



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:43 AM UTC

PDB ID : 2JXM / pdb_00002jxm
Title : Ensemble of twenty structures of the Prochlorothrix hollandica plastocyanin-cytochrome f complex
Authors : Hulsker, R.; Baranova, M.; Bullerjahn, G.; Ubbink, M.
Deposited on : 2007-11-22

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 ⓘ 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 ⓘ](#)) 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

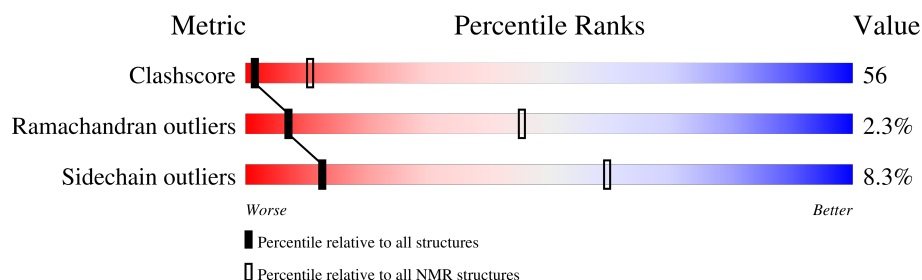
1 Overall quality at a glance

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	97	
2	B	249	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:97 (97)	0.00	20
2	B:1-B:249 (249)	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, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 13, 14, 17
2	12, 15, 16, 18
3	19, 20

3 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5179 atoms, of which 2547 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Plastocyanin.

Mol	Chain	Residues	Atoms						Trace
1	A	97	Total	C	H	N	O	S	0
			1424	457	711	114	138	4	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	THR	engineered mutation	UNP P50057

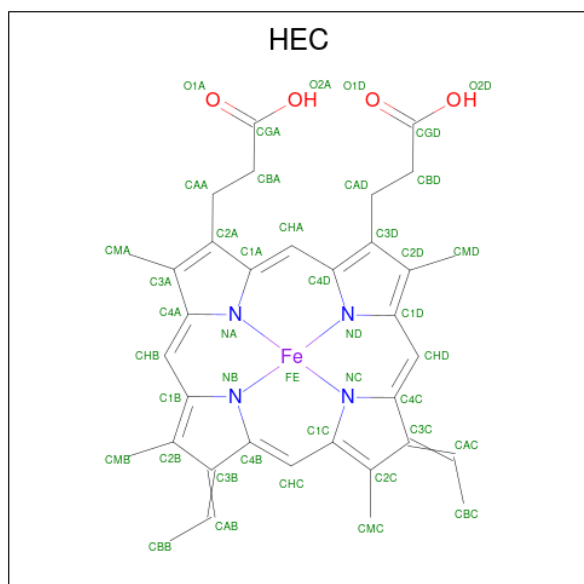
- Molecule 2 is a protein called Cytochrome f.

Mol	Chain	Residues	Atoms						Trace
2	B	249	Total	C	H	N	O	S	0
			3679	1192	1804	295	382	6	

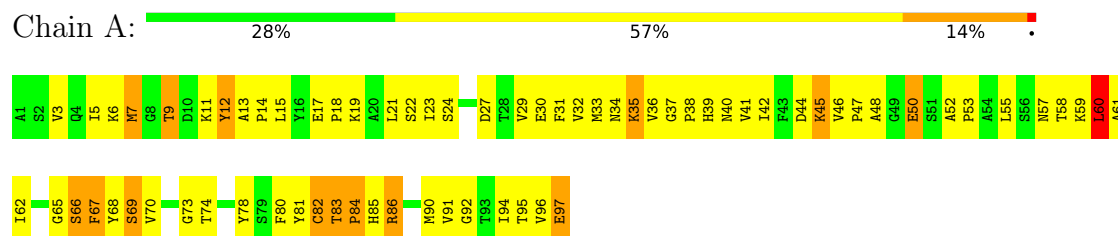
- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	
3	A	1	Total	Cu
			1	1

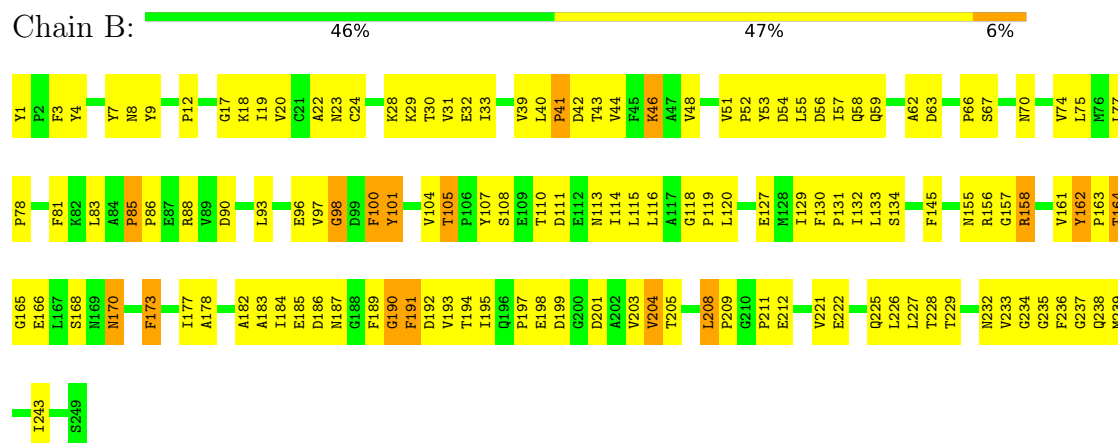
- Molecule 4 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

