85	10	4
1:A:66:MET:HE2	2:B:119:LEU:CG	0.44	2.43	6	1
1:A:41:VAL:O	1:A:41:VAL:HG23	0.44	2.11	9	8
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	4
2:B:102:TYR:CD2	2:B:102:TYR:O	0.44	2.71	9	6
1:A:57:LYS:C	1:A:59:LEU:N	0.44	2.71	4	10
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:CG2	2:B:149:VAL:O	0.44	2.65	3	1
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
2:B:196:LEU:CD1	2:B:196:LEU:N	0.43	2.82	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:GLU:H2	1:A:27:ASP:CG	0.43	2.17	1	5
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:CBC	4:B:255:HEC:HMC1	0.43	2.44	1	5
4:B:255:HEC:HMC1	4:B:255:HEC:CBC	0.43	2.44	2	5
2:B:149:VAL:O	2:B:149:VAL:CG2	0.43	2.67	6	2
1:A:66:MET:HG3	2:B:119:LEU:HA	0.43	1.91	6	1
1:A:86:THR:HG23	1:A:99:GLY:O	0.42	2.14	4	3
2:B:171:LEU:C	2:B:171:LEU:CD2	0.42	2.87	4	2
1:A:93:ARG:CD	1:A:93:ARG:O	0.42	2.68	6	2
1:A:81:PRO:O	1:A:83:GLY:N	0.42	2.53	7	10
1:A:39:HIS:CA	1:A:89:CYS:SG	0.42	3.08	9	10
1:A:37:PRO:HG2	2:B:102:TYR:CD1	0.42	2.50	1	1
1:A:64:LEU:HD22	2:B:1:TYR:OH	0.42	2.11	2	1
1:A:43:PHE:HB2	1:A:60:SER:CA	0.42	2.45	9	8
1:A:85:TYR:CD1	1:A:85:TYR:N	0.42	2.84	3	5
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:79:ASP:N	1:A:79:ASP:OD1	0.42	2.52	9	1
1:A:93:ARG:O	1:A:93:ARG:CD	0.42	2.67	4	2
1:A:23:ILE:CD1	1:A:103:VAL:CG2	0.42	2.98	7	4
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:101:ILE:HG22	1:A:101:ILE:O	0.42	2.15	5	1
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:HG13	2:B:131:VAL:N	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
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: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:131:VAL:HG23	2:B:131:VAL:C	0.40	2.36	5	1

5.2 Torsion angles (i)

5.2.1 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	53	ALA	10
1	A	27	ASP	10
1	A	68	PRO	10
1	A	85	TYR	10
1	A	96	GLY	10
1	A	28	THR	10
1	A	7	LEU	10
1	A	104	ALA	10
1	A	82	ALA	10
1	A	18	PRO	10
1	A	63	GLN	10
1	A	10	ASP	10
1	A	25	PRO	10
1	A	19	ALA	10
1	A	89	CYS	10
1	A	64	LEU	10
1	A	62	LYS	10
1	A	56	ALA	10
1	A	9	SER	10
1	A	2	THR	10
1	A	90	GLU	10
1	A	44	ASP	10
1	A	93	ARG	10

5.2.2 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%)	73±0 (86±0%)	12±0 (14±0%)	6 45
2	B	209/209 (100%)	193±1 (93±0%)	16±1 (7±0%)	17 65
All	All	2940/2940 (100%)	2662 (91%)	278 (9%)	12 58

All 31 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)
2	B	116	VAL	10
2	B	123	GLN	10
2	B	47	LYS	10
1	A	79	ASP	10
2	B	115	ILE	10
2	B	138	ASN	10
2	B	170	ASN	10
1	A	101	ILE	10
1	A	11	LYS	10
2	B	225	VAL	10
1	A	20	LYS	10
1	A	51	LYS	10
2	B	197	VAL	10
2	B	199	ILE	10
1	A	40	ASN	10
2	B	155	ARG	10
1	A	10	ASP	10
1	A	21	LEU	10
1	A	24	LYS	10
1	A	62	LYS	10
1	A	48	ASN	10
2	B	84	ILE	10
2	B	196	LEU	10
2	B	142	ILE	10
1	A	93	ARG	10
2	B	131	VAL	7
2	B	34	VAL	6
2	B	160	VAL	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	B	193	VAL	4
2	B	149	VAL	3
1	A	17	GLU	2

5.2.3 RNA

There are no RNA molecules in this entry.

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

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

5.4 Carbohydrates

There are no carbohydrates in this entry.

LIGAND-GEOMETRY INFOmissingINFO

5.5 Other polymers

There are no such molecules in this entry.

5.6 Polymer linkage issues

There are no chain breaks in this entry.

6 Chemical shift validation

No chemical shift data were provided