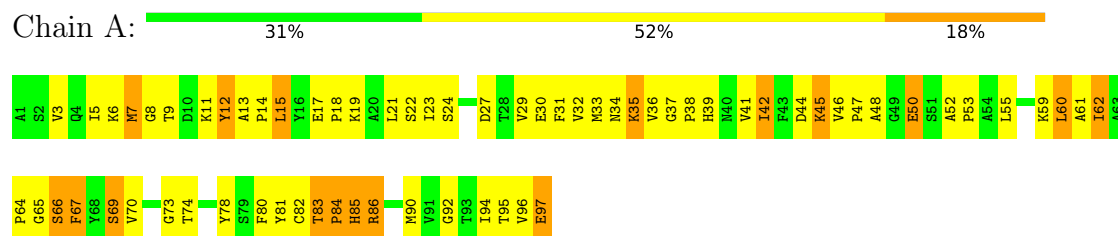


• Molecule 2: Cytochrome f

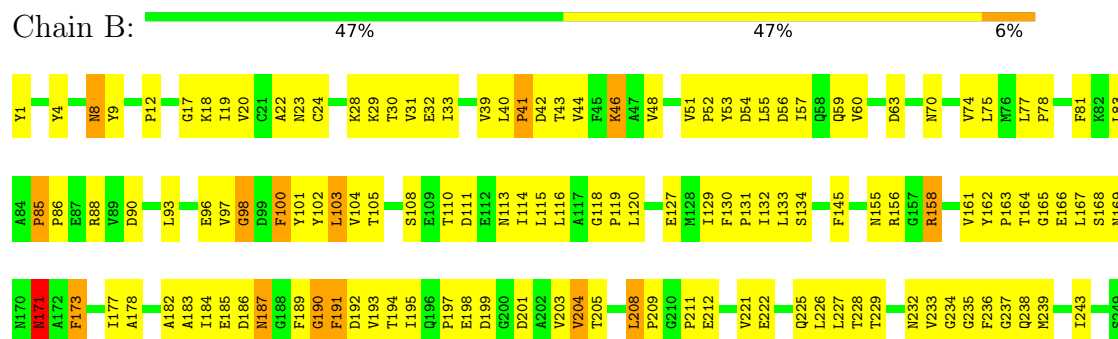


4.2.2 Score per residue for model 2

• Molecule 1: Plastocyanin

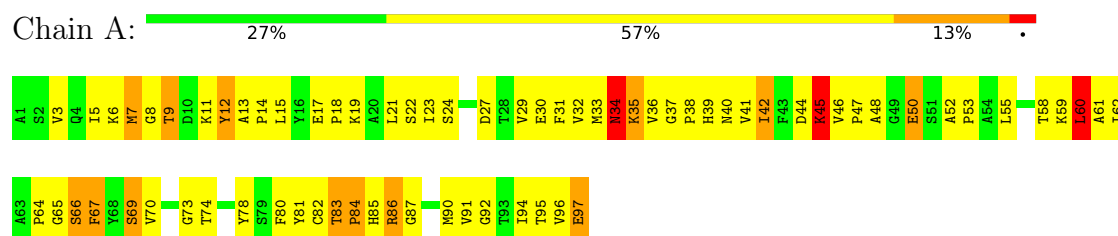


• Molecule 2: Cytochrome f

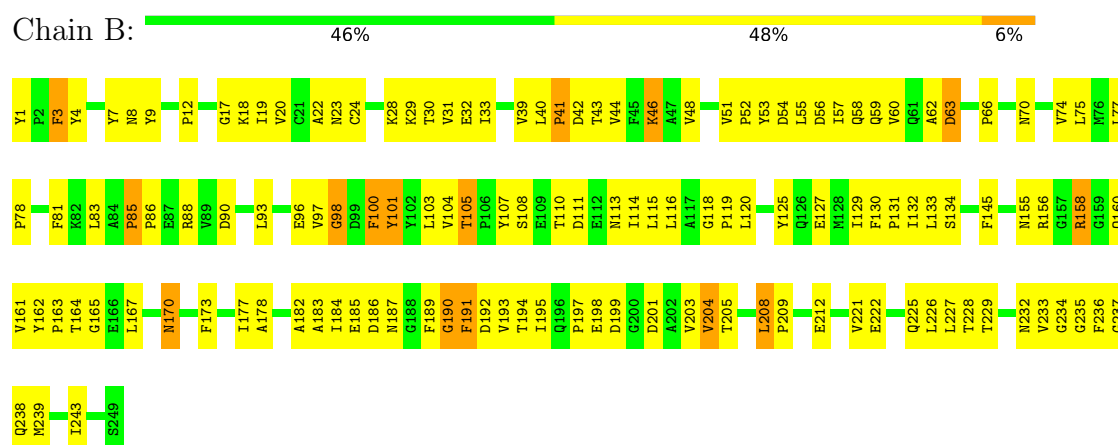


4.2.3 Score per residue for model 3

• Molecule 1: Plastocyanin

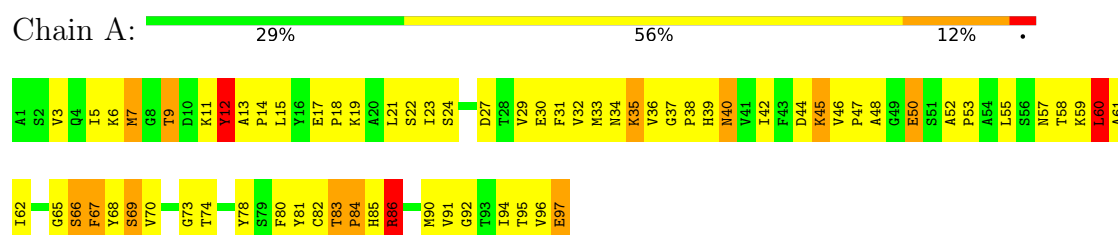


• Molecule 2: Cytochrome f



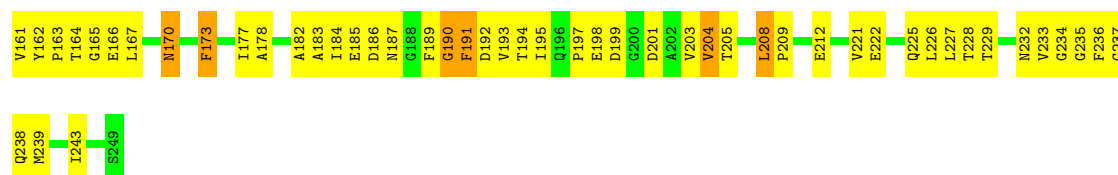
4.2.4 Score per residue for model 4

• Molecule 1: Plastocyanin



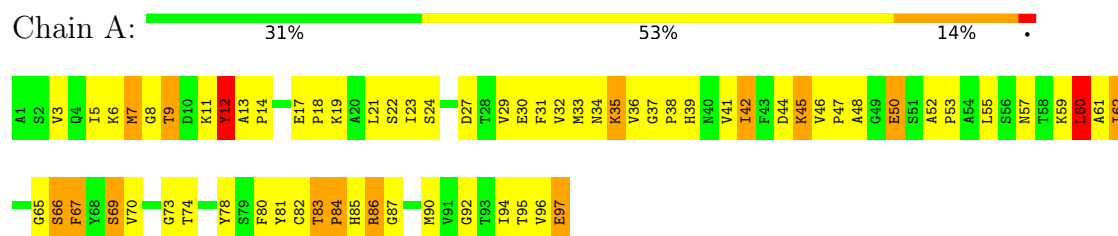
• Molecule 2: Cytochrome f



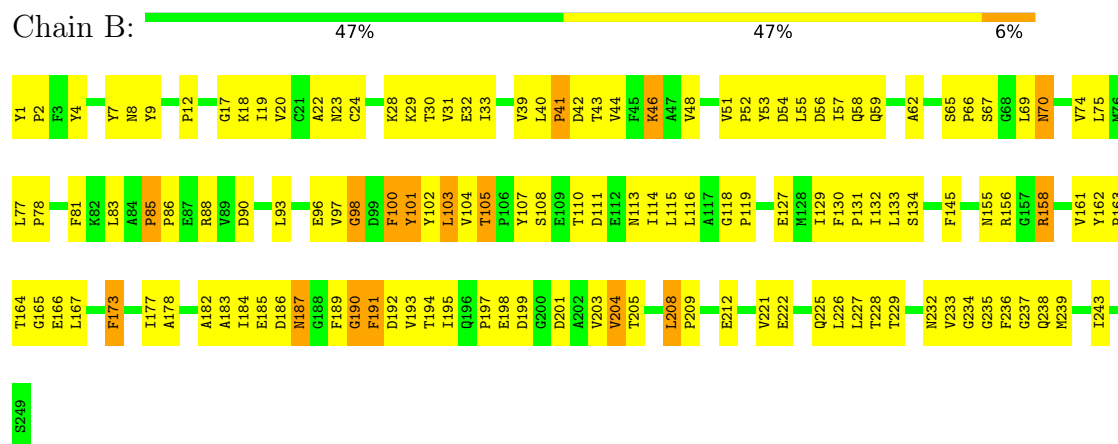


4.2.5 Score per residue for model 5

- Molecule 1: Plastocyanin

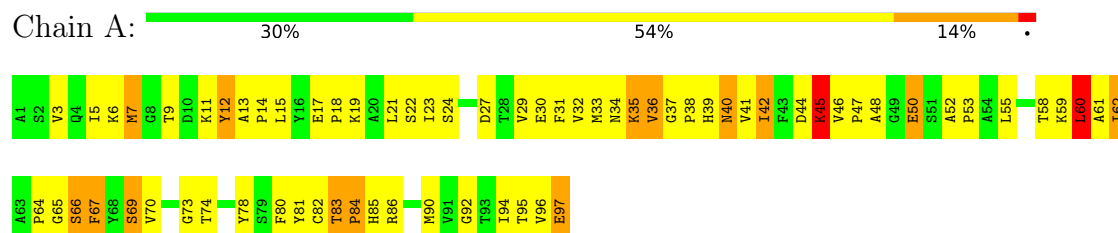


- Molecule 2: Cytochrome f

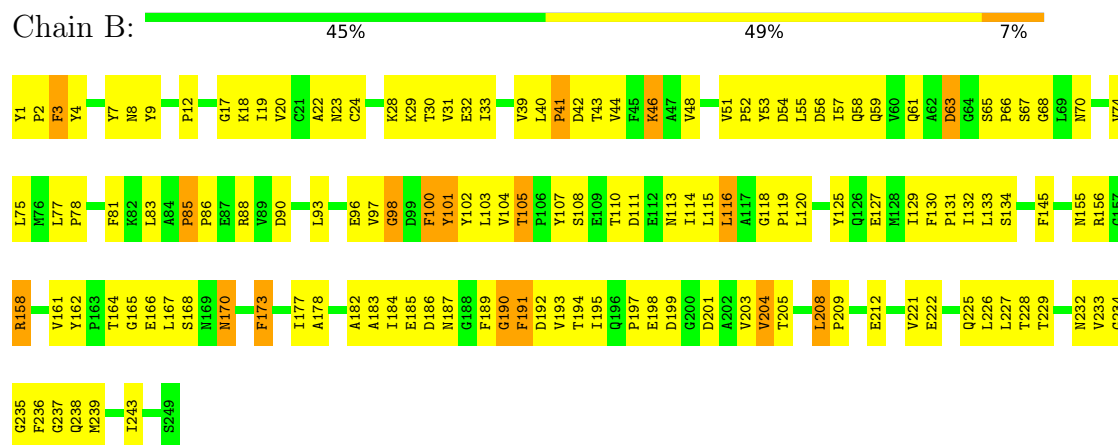


4.2.6 Score per residue for model 6

- Molecule 1: Plastocyanin

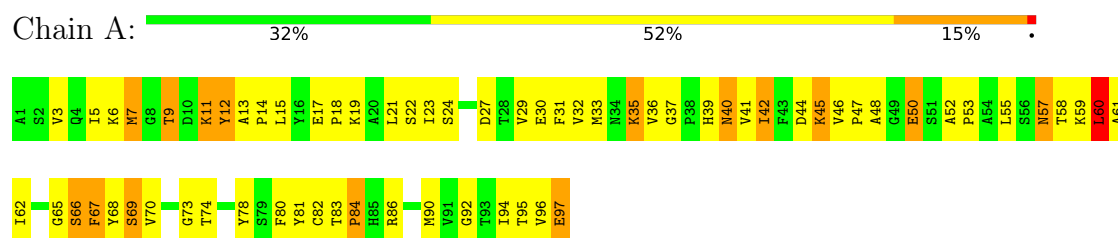


- Molecule 2: Cytochrome f

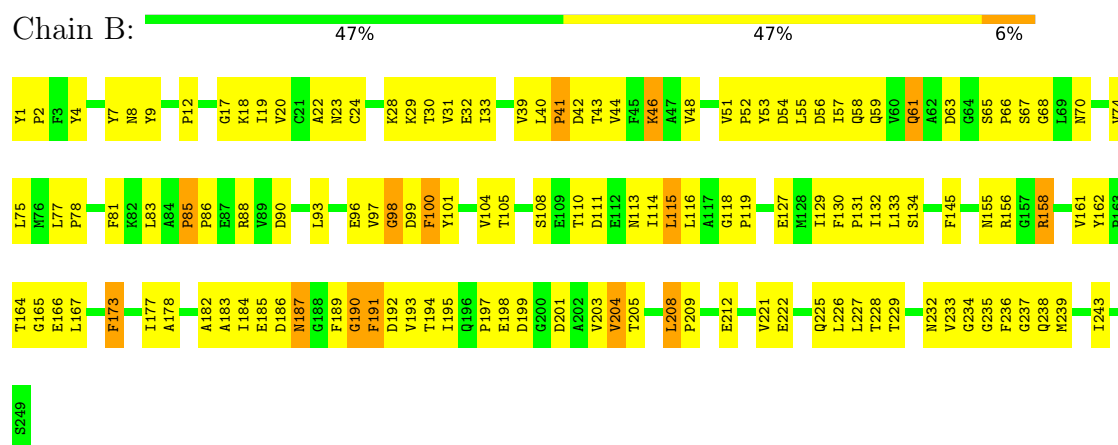


4.2.7 Score per residue for model 7

- Molecule 1: Plastocyanin



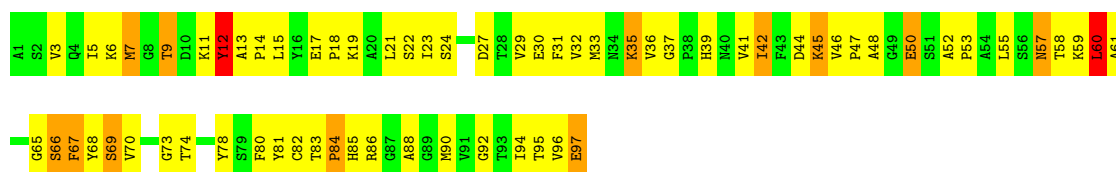
- Molecule 2: Cytochrome f



4.2.8 Score per residue for model 8

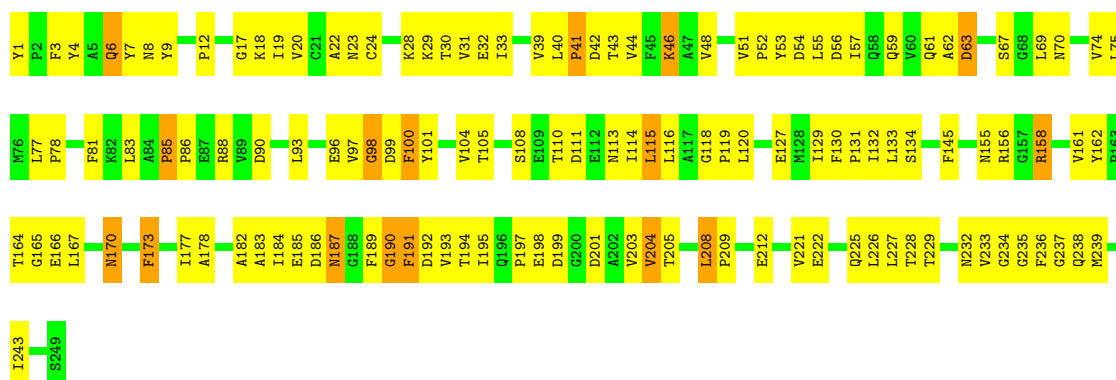
- Molecule 1: Plastocyanin





• Molecule 2: Cytochrome f

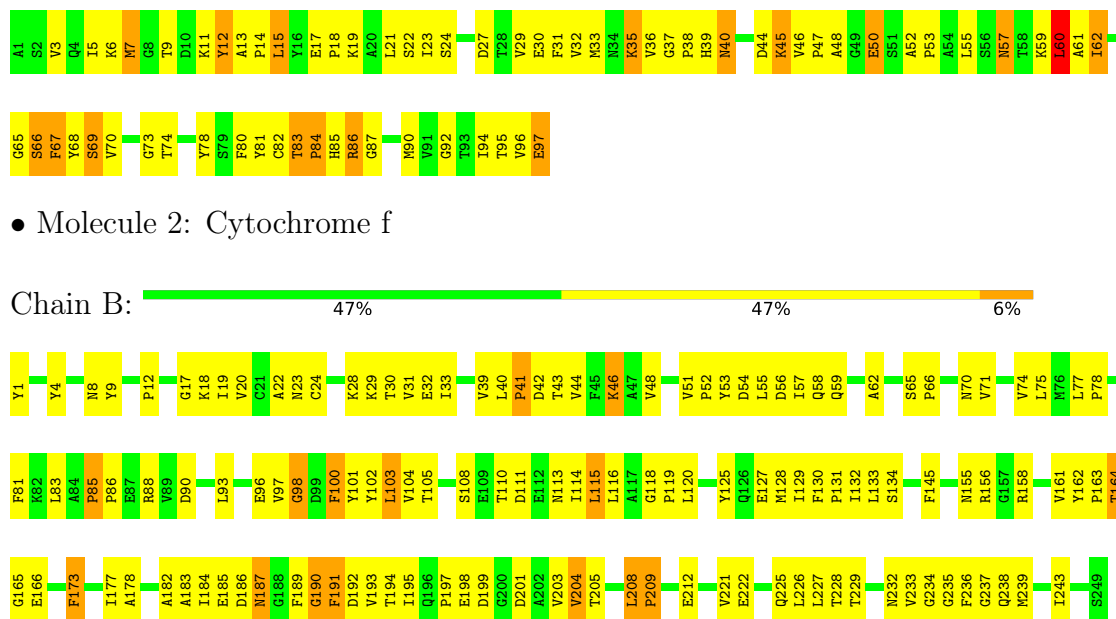
Chain B: 47% 47% 6%



4.2.9 Score per residue for model 9

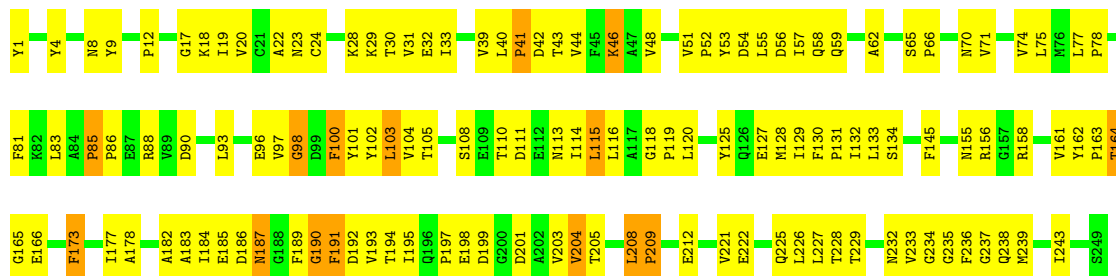
• Molecule 1: Plastocyanin

Chain A: 32% 51% 16%



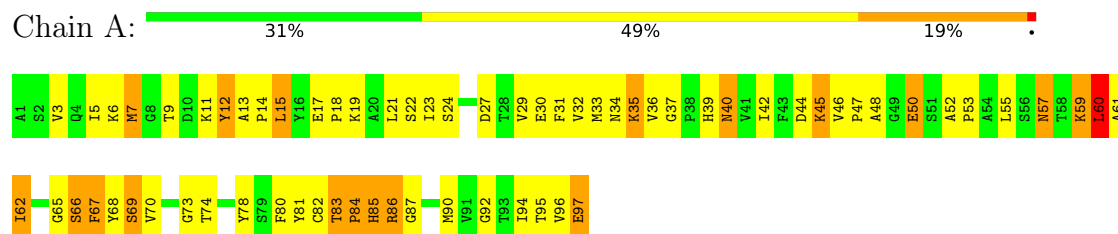
• Molecule 2: Cytochrome f

Chain B: 47% 47% 6%

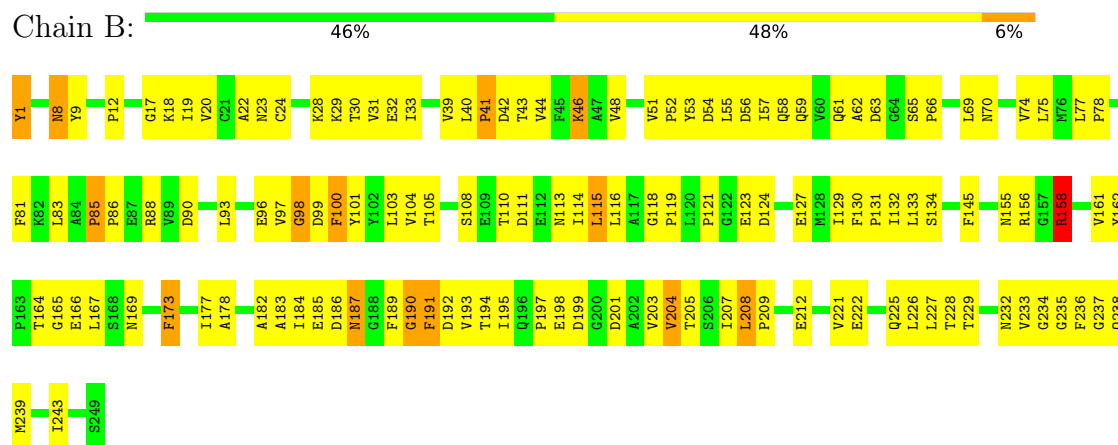


4.2.10 Score per residue for model 10

• Molecule 1: Plastocyanin

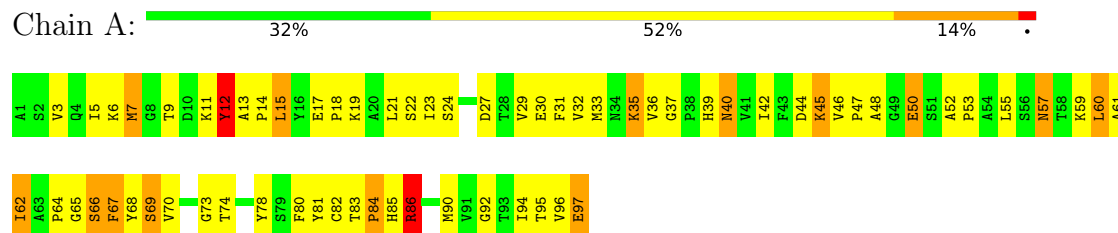


• Molecule 2: Cytochrome f

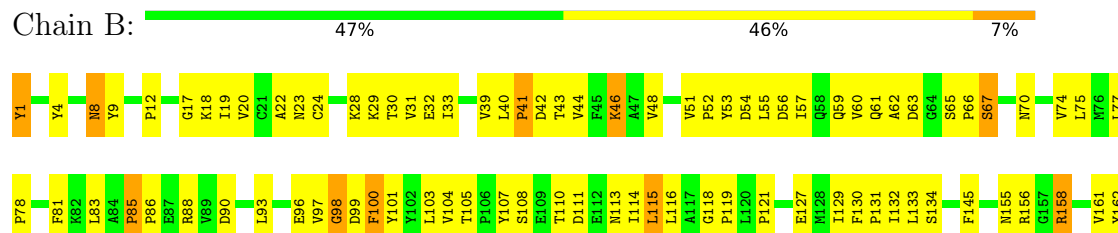


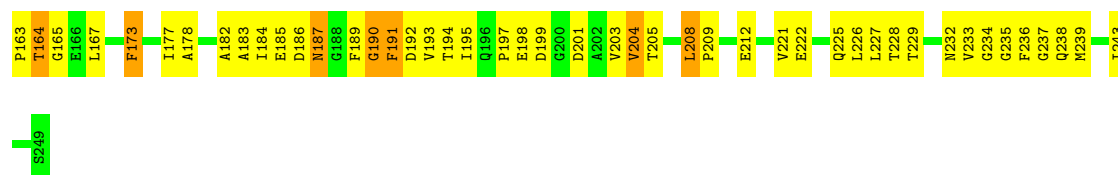
4.2.11 Score per residue for model 11

• Molecule 1: Plastocyanin



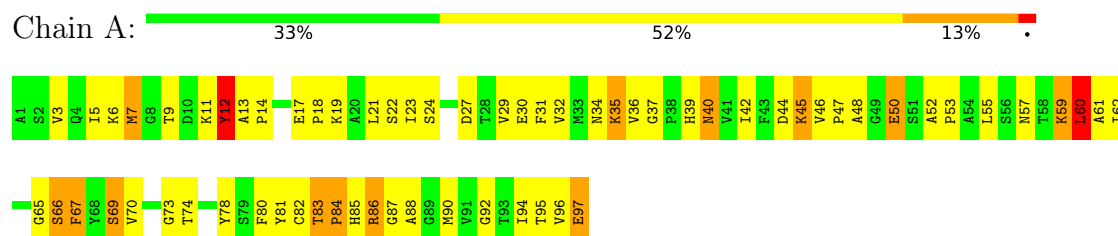
• Molecule 2: Cytochrome f



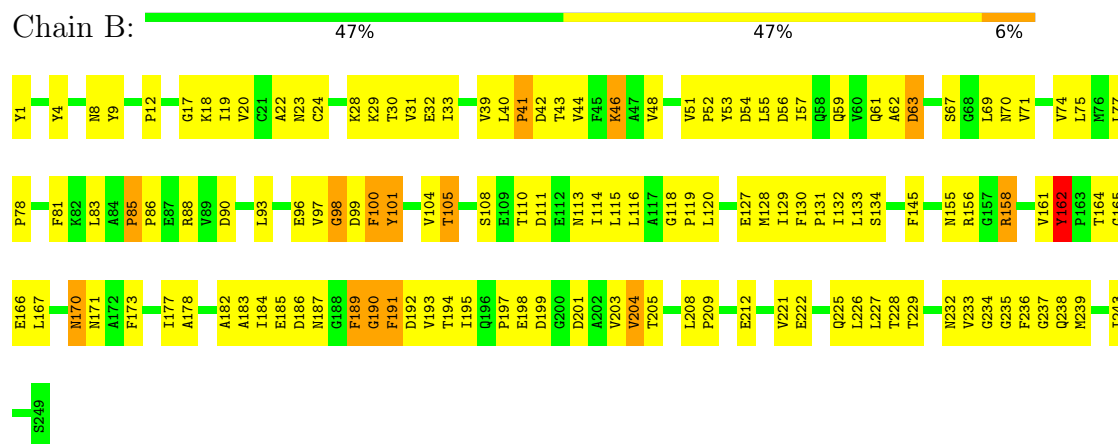


4.2.12 Score per residue for model 12

- Molecule 1: Plastocyanin

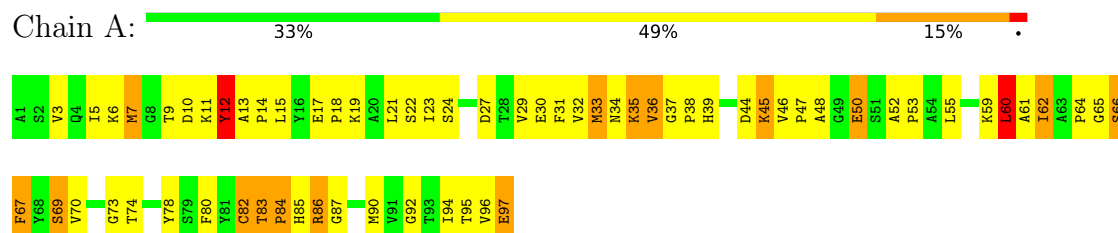


- Molecule 2: Cytochrome f

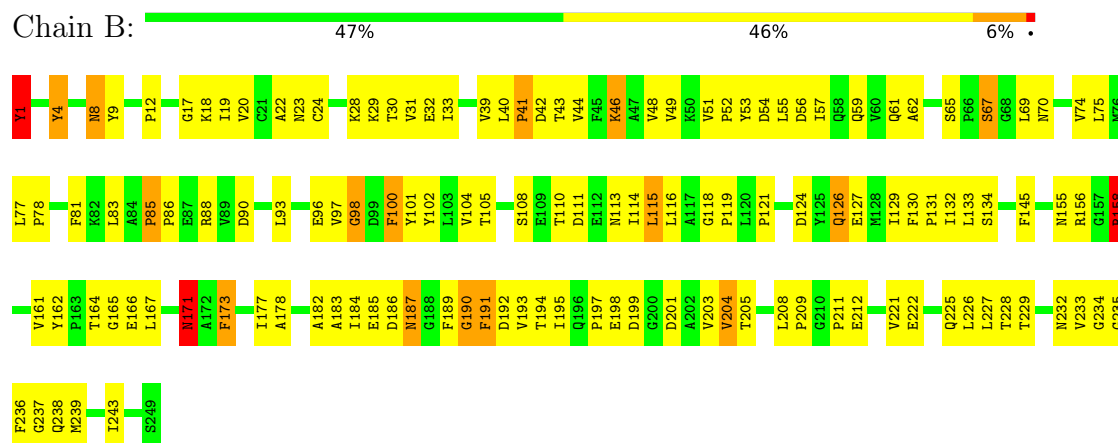


4.2.13 Score per residue for model 13

- Molecule 1: Plastocyanin

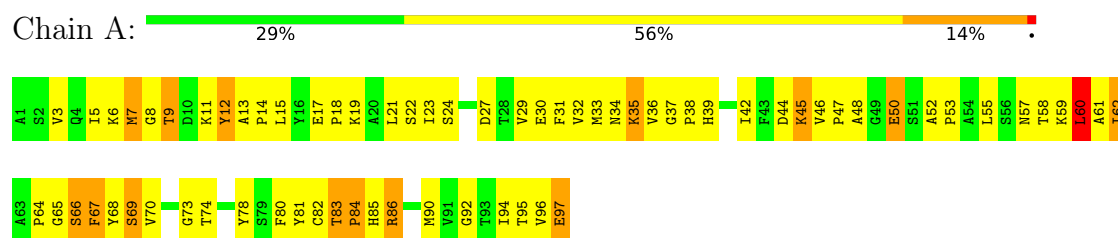


- Molecule 2: Cytochrome f

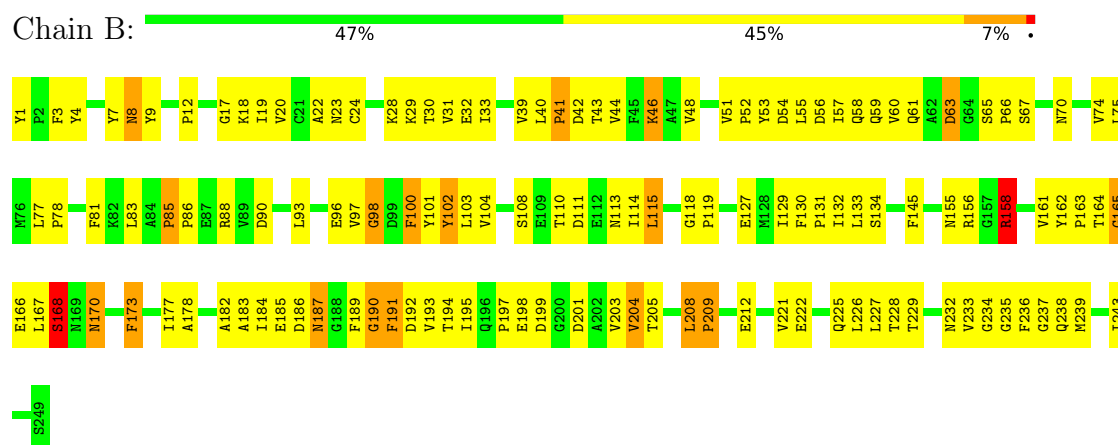


4.2.14 Score per residue for model 14

- Molecule 1: Plastocyanin



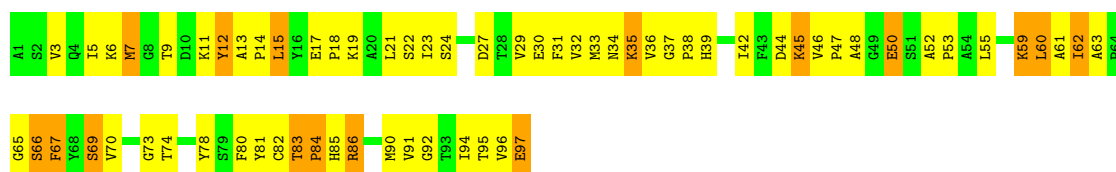
- Molecule 2: Cytochrome f



4.2.15 Score per residue for model 15

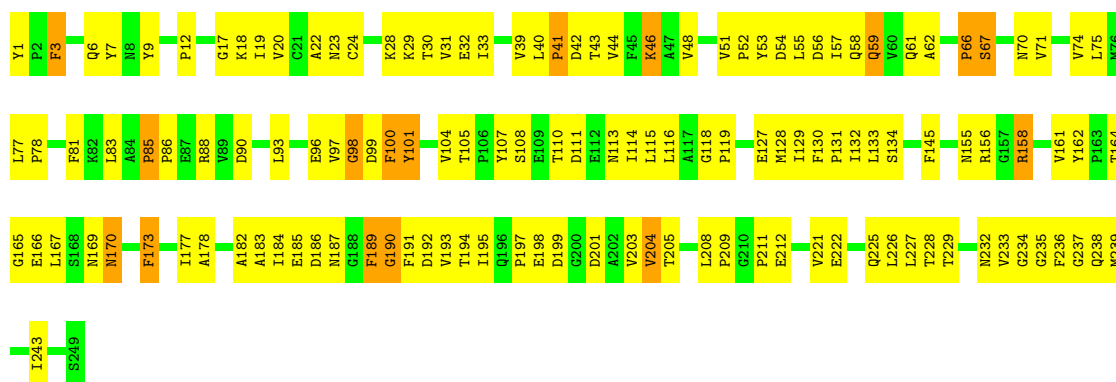
- Molecule 1: Plastocyanin





• Molecule 2: Cytochrome f

Chain B: 46% 47% 6%



4.2.16 Score per residue for model 16

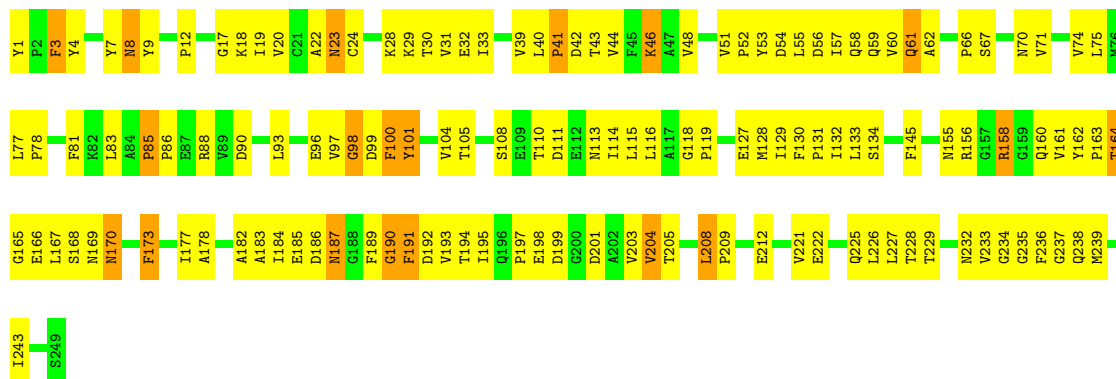
• Molecule 1: Plastocyanin

Chain A: 33% 51% 13%



• Molecule 2: Cytochrome f

Chain B: 45% 47% 8%

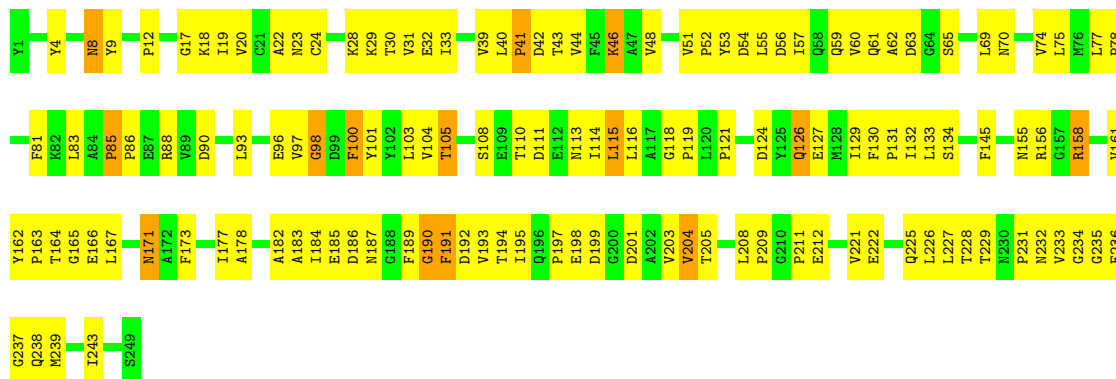
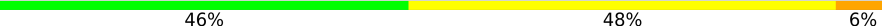


4.2.17 Score per residue for model 17

• Molecule 1: Plastocyanin

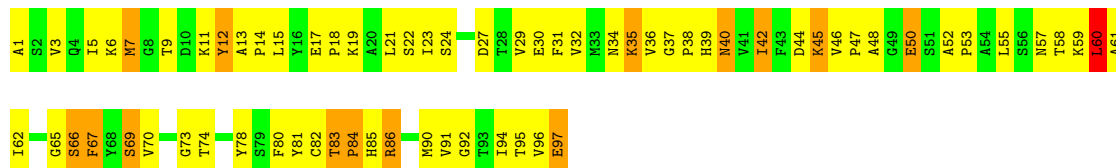
Chain A: 

• Molecule 2: Cytochrome f

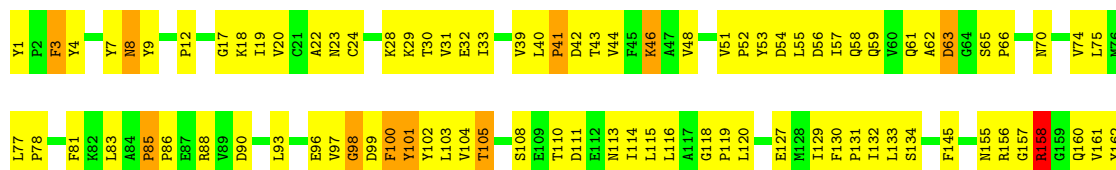
Chain B: 

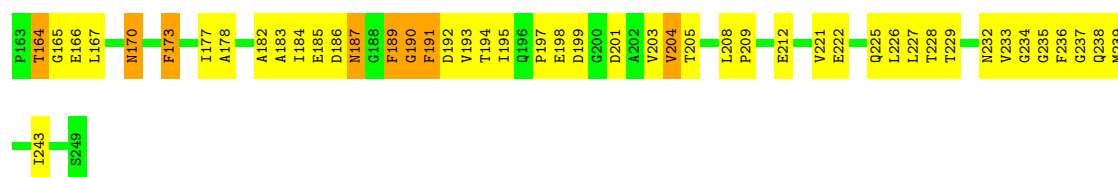
4.2.18 Score per residue for model 18

• Molecule 1: Plastocyanin

Chain A: 

• Molecule 2: Cytochrome f

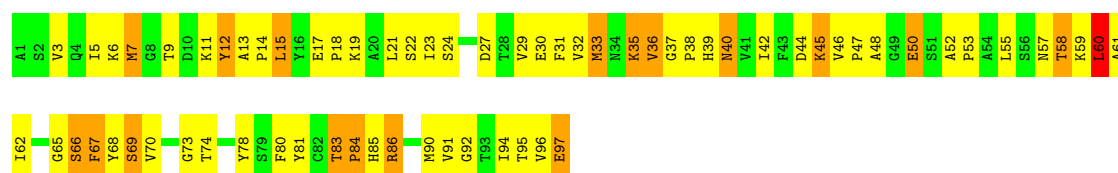
Chain B: 



4.2.19 Score per residue for model 19

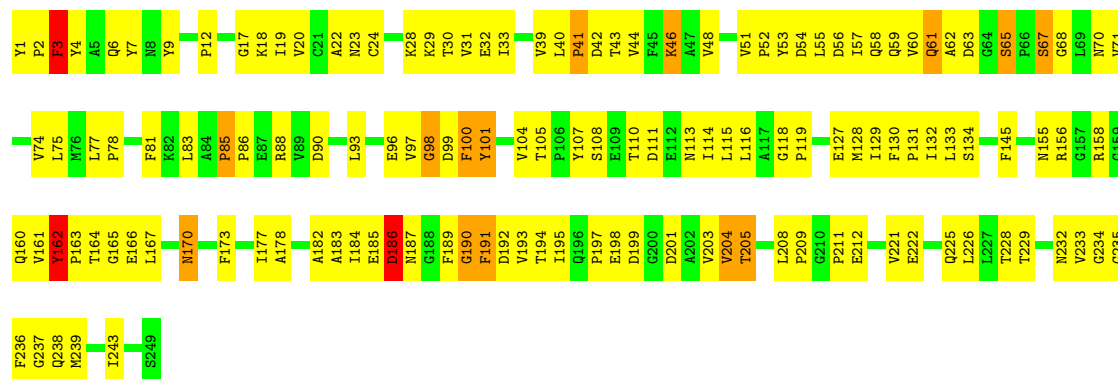
- Molecule 1: Plastocyanin

Chain A: 31% 51% 18%



- Molecule 2: Cytochrome f

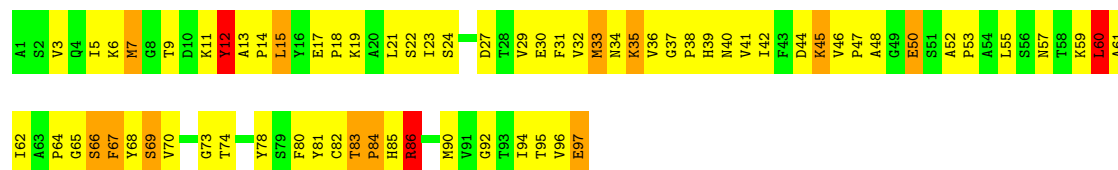
Chain B: 44% 49% 6%



4.2.20 Score per residue for model 20

- Molecule 1: Plastocyanin

Chain A: 29% 56% 12%



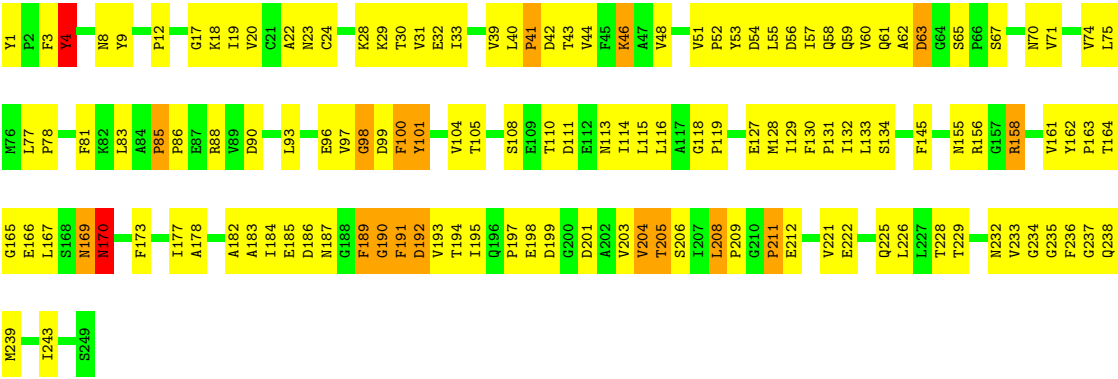
- Molecule 2: Cytochrome f

Chain B:

45%

47%

7%



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *Rigid Body docking, Energy minimisation*.

Of the 1000 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.74±0.05	0±1/731 (0.1± 0.1%)	1.15±0.04	1±1/995 (0.1± 0.1%)
2	B	1.30±0.03	1±1/1918 (0.0± 0.0%)	1.64±0.08	26±2/2621 (1.0± 0.1%)
All	All	1.17	22/52980 (0.0%)	1.52	547/72320 (0.8%)

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	0.2±0.4
2	B	0.0±0.0	1.2±0.4
All	All	0	29

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	23	ASN	CA-CB	22.76	1.88	1.53	16	1
2	B	171	ASN	CG-OD1	20.84	1.63	1.23	17	1
2	B	170	ASN	CA-CB	15.94	1.76	1.53	3	6
1	A	34	ASN	CA-CB	-10.32	1.40	1.53	18	4
1	A	57	ASN	CA-CB	-9.40	1.40	1.53	7	1
1	A	57	ASN	CB-CG	-8.55	1.30	1.52	11	2
2	B	171	ASN	CB-CG	-8.46	1.30	1.52	17	1
2	B	4	TYR	CA-CB	7.86	1.65	1.53	20	1
2	B	58	GLN	CG-CD	-6.48	1.35	1.52	7	1
1	A	57	ASN	CG-ND2	-6.24	1.20	1.33	7	1
2	B	168	SER	CA-CB	5.86	1.61	1.53	14	1
2	B	58	GLN	CA-CB	5.65	1.62	1.53	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	86	ARG	CD-NE	5.60	1.54	1.46	20	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(°)	Ideal(°)	Models	
								Worst	Total
2	B	171	ASN	OD1-CG-ND2	-34.83	87.77	122.60	12	2
2	B	187	ASN	OD1-CG-ND2	-30.53	92.07	122.60	2	1
2	B	171	ASN	CB-CA-C	-27.05	58.15	111.17	17	4
2	B	171	ASN	N-CA-CB	25.47	150.69	111.46	13	3
2	B	8	ASN	OD1-CG-ND2	-22.21	100.39	122.60	11	1
2	B	187	ASN	CB-CG-ND2	19.65	145.87	116.40	2	1
2	B	171	ASN	CB-CG-ND2	18.30	143.85	116.40	12	4
2	B	23	ASN	CA-CB-CG	-16.93	95.67	112.60	16	1
2	B	170	ASN	CA-CB-CG	-13.20	99.40	112.60	3	8
1	A	57	ASN	N-CA-CB	13.20	131.27	110.55	11	2
2	B	8	ASN	CB-CG-ND2	12.86	135.69	116.40	11	1
2	B	171	ASN	CB-CG-OD1	-11.93	96.95	120.80	17	3
2	B	168	SER	CB-CA-C	-11.65	86.16	111.78	14	1
2	B	58	GLN	CG-CD-NE2	11.17	133.16	116.40	7	3
2	B	23	ASN	N-CA-CB	10.77	125.95	110.12	16	1
2	B	4	TYR	CA-CB-CG	-10.45	95.09	113.90	13	3
2	B	58	GLN	OE1-CD-NE2	-9.74	112.86	122.60	7	1
2	B	162	TYR	CB-CA-C	-9.65	94.15	108.91	19	2
2	B	1	TYR	CA-CB-CG	9.14	130.36	113.90	4	2
2	B	191	PHE	N-CA-C	-9.12	101.34	111.28	1	20
2	B	3	PHE	CA-CB-CG	-9.08	104.72	113.80	16	6
1	A	34	ASN	N-CA-CB	9.00	122.88	110.10	18	4
2	B	126	GLN	CB-CG-CD	-8.88	97.50	112.60	17	2
2	B	186	ASP	N-CA-C	8.60	122.57	107.61	1	20
2	B	170	ASN	OD1-CG-ND2	-8.47	114.13	122.60	15	1
2	B	162	TYR	CA-CB-CG	-8.40	98.79	113.90	19	2
2	B	170	ASN	CB-CG-ND2	8.15	128.63	116.40	15	1
1	A	57	ASN	CA-CB-CG	7.98	120.58	112.60	11	1
2	B	100	PHE	CA-C-N	-7.85	109.95	120.63	1	20
2	B	100	PHE	C-N-CA	-7.85	109.95	120.63	1	20
1	A	34	ASN	OD1-CG-ND2	7.84	130.44	122.60	3	1
2	B	211	PRO	N-CA-CB	7.53	110.33	103.33	20	1
2	B	191	PHE	CA-CB-CG	-7.36	106.44	113.80	2	14
2	B	190	GLY	N-CA-C	-7.34	95.78	113.18	1	20
2	B	4	TYR	CB-CA-C	-7.18	98.87	110.79	20	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	85	HIS	CA-CB-CG	-7.12	106.68	113.80	2	5
2	B	100	PHE	CA-CB-CG	-7.07	106.73	113.80	1	20
2	B	168	SER	N-CA-CB	6.88	121.02	110.49	14	1
2	B	1	TYR	CB-CA-C	-6.80	97.17	110.10	4	1
2	B	173	PHE	CA-CB-CG	-6.64	107.16	113.80	2	15
2	B	23	ASN	CB-CG-OD1	-6.58	107.63	120.80	16	1
2	B	98	GLY	N-CA-C	-6.51	105.17	112.33	1	20
2	B	23	ASN	CB-CG-ND2	6.41	126.02	116.40	16	1
2	B	209	PRO	N-CA-CB	6.39	108.91	103.35	14	2
2	B	209	PRO	CB-CA-C	-6.23	103.26	111.23	9	1
2	B	170	ASN	N-CA-CB	-6.02	103.42	110.35	20	1
1	A	12	TYR	CA-CB-CG	-5.89	103.29	113.90	20	1
2	B	110	THR	CA-C-N	5.87	134.47	122.55	1	20
2	B	110	THR	C-N-CA	5.87	134.47	122.55	1	20
2	B	66	PRO	CB-CA-C	5.84	118.98	110.63	15	2
2	B	66	PRO	N-CD-CG	-5.83	94.46	103.20	7	2
2	B	85	PRO	N-CA-CB	5.75	106.21	103.22	1	20
2	B	3	PHE	N-CA-CB	5.75	118.57	110.12	19	1
2	B	170	ASN	CB-CA-C	5.74	119.60	111.74	4	6
2	B	99	ASP	CA-CB-CG	-5.68	106.92	112.60	8	8
1	A	34	ASN	CA-CB-CG	5.67	118.27	112.60	4	5
1	A	34	ASN	CB-CA-C	-5.49	102.66	111.39	18	4
2	B	160	GLN	CA-CB-CG	-5.47	103.16	114.10	3	2
2	B	85	PRO	O-C-N	5.45	123.71	121.15	1	20
2	B	101	TYR	CB-CA-C	-5.45	102.51	110.95	1	11
2	B	17	GLY	N-CA-C	-5.44	107.17	115.00	1	20
1	A	34	ASN	CB-CG-ND2	-5.36	108.37	116.40	3	1
2	B	56	ASP	CA-CB-CG	-5.17	107.43	112.60	1	20
2	B	187	ASN	CA-CB-CG	-5.16	107.44	112.60	2	11
2	B	8	ASN	CA-CB-CG	-5.14	107.46	112.60	2	5
1	A	57	ASN	CB-CG-ND2	-5.13	108.70	116.40	7	1
2	B	4	TYR	N-CA-CB	5.10	117.62	110.12	20	1
2	B	63	ASP	CA-CB-CG	-5.09	107.51	112.60	20	1
2	B	199	ASP	CA-CB-CG	-5.08	107.52	112.60	1	20
2	B	232	ASN	CA-C-N	5.08	128.68	121.02	1	20
2	B	232	ASN	C-N-CA	5.08	128.68	121.02	1	20
2	B	145	PHE	CA-CB-CG	-5.05	108.75	113.80	1	20
2	B	186	ASP	CB-CA-C	-5.02	103.81	110.79	1	18
2	B	165	GLY	N-CA-C	-5.00	107.63	114.64	1	20

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	158	ARG	Sidechain	20
1	A	86	ARG	Sidechain	5
2	B	171	ASN	Sidechain	3
2	B	1	TYR	Sidechain	1

6.2 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	713	711	711	100±16
2	B	1875	1804	1805	211±16
4	B	43	32	31	12±2
All	All	52640	50940	50951	5827

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 56.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:4:TYR:CZ	2:B:163:PRO:HG2	1.59	1.28	4	1
2:B:170:ASN:CB	2:B:170:ASN:CA	1.58	1.76	1	6
1:A:60:LEU:HD23	2:B:63:ASP:CB	1.51	1.29	19	1
1:A:37:GLY:O	2:B:1:TYR:CE1	1.49	1.65	4	1
2:B:23:ASN:CB	2:B:23:ASN:CA	1.48	1.88	16	1
2:B:4:TYR:CE2	2:B:163:PRO:HG2	1.47	1.43	4	1
1:A:81:TYR:HB2	1:A:86:ARG:NH2	1.46	1.11	3	2
1:A:60:LEU:CD1	2:B:63:ASP:HB3	1.45	1.35	12	1
1:A:60:LEU:CD2	2:B:63:ASP:CB	1.43	1.95	19	2
2:B:4:TYR:CZ	2:B:163:PRO:CG	1.40	2.03	4	1
1:A:37:GLY:C	2:B:1:TYR:OH	1.40	1.64	4	1
2:B:162:TYR:O	2:B:162:TYR:CD1	1.38	1.76	19	1
1:A:60:LEU:HD11	2:B:63:ASP:CB	1.34	1.52	12	1
2:B:1:TYR:CD2	2:B:4:TYR:HE2	1.33	1.40	7	2
1:A:82:CYS:O	1:A:86:ARG:NE	1.33	1.60	16	1
1:A:60:LEU:CD2	2:B:63:ASP:HB2	1.33	1.50	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:TYR:OH	2:B:3:PHE:HB2	1.30	1.19	20	2
2:B:4:TYR:CE2	2:B:163:PRO:CG	1.29	2.13	4	1
2:B:161:VAL:C	2:B:162:TYR:HD1	1.28	1.34	12	1
2:B:1:TYR:CD2	2:B:4:TYR:CE2	1.27	2.22	7	5
2:B:162:TYR:OH	2:B:168:SER:HA	1.26	1.25	6	2
1:A:81:TYR:CB	1:A:86:ARG:HH21	1.25	1.42	3	1
1:A:86:ARG:HH12	1:A:87:GLY:CA	1.25	1.42	10	1
1:A:86:ARG:O	1:A:86:ARG:HD3	1.24	1.27	3	3
1:A:37:GLY:O	2:B:1:TYR:CZ	1.24	1.90	4	1
2:B:162:TYR:CD2	2:B:163:PRO:HD2	1.23	1.66	9	2
1:A:37:GLY:O	4:B:250:HEC:CGD	1.23	1.84	20	2
1:A:60:LEU:CD1	2:B:61:GLN:NE2	1.22	2.02	19	1
2:B:189:PHE:CD1	2:B:209:PRO:HG3	1.21	1.70	15	12
1:A:38:PRO:HD3	2:B:119:PRO:O	1.21	1.09	2	1
1:A:60:LEU:CG	2:B:63:ASP:HB2	1.21	1.64	12	1
2:B:162:TYR:CD1	2:B:162:TYR:C	1.20	2.06	19	1
1:A:60:LEU:CG	2:B:63:ASP:CB	1.20	2.19	12	1
2:B:162:TYR:CG	2:B:164:THR:HG22	1.19	1.71	19	2
1:A:81:TYR:CB	1:A:86:ARG:NH2	1.19	2.04	3	3
1:A:60:LEU:HD21	2:B:63:ASP:CB	1.19	1.67	12	1
1:A:83:THR:O	2:B:62:ALA:HB3	1.19	1.36	13	2
2:B:24:CYS:SG	4:B:250:HEC:CHD	1.17	2.31	5	20
2:B:1:TYR:CZ	2:B:119:PRO:CG	1.17	2.27	20	1
2:B:1:TYR:CZ	2:B:119:PRO:HG2	1.17	1.74	20	1
1:A:12:TYR:CZ	2:B:3:PHE:HB2	1.17	1.75	19	2
2:B:161:VAL:C	2:B:162:TYR:CD1	1.17	2.22	12	1
1:A:86:ARG:HH22	1:A:91:VAL:CG1	1.16	1.53	19	3
1:A:38:PRO:HB2	1:A:60:LEU:CD1	1.16	1.70	15	1
1:A:86:ARG:NH1	1:A:87:GLY:CA	1.15	2.10	10	1
1:A:86:ARG:HD2	1:A:86:ARG:C	1.14	1.67	9	1
1:A:12:TYR:OH	2:B:3:PHE:CB	1.14	1.94	20	2
1:A:60:LEU:CD1	2:B:61:GLN:CD	1.14	2.21	19	2
2:B:162:TYR:OH	2:B:168:SER:CA	1.14	1.93	6	1
1:A:37:GLY:C	2:B:1:TYR:CZ	1.12	2.25	4	1
1:A:60:LEU:CD2	2:B:62:ALA:HB1	1.12	1.72	15	1
2:B:162:TYR:CG	2:B:163:PRO:HD2	1.12	1.78	9	1
1:A:58:THR:OG1	2:B:63:ASP:CB	1.11	1.97	8	1
2:B:1:TYR:CD1	2:B:1:TYR:N	1.11	2.15	13	3
2:B:104:VAL:CG1	2:B:115:LEU:HD12	1.11	1.76	17	3
2:B:189:PHE:CD2	2:B:209:PRO:HD3	1.10	1.80	5	19
1:A:58:THR:OG1	2:B:63:ASP:HB2	1.10	1.42	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:61:GLN:HG2	2:B:65:SER:O	1.10	1.43	19	8
1:A:86:ARG:NH2	1:A:91:VAL:CG1	1.10	2.14	19	2
1:A:60:LEU:CD1	2:B:63:ASP:CB	1.09	2.15	12	1
1:A:87:GLY:HA3	2:B:164:THR:HG23	1.09	1.13	3	1
1:A:86:ARG:HH12	1:A:91:VAL:CG1	1.09	1.61	18	3
2:B:1:TYR:HD2	2:B:4:TYR:CE2	1.09	1.54	7	3
1:A:38:PRO:CD	2:B:119:PRO:O	1.08	2.00	2	1
1:A:38:PRO:HD2	2:B:62:ALA:HB2	1.08	1.20	20	2
1:A:60:LEU:HD21	2:B:63:ASP:CA	1.08	1.77	12	1
1:A:86:ARG:CA	1:A:86:ARG:HE	1.08	1.61	18	1
2:B:189:PHE:CE1	2:B:209:PRO:HG3	1.07	1.84	4	14
2:B:162:TYR:HB3	2:B:164:THR:HG22	1.07	1.16	9	13
1:A:86:ARG:NH1	1:A:87:GLY:N	1.07	2.02	10	2
2:B:162:TYR:HB3	2:B:164:THR:CG2	1.07	1.78	9	2
1:A:60:LEU:HD23	2:B:62:ALA:CB	1.07	1.79	18	2
1:A:86:ARG:HH22	1:A:91:VAL:HG11	1.06	0.96	19	1
2:B:104:VAL:HG13	2:B:115:LEU:HG	1.06	1.25	6	16
1:A:60:LEU:CG	2:B:62:ALA:HB1	1.06	1.81	15	1
1:A:86:ARG:HG2	1:A:86:ARG:HH11	1.05	0.90	1	2
2:B:104:VAL:HG11	2:B:115:LEU:HD12	1.05	1.28	17	3
1:A:38:PRO:CD	2:B:119:PRO:HG2	1.05	1.81	4	7
1:A:46:VAL:HG13	1:A:52:ALA:HB2	1.05	1.29	17	20
1:A:62:ILE:HG23	2:B:121:PRO:CG	1.05	1.81	17	2
2:B:162:TYR:CD2	2:B:163:PRO:N	1.05	2.20	19	1
1:A:38:PRO:HD3	2:B:119:PRO:CG	1.04	1.82	3	5
2:B:162:TYR:HB2	2:B:164:THR:HG22	1.04	1.14	6	12
1:A:60:LEU:CD2	2:B:63:ASP:HB3	1.04	1.68	19	1
2:B:162:TYR:CG	2:B:163:PRO:N	1.04	2.17	19	1
1:A:60:LEU:HD23	2:B:62:ALA:HB2	1.03	1.13	18	1
1:A:8:GLY:O	1:A:34:ASN:ND2	1.03	1.91	5	4
2:B:162:TYR:HD1	2:B:162:TYR:N	1.03	1.35	12	1
2:B:164:THR:HG23	2:B:166:GLU:H	1.02	1.11	14	16
1:A:82:CYS:C	1:A:86:ARG:HE	1.02	1.60	16	1
1:A:38:PRO:HD3	2:B:119:PRO:HG2	1.01	1.22	1	7
1:A:57:ASN:OD1	1:A:68:TYR:OH	1.01	1.77	11	1
2:B:4:TYR:CE1	2:B:163:PRO:CG	1.00	2.44	4	3
1:A:60:LEU:HD11	2:B:61:GLN:OE1	1.00	1.55	20	3
2:B:1:TYR:CD2	2:B:3:PHE:CZ	1.00	2.49	19	1
1:A:37:GLY:C	2:B:1:TYR:CE1	1.00	2.40	4	1
1:A:60:LEU:HD13	2:B:61:GLN:NE2	1.00	1.71	19	1
1:A:86:ARG:HH12	1:A:91:VAL:HG13	1.00	1.10	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ILE:HG23	2:B:121:PRO:HG2	1.00	1.28	17	2
1:A:87:GLY:CA	2:B:164:THR:HG23	0.99	1.87	3	1
2:B:162:TYR:HE1	2:B:168:SER:N	0.99	1.55	6	1
2:B:162:TYR:CZ	2:B:168:SER:HA	0.99	1.93	6	1
1:A:60:LEU:HD21	2:B:63:ASP:HB2	0.99	1.17	12	1
2:B:59:GLN:HG3	2:B:233:VAL:HG22	0.99	1.28	12	7
1:A:60:LEU:HD21	2:B:61:GLN:CG	0.99	1.88	8	1
1:A:83:THR:O	1:A:86:ARG:CG	0.99	2.11	11	2
1:A:83:THR:HG21	2:B:61:GLN:NE2	0.98	1.73	17	1
1:A:86:ARG:O	1:A:86:ARG:NE	0.98	1.96	18	2
1:A:86:ARG:HG2	1:A:86:ARG:NH1	0.98	1.68	1	1
2:B:164:THR:HG22	2:B:166:GLU:H	0.98	1.12	1	1
1:A:58:THR:HG21	2:B:63:ASP:HB3	0.98	1.00	14	2
1:A:12:TYR:O	2:B:3:PHE:CZ	0.98	2.16	16	1
1:A:14:PRO:HG3	2:B:3:PHE:HE2	0.98	1.17	18	1
2:B:162:TYR:CB	2:B:164:THR:HG22	0.98	1.87	14	17
2:B:24:CYS:SG	4:B:250:HEC:HHD	0.98	1.99	20	20
1:A:38:PRO:CB	1:A:60:LEU:HD11	0.98	1.87	15	1
1:A:14:PRO:HG3	1:A:36:VAL:HG21	0.97	0.98	16	7
1:A:40:ASN:HB3	1:A:60:LEU:HD22	0.97	1.30	16	1
1:A:86:ARG:HE	1:A:86:ARG:C	0.97	1.65	18	1
1:A:62:ILE:HD11	2:B:120:LEU:HA	0.97	1.32	2	1
1:A:83:THR:O	2:B:62:ALA:CB	0.97	2.12	17	2
1:A:38:PRO:HD3	2:B:70:ASN:OD1	0.97	1.59	17	1
1:A:86:ARG:NE	1:A:86:ARG:HA	0.97	1.74	18	1
1:A:86:ARG:HB3	2:B:164:THR:HG23	0.97	1.34	18	1
2:B:4:TYR:CE1	2:B:163:PRO:CB	0.96	2.48	4	1
1:A:60:LEU:CD2	2:B:62:ALA:HB2	0.96	1.88	18	1
1:A:86:ARG:HD3	1:A:86:ARG:C	0.96	1.81	3	2
1:A:38:PRO:HD3	2:B:119:PRO:C	0.96	1.84	2	1
1:A:83:THR:O	1:A:86:ARG:HG2	0.96	1.60	11	3
1:A:60:LEU:CD1	2:B:61:GLN:OE1	0.96	2.14	20	1
1:A:38:PRO:CD	2:B:70:ASN:OD1	0.96	2.14	17	2
1:A:86:ARG:NH1	1:A:91:VAL:CG1	0.95	2.28	18	3
2:B:162:TYR:HB2	2:B:164:THR:CG2	0.95	1.91	6	13
1:A:14:PRO:HG3	1:A:36:VAL:CG2	0.95	1.90	16	1
1:A:60:LEU:HD21	2:B:61:GLN:HG3	0.95	1.36	8	1
1:A:86:ARG:CZ	1:A:86:ARG:HA	0.95	1.91	16	1
1:A:58:THR:HG21	2:B:63:ASP:CB	0.94	1.93	14	1
1:A:39:HIS:O	1:A:60:LEU:CD1	0.94	2.15	15	1
2:B:24:CYS:HB2	4:B:250:HEC:CAC	0.94	1.93	20	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:162:TYR:CG	2:B:164:THR:CG2	0.94	2.49	19	1
2:B:162:TYR:CD1	2:B:162:TYR:N	0.94	2.11	12	2
2:B:4:TYR:CD1	2:B:163:PRO:HG3	0.93	1.99	3	6
1:A:60:LEU:HD23	2:B:63:ASP:HB2	0.93	0.95	19	1
1:A:14:PRO:CG	1:A:36:VAL:HG21	0.93	1.93	16	3
1:A:86:ARG:HH12	1:A:91:VAL:HG11	0.92	1.19	18	1
1:A:60:LEU:HG	2:B:62:ALA:HB1	0.92	1.40	15	1
1:A:86:ARG:NH2	1:A:91:VAL:HG11	0.92	1.71	19	1
2:B:162:TYR:HD1	2:B:166:GLU:O	0.92	1.47	6	1
2:B:115:LEU:HD23	2:B:115:LEU:O	0.92	1.64	14	8
2:B:1:TYR:OH	4:B:250:HEC:CBD	0.92	2.18	11	2
1:A:60:LEU:HD23	2:B:63:ASP:HB3	0.92	1.23	19	1
1:A:38:PRO:CD	2:B:62:ALA:HB2	0.92	1.95	20	2
2:B:7:TYR:CD1	2:B:7:TYR:O	0.92	2.23	19	1
1:A:60:LEU:HD13	2:B:61:GLN:CD	0.91	1.88	19	1
2:B:162:TYR:OH	2:B:168:SER:CB	0.91	2.19	6	1
2:B:162:TYR:CE1	2:B:168:SER:CA	0.91	2.53	6	2
2:B:1:TYR:OH	2:B:119:PRO:HG2	0.91	1.66	20	1
2:B:59:GLN:HG3	2:B:233:VAL:CG2	0.91	1.96	12	4
2:B:162:TYR:CZ	2:B:168:SER:CA	0.91	2.54	6	1
1:A:86:ARG:HH12	1:A:87:GLY:HA3	0.90	1.25	10	1
1:A:38:PRO:HB2	1:A:60:LEU:HD11	0.90	0.96	15	1
1:A:83:THR:O	1:A:86:ARG:CD	0.90	2.20	11	1
2:B:189:PHE:HD1	2:B:209:PRO:CG	0.90	1.78	15	1
1:A:60:LEU:HG	2:B:61:GLN:CD	0.90	1.90	20	1
1:A:86:ARG:CA	1:A:86:ARG:NE	0.90	2.30	18	1
2:B:115:LEU:HD23	2:B:115:LEU:C	0.90	1.90	14	16
2:B:59:GLN:NE2	2:B:158:ARG:HG3	0.90	1.81	4	7
2:B:1:TYR:CZ	2:B:119:PRO:HG3	0.89	2.01	20	1
1:A:60:LEU:HD11	2:B:61:GLN:CD	0.89	1.89	19	3
1:A:38:PRO:N	2:B:1:TYR:OH	0.89	2.06	4	1
1:A:40:ASN:HB3	1:A:60:LEU:CD2	0.89	1.97	16	1
1:A:86:ARG:HH11	1:A:86:ARG:CG	0.89	1.79	1	2
2:B:189:PHE:CG	2:B:209:PRO:HD3	0.88	2.03	3	13
1:A:60:LEU:HD22	2:B:63:ASP:CB	0.88	1.97	19	1
2:B:4:TYR:CD2	2:B:163:PRO:HG3	0.88	2.03	4	3
1:A:14:PRO:HG3	2:B:3:PHE:CE2	0.88	2.02	18	3
1:A:83:THR:O	2:B:164:THR:HB	0.88	1.69	16	1
1:A:38:PRO:CD	2:B:1:TYR:CE1	0.88	2.57	4	2
1:A:62:ILE:HG23	2:B:121:PRO:CB	0.87	1.99	13	2
2:B:162:TYR:CG	2:B:163:PRO:CD	0.87	2.57	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:1:TYR:OH	4:B:250:HEC:HBD2	0.87	1.69	11	1
2:B:3:PHE:O	2:B:6:GLN:HG3	0.87	1.70	8	1
1:A:86:ARG:CZ	1:A:87:GLY:N	0.87	2.37	10	1
1:A:83:THR:HG21	2:B:62:ALA:CB	0.86	1.99	3	6
2:B:162:TYR:CD2	2:B:163:PRO:CD	0.86	2.57	9	2
2:B:162:TYR:CE1	2:B:168:SER:N	0.86	2.42	6	1
2:B:187:ASN:HB2	2:B:189:PHE:CD1	0.86	2.05	18	5
2:B:162:TYR:CD1	2:B:164:THR:CG2	0.86	2.58	19	1
1:A:83:THR:O	1:A:86:ARG:HD2	0.86	1.69	11	1
1:A:85:HIS:HA	2:B:4:TYR:OH	0.86	1.69	3	3
1:A:86:ARG:C	1:A:86:ARG:CD	0.86	2.49	9	3
1:A:86:ARG:NH1	1:A:91:VAL:HG13	0.86	1.86	19	3
2:B:23:ASN:CA	2:B:23:ASN:CG	0.85	2.49	16	1
2:B:104:VAL:CG1	2:B:115:LEU:CD1	0.85	2.54	17	3
1:A:60:LEU:CG	2:B:61:GLN:CD	0.85	2.48	20	1
1:A:37:GLY:O	2:B:1:TYR:HE1	0.85	1.49	4	1
2:B:189:PHE:CD1	2:B:209:PRO:CG	0.85	2.58	15	6
2:B:1:TYR:CE1	2:B:119:PRO:HG3	0.85	2.06	20	1
1:A:38:PRO:HG2	1:A:60:LEU:HD21	0.85	1.47	15	1
1:A:42:ILE:HG13	1:A:83:THR:OG1	0.85	1.71	11	8
1:A:83:THR:HG21	2:B:62:ALA:HB2	0.85	1.49	3	3
2:B:162:TYR:HE1	2:B:167:LEU:C	0.85	1.80	6	1
1:A:39:HIS:O	1:A:60:LEU:HD12	0.85	1.70	15	1
1:A:38:PRO:HD3	2:B:1:TYR:CZ	0.85	2.06	16	2
1:A:87:GLY:CA	2:B:164:THR:CG2	0.84	2.54	3	1
1:A:86:ARG:HE	1:A:86:ARG:HA	0.84	1.23	18	1
1:A:82:CYS:H	1:A:86:ARG:NH2	0.84	1.68	16	1
1:A:62:ILE:HG22	2:B:121:PRO:HB3	0.84	1.49	11	1
2:B:46:LYS:HG2	2:B:129:ILE:HD11	0.84	1.48	1	20
2:B:170:ASN:CA	2:B:170:ASN:CG	0.84	2.50	1	6
2:B:189:PHE:HD1	2:B:209:PRO:HG3	0.83	1.07	15	1
2:B:86:PRO:HB3	2:B:100:PHE:CE2	0.83	2.08	1	20
2:B:32:GLU:HA	2:B:239:MET:CE	0.83	2.04	1	20
1:A:86:ARG:NH1	2:B:164:THR:HG21	0.83	1.87	12	1
1:A:62:ILE:HG23	2:B:70:ASN:ND2	0.83	1.89	10	2
2:B:192:ASP:HB3	2:B:204:VAL:HG22	0.83	1.48	1	20
1:A:36:VAL:HG13	1:A:36:VAL:O	0.83	1.74	19	10
1:A:86:ARG:CZ	1:A:91:VAL:CG1	0.82	2.57	19	1
2:B:104:VAL:CG1	2:B:115:LEU:HG	0.82	2.02	4	12
2:B:1:TYR:HD2	2:B:4:TYR:HE2	0.82	1.16	9	1
2:B:9:TYR:CD1	2:B:20:VAL:HG11	0.82	2.09	16	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:4:TYR:CG	2:B:163:PRO:HG3	0.82	2.10	4	1
1:A:12:TYR:O	2:B:3:PHE:HZ	0.82	1.54	16	1
1:A:58:THR:O	2:B:62:ALA:CB	0.82	2.27	18	1
2:B:4:TYR:CD2	2:B:163:PRO:CG	0.82	2.62	4	2
2:B:115:LEU:C	2:B:115:LEU:HD23	0.82	1.99	7	2
2:B:162:TYR:CD1	2:B:164:THR:HG22	0.82	2.10	19	1
2:B:162:TYR:HH	2:B:168:SER:HA	0.81	0.99	6	1
1:A:86:ARG:HB3	2:B:164:THR:CG2	0.81	2.05	18	1
2:B:4:TYR:CE2	2:B:163:PRO:HG3	0.81	2.11	4	1
2:B:162:TYR:CD1	2:B:166:GLU:O	0.81	2.33	6	1
2:B:162:TYR:CZ	2:B:168:SER:CB	0.81	2.64	6	1
2:B:1:TYR:HD2	2:B:3:PHE:CZ	0.81	1.92	19	1
1:A:60:LEU:HG	2:B:63:ASP:HB2	0.81	1.49	12	1
2:B:189:PHE:CD2	2:B:209:PRO:CD	0.81	2.64	16	17
2:B:83:LEU:HD11	2:B:131:PRO:HD2	0.80	1.49	17	20
1:A:58:THR:HG1	2:B:63:ASP:HB2	0.80	1.27	8	1
2:B:1:TYR:CE1	2:B:4:TYR:CE2	0.80	2.68	11	1
1:A:46:VAL:CG1	1:A:52:ALA:HB2	0.80	2.07	4	20
1:A:14:PRO:HD2	2:B:7:TYR:HE2	0.80	1.36	16	1
1:A:37:GLY:CA	2:B:1:TYR:OH	0.80	2.29	4	1
1:A:62:ILE:HD12	1:A:62:ILE:H	0.80	1.37	10	2
2:B:162:TYR:CB	2:B:164:THR:CG2	0.80	2.59	11	10
1:A:58:THR:CG2	2:B:63:ASP:HB3	0.80	1.96	14	2
2:B:164:THR:CG2	2:B:166:GLU:H	0.80	1.90	15	3
1:A:40:ASN:HB3	2:B:63:ASP:OD2	0.80	1.77	20	1
2:B:4:TYR:CZ	2:B:163:PRO:CB	0.79	2.63	4	1
1:A:58:THR:O	2:B:62:ALA:HB3	0.79	1.75	18	1
2:B:162:TYR:CE2	2:B:163:PRO:HD2	0.79	2.12	9	1
1:A:33:MET:SD	1:A:39:HIS:HD2	0.79	2.00	19	16
1:A:36:VAL:HG22	1:A:36:VAL:O	0.79	1.77	13	6
1:A:62:ILE:HG23	2:B:121:PRO:HB2	0.79	1.51	13	1
1:A:12:TYR:CG	2:B:4:TYR:CE1	0.79	2.70	19	1
2:B:1:TYR:CD1	2:B:119:PRO:HG3	0.79	2.12	18	5
1:A:88:ALA:HB2	2:B:4:TYR:OH	0.79	1.78	12	2
2:B:208:LEU:HD22	2:B:208:LEU:H	0.79	1.37	9	12
1:A:87:GLY:HA3	2:B:164:THR:CG2	0.79	2.00	3	1
2:B:1:TYR:CE2	2:B:119:PRO:CG	0.79	2.65	20	2
1:A:38:PRO:O	2:B:1:TYR:OH	0.78	2.02	4	1
1:A:60:LEU:HD12	2:B:61:GLN:NE2	0.78	1.91	19	1
1:A:3:VAL:HG21	1:A:21:LEU:HD11	0.78	1.56	4	20
2:B:97:VAL:HA	2:B:129:ILE:CG2	0.78	2.09	1	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:104:VAL:HG13	2:B:115:LEU:CG	0.78	2.08	4	14
2:B:104:VAL:HG13	2:B:115:LEU:CD1	0.78	2.07	17	3
2:B:1:TYR:H3	2:B:4:TYR:HD2	0.78	1.17	14	1
1:A:86:ARG:HD2	1:A:87:GLY:N	0.78	1.94	9	1
1:A:60:LEU:HG	2:B:62:ALA:CB	0.78	2.08	15	1
2:B:40:LEU:HB3	2:B:41:PRO:HD2	0.78	1.53	1	20
1:A:81:TYR:HB2	1:A:86:ARG:HH22	0.78	1.38	3	1
1:A:38:PRO:HD2	2:B:70:ASN:CG	0.78	2.04	13	1
1:A:12:TYR:HB3	2:B:4:TYR:CE1	0.78	2.13	19	1
1:A:58:THR:OG1	2:B:63:ASP:HB3	0.77	1.79	8	1
1:A:38:PRO:HD2	2:B:70:ASN:ND2	0.77	1.95	13	1
2:B:189:PHE:CE2	2:B:209:PRO:HD3	0.77	2.14	14	13
1:A:64:PRO:HD3	2:B:121:PRO:HG3	0.77	1.56	11	1
2:B:208:LEU:HD13	2:B:208:LEU:N	0.77	1.94	10	4
1:A:46:VAL:HG11	1:A:78:TYR:CD2	0.77	2.15	5	20
2:B:42:ASP:OD1	2:B:133:LEU:HD11	0.77	1.79	1	20
2:B:107:TYR:HA	2:B:116:LEU:HD11	0.77	1.57	6	2
1:A:60:LEU:CD2	2:B:63:ASP:CA	0.77	2.58	12	1
2:B:187:ASN:HB2	2:B:189:PHE:HD1	0.77	1.36	18	5
2:B:1:TYR:CD2	2:B:4:TYR:CG	0.77	2.44	13	1
2:B:1:TYR:H1	2:B:1:TYR:HD1	0.77	1.22	13	2
1:A:12:TYR:HE2	2:B:3:PHE:O	0.77	1.63	19	1
1:A:86:ARG:NH2	1:A:91:VAL:HG12	0.77	1.93	19	2
1:A:14:PRO:HG3	2:B:3:PHE:CZ	0.77	2.15	6	1
1:A:12:TYR:HD2	2:B:3:PHE:HE1	0.77	1.19	16	1
1:A:82:CYS:H	1:A:86:ARG:HH21	0.77	1.23	16	1
1:A:38:PRO:HD3	2:B:1:TYR:CE1	0.76	2.14	16	2
1:A:62:ILE:HG12	2:B:121:PRO:HB3	0.76	1.58	13	2
2:B:83:LEU:HD22	2:B:104:VAL:CG1	0.76	2.10	2	20
2:B:158:ARG:HE	4:B:250:HEC:CGD	0.76	1.93	17	9
1:A:60:LEU:HD21	2:B:63:ASP:HA	0.76	1.56	12	1
2:B:208:LEU:HD22	2:B:208:LEU:N	0.76	1.96	3	9
1:A:62:ILE:HD12	2:B:70:ASN:ND2	0.76	1.95	14	2
1:A:24:SER:HA	1:A:97:GLU:OXT	0.76	1.81	1	20
1:A:38:PRO:HD2	2:B:1:TYR:CZ	0.76	2.16	3	3
1:A:86:ARG:O	1:A:86:ARG:CD	0.76	2.23	3	2
2:B:24:CYS:HB2	4:B:250:HEC:HAC	0.75	1.55	20	20
2:B:61:GLN:CG	2:B:65:SER:O	0.75	2.31	19	1
2:B:170:ASN:O	2:B:170:ASN:ND2	0.75	2.18	20	1
2:B:59:GLN:HB2	2:B:233:VAL:HG21	0.75	1.58	10	18
1:A:34:ASN:ND2	1:A:35:LYS:HD3	0.75	1.96	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:PRO:CG	2:B:62:ALA:HB2	0.75	2.12	15	1
1:A:40:ASN:HD22	1:A:40:ASN:C	0.75	1.90	16	1
1:A:60:LEU:HD23	2:B:62:ALA:HB1	0.75	1.58	15	1
1:A:60:LEU:HD21	2:B:61:GLN:NE2	0.74	1.97	20	1
1:A:81:TYR:HB3	1:A:86:ARG:NH2	0.74	1.96	4	2
1:A:37:GLY:O	4:B:250:HEC:O2D	0.74	2.05	20	2
2:B:83:LEU:HD22	2:B:104:VAL:CB	0.74	2.12	5	20
1:A:12:TYR:HH	2:B:3:PHE:HB2	0.74	1.43	20	1
1:A:14:PRO:HD2	2:B:7:TYR:CE2	0.74	2.18	16	1
1:A:37:GLY:O	2:B:119:PRO:HD2	0.74	1.82	2	3
1:A:62:ILE:HB	2:B:121:PRO:HG3	0.74	1.57	10	1
1:A:36:VAL:HG23	2:B:119:PRO:HG2	0.74	1.58	13	1
2:B:170:ASN:ND2	2:B:170:ASN:O	0.74	2.19	19	3
2:B:162:TYR:O	2:B:162:TYR:CE1	0.74	2.38	19	1
1:A:46:VAL:HG13	1:A:52:ALA:CB	0.73	2.13	20	20
2:B:30:THR:CG2	2:B:52:PRO:HG2	0.73	2.13	1	20
2:B:1:TYR:HD1	2:B:119:PRO:HG3	0.73	1.40	18	3
2:B:61:GLN:OE1	2:B:65:SER:HB2	0.73	1.84	13	2
1:A:14:PRO:HB3	1:A:36:VAL:CG1	0.73	2.13	19	11
2:B:24:CYS:SG	4:B:250:HEC:C4C	0.73	2.76	5	20
2:B:208:LEU:N	2:B:208:LEU:HD22	0.73	1.98	13	5
1:A:62:ILE:HD13	2:B:121:PRO:HB2	0.73	1.60	13	2
1:A:36:VAL:HG23	2:B:3:PHE:CG	0.72	2.19	3	2
2:B:75:LEU:HB3	2:B:115:LEU:HD22	0.72	1.60	9	7
1:A:12:TYR:CB	2:B:4:TYR:HE1	0.72	1.96	19	1
1:A:86:ARG:NH1	1:A:86:ARG:CG	0.72	2.45	1	2
1:A:86:ARG:HH12	1:A:87:GLY:HA2	0.72	1.37	10	1
1:A:60:LEU:CD2	2:B:62:ALA:CB	0.72	2.63	15	1
1:A:38:PRO:HD3	4:B:250:HEC:O2D	0.72	1.85	20	2
1:A:36:VAL:HG23	2:B:119:PRO:HD2	0.72	1.61	17	1
1:A:64:PRO:HG3	2:B:102:TYR:CD1	0.72	2.20	2	1
2:B:162:TYR:CE1	2:B:167:LEU:C	0.72	2.67	6	1
1:A:12:TYR:CB	2:B:4:TYR:CE1	0.72	2.72	19	1
1:A:60:LEU:HG	2:B:61:GLN:CG	0.72	2.15	20	1
2:B:212:GLU:HG2	2:B:229:THR:HG22	0.72	1.62	1	20
2:B:1:TYR:HD1	2:B:1:TYR:H3	0.72	1.27	11	1
1:A:87:GLY:HA3	2:B:162:TYR:HE2	0.72	1.45	17	2
1:A:82:CYS:O	1:A:86:ARG:CZ	0.72	2.38	16	1
2:B:212:GLU:HG2	2:B:229:THR:CG2	0.71	2.14	1	20
2:B:7:TYR:CD1	2:B:7:TYR:C	0.71	2.66	19	1
2:B:83:LEU:HD22	2:B:104:VAL:HB	0.71	1.61	15	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:61:GLN:CG	2:B:62:ALA:N	0.71	2.53	16	1
2:B:162:TYR:CE1	2:B:168:SER:HA	0.71	2.19	6	2
2:B:107:TYR:HD1	2:B:116:LEU:HD21	0.71	1.43	6	1
1:A:14:PRO:CB	1:A:36:VAL:HG11	0.71	2.14	19	6
2:B:24:CYS:CB	4:B:250:HEC:C3C	0.71	2.69	2	20
2:B:120:LEU:HD22	2:B:125:TYR:CE2	0.71	2.21	9	3
1:A:40:ASN:OD1	1:A:42:ILE:CG1	0.71	2.38	20	1
2:B:107:TYR:CD1	2:B:116:LEU:HD21	0.71	2.21	6	1
2:B:7:TYR:O	2:B:7:TYR:HD1	0.71	1.69	19	1
1:A:12:TYR:CD2	2:B:3:PHE:HE1	0.70	2.03	16	1
1:A:40:ASN:CG	2:B:63:ASP:OD1	0.70	2.35	20	1
1:A:81:TYR:HB2	1:A:86:ARG:CZ	0.70	2.16	16	3
2:B:162:TYR:CE1	4:B:250:HEC:CMD	0.70	2.74	12	1
1:A:82:CYS:O	1:A:86:ARG:CD	0.70	2.40	16	1
2:B:83:LEU:HD22	2:B:104:VAL:HG11	0.70	1.63	2	9
1:A:62:ILE:CG2	2:B:121:PRO:HB2	0.70	2.16	13	1
1:A:60:LEU:HD12	1:A:62:ILE:HD11	0.70	1.61	4	3
2:B:24:CYS:HB2	4:B:250:HEC:C3C	0.70	2.16	14	20
2:B:115:LEU:C	2:B:115:LEU:CD2	0.70	2.65	14	18
2:B:115:LEU:HD23	2:B:116:LEU:N	0.70	2.02	5	12
1:A:37:GLY:O	2:B:119:PRO:HG2	0.70	1.86	11	4
1:A:14:PRO:CD	2:B:7:TYR:HE2	0.70	1.99	16	1
2:B:4:TYR:CE1	2:B:163:PRO:HG2	0.70	2.22	3	2
1:A:12:TYR:CZ	2:B:3:PHE:CB	0.70	2.66	20	2
1:A:60:LEU:CG	2:B:61:GLN:NE2	0.70	2.55	20	1
2:B:164:THR:HG22	2:B:166:GLU:N	0.69	1.97	1	1
2:B:164:THR:CG2	2:B:166:GLU:HB2	0.69	2.17	1	1
1:A:36:VAL:HG22	1:A:85:HIS:HE2	0.69	1.46	4	1
2:B:187:ASN:O	2:B:189:PHE:CD1	0.69	2.45	20	5
2:B:61:GLN:HG3	2:B:62:ALA:H	0.69	1.47	16	1
1:A:96:VAL:HG12	1:A:96:VAL:O	0.69	1.88	16	20
2:B:1:TYR:CD2	2:B:119:PRO:HG3	0.69	2.23	16	3
2:B:164:THR:HG23	2:B:166:GLU:N	0.69	1.97	10	12
1:A:82:CYS:N	1:A:86:ARG:NH2	0.69	2.41	16	1
1:A:86:ARG:HD3	1:A:87:GLY:N	0.69	2.03	12	1
2:B:1:TYR:CE2	2:B:4:TYR:HE2	0.68	2.05	7	1
2:B:62:ALA:HA	2:B:158:ARG:NH2	0.68	2.02	15	7
1:A:38:PRO:CD	2:B:1:TYR:HE1	0.68	2.01	4	1
1:A:12:TYR:OH	2:B:3:PHE:HB3	0.68	1.85	19	1
1:A:86:ARG:NH1	1:A:86:ARG:HA	0.68	2.03	3	2
1:A:33:MET:SD	1:A:39:HIS:CD2	0.68	2.87	19	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:PRO:CB	1:A:85:HIS:CD2	0.68	2.76	4	1
2:B:32:GLU:HA	2:B:239:MET:HE2	0.68	1.65	1	20
2:B:1:TYR:OH	4:B:250:HEC:HBD1	0.68	1.87	11	3
2:B:53:TYR:CE2	2:B:69:LEU:HD13	0.68	2.23	10	1
2:B:4:TYR:CD1	4:B:250:HEC:HBC2	0.68	2.24	20	1
1:A:38:PRO:HD2	2:B:1:TYR:CE2	0.68	2.24	6	3
2:B:168:SER:HB3	2:B:170:ASN:H	0.67	1.48	14	1
1:A:12:TYR:HD2	2:B:105:THR:HG21	0.67	1.47	13	1
1:A:38:PRO:CG	2:B:62:ALA:CB	0.67	2.72	15	2
2:B:1:TYR:HB2	2:B:4:TYR:CD2	0.67	2.25	19	1
1:A:12:TYR:OH	2:B:3:PHE:CG	0.67	2.47	20	1
2:B:46:LYS:CG	2:B:129:ILE:HD11	0.67	2.19	1	20
1:A:86:ARG:HB2	1:A:86:ARG:CZ	0.67	2.18	11	1
2:B:189:PHE:HD2	2:B:209:PRO:HD3	0.67	1.47	13	4
1:A:86:ARG:NH1	1:A:86:ARG:HG2	0.67	1.98	10	1
2:B:4:TYR:CD1	2:B:163:PRO:CG	0.67	2.77	3	4
2:B:187:ASN:HB2	2:B:189:PHE:CD2	0.67	2.25	15	1
1:A:9:THR:CG2	1:A:15:LEU:HD11	0.67	2.20	9	8
1:A:38:PRO:HD2	2:B:1:TYR:CE1	0.67	2.24	4	2
1:A:81:TYR:HB2	1:A:86:ARG:NH1	0.67	2.05	1	2
1:A:39:HIS:O	1:A:60:LEU:HD13	0.67	1.89	15	1
2:B:1:TYR:N	2:B:4:TYR:HD2	0.66	1.87	14	2
1:A:12:TYR:CD2	2:B:4:TYR:CD1	0.66	2.83	19	1
1:A:36:VAL:O	1:A:85:HIS:CE1	0.66	2.47	4	14
1:A:14:PRO:CG	2:B:3:PHE:HE2	0.66	2.00	18	1
1:A:38:PRO:HG2	2:B:62:ALA:CB	0.66	2.20	15	2
1:A:60:LEU:HD22	2:B:63:ASP:HB2	0.66	1.55	19	1
1:A:62:ILE:HG23	2:B:70:ASN:HD21	0.66	1.49	10	1
1:A:36:VAL:HA	2:B:119:PRO:HD2	0.66	1.67	13	1
1:A:60:LEU:CD2	2:B:61:GLN:NE2	0.66	2.58	20	1
2:B:90:ASP:OD1	2:B:93:LEU:HD13	0.66	1.91	1	20
1:A:62:ILE:HG22	2:B:121:PRO:CB	0.66	2.20	11	1
1:A:60:LEU:HG	2:B:63:ASP:CB	0.66	2.10	12	1
2:B:167:LEU:N	2:B:167:LEU:HD22	0.66	2.04	10	16
2:B:61:GLN:CD	2:B:67:SER:HB3	0.66	2.16	19	1
1:A:82:CYS:O	1:A:86:ARG:HG2	0.66	1.91	16	3
1:A:60:LEU:CD1	1:A:62:ILE:HD11	0.66	2.21	18	1
1:A:36:VAL:CB	2:B:119:PRO:HD2	0.66	2.21	13	1
1:A:60:LEU:CD2	2:B:61:GLN:HB2	0.66	2.21	8	1
2:B:61:GLN:OE1	2:B:65:SER:HB3	0.66	1.91	11	1
2:B:187:ASN:HB2	2:B:191:PHE:CE1	0.65	2.26	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:4:TYR:CE1	2:B:163:PRO:HB3	0.65	2.26	4	1
2:B:1:TYR:CE1	4:B:250:HEC:CHA	0.65	2.80	19	3
1:A:38:PRO:HD3	4:B:250:HEC:CGD	0.65	2.21	15	1
2:B:170:ASN:O	2:B:170:ASN:CG	0.65	2.40	15	1
1:A:82:CYS:N	1:A:86:ARG:HH21	0.65	1.89	16	1
2:B:105:THR:HG23	2:B:116:LEU:HB2	0.65	1.69	7	13
2:B:189:PHE:CE1	2:B:209:PRO:CG	0.65	2.77	17	10
1:A:84:PRO:HB3	2:B:1:TYR:OH	0.65	1.91	14	2
1:A:62:ILE:CG2	2:B:124:ASP:HB2	0.65	2.22	13	1
1:A:38:PRO:HG2	2:B:62:ALA:H	0.65	1.50	20	1
2:B:75:LEU:HD22	2:B:130:PHE:CD2	0.64	2.27	1	20
1:A:62:ILE:CD1	2:B:70:ASN:ND2	0.64	2.61	14	2
1:A:12:TYR:CD2	2:B:105:THR:HG21	0.64	2.27	13	1
2:B:3:PHE:CD1	2:B:3:PHE:C	0.64	2.74	3	1
2:B:24:CYS:HA	2:B:161:VAL:HG12	0.64	1.68	15	19
1:A:60:LEU:HB3	2:B:63:ASP:HB2	0.64	1.68	20	1
2:B:24:CYS:CB	4:B:250:HEC:CAC	0.64	2.75	20	20
1:A:81:TYR:HD1	1:A:86:ARG:NE	0.64	1.90	16	1
1:A:88:ALA:HB1	2:B:7:TYR:CE2	0.64	2.27	16	1
2:B:103:LEU:HD23	2:B:120:LEU:HD11	0.64	1.70	9	1
2:B:4:TYR:N	2:B:4:TYR:CD1	0.64	2.59	13	2
1:A:64:PRO:HG3	2:B:102:TYR:CG	0.64	2.28	2	1
1:A:62:ILE:HD13	1:A:63:ALA:N	0.64	2.08	15	1
1:A:61:ALA:HB3	1:A:67:PHE:CZ	0.64	2.27	2	20
2:B:97:VAL:HA	2:B:129:ILE:HG21	0.64	1.68	1	20
2:B:1:TYR:CE2	2:B:119:PRO:HG2	0.64	2.24	20	2
2:B:6:GLN:NE2	2:B:116:LEU:HD12	0.64	2.08	19	1
1:A:62:ILE:CG2	2:B:70:ASN:ND2	0.63	2.60	10	3
1:A:36:VAL:O	1:A:36:VAL:CG1	0.63	2.44	19	3
1:A:60:LEU:CD1	2:B:63:ASP:H	0.63	2.05	12	1
1:A:62:ILE:CG2	2:B:121:PRO:HG2	0.63	2.17	17	1
1:A:12:TYR:CE2	2:B:3:PHE:O	0.63	2.50	19	1
2:B:187:ASN:HB2	2:B:191:PHE:HE1	0.63	1.52	1	3
1:A:40:ASN:CB	1:A:60:LEU:CD2	0.63	2.76	16	1
1:A:38:PRO:HB2	1:A:60:LEU:CG	0.63	2.22	15	1
2:B:192:ASP:OD1	2:B:204:VAL:HG13	0.63	1.93	19	19
2:B:100:PHE:CE2	2:B:101:TYR:HD2	0.63	2.11	2	9
1:A:62:ILE:HG21	2:B:61:GLN:HG3	0.63	1.71	15	1
2:B:58:GLN:OE1	2:B:66:PRO:HB2	0.63	1.94	4	11
1:A:60:LEU:HD13	2:B:61:GLN:CG	0.63	2.23	19	1
2:B:162:TYR:CG	2:B:164:THR:CB	0.63	2.78	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:189:PHE:CE2	2:B:209:PRO:CD	0.63	2.82	17	12
2:B:74:VAL:HG23	2:B:116:LEU:CD2	0.63	2.23	19	2
1:A:60:LEU:CD1	2:B:61:GLN:HG3	0.63	2.24	12	1
2:B:48:VAL:HG13	2:B:127:GLU:CG	0.63	2.23	1	20
2:B:3:PHE:CE2	2:B:4:TYR:CE2	0.63	2.87	19	1
2:B:4:TYR:CD1	2:B:163:PRO:HB3	0.63	2.27	20	1
2:B:113:ASN:CG	2:B:114:ILE:HD12	0.62	2.18	1	20
1:A:38:PRO:CD	2:B:1:TYR:CE2	0.62	2.82	18	1
2:B:83:LEU:HD12	2:B:131:PRO:O	0.62	1.94	1	20
2:B:192:ASP:HB3	2:B:204:VAL:CG2	0.62	2.22	1	20
2:B:205:THR:HG21	2:B:227:LEU:CD1	0.62	2.24	1	18
2:B:222:GLU:H	2:B:225:GLN:NE2	0.62	1.92	1	20
1:A:86:ARG:CB	2:B:164:THR:CG2	0.62	2.77	18	1
2:B:208:LEU:HB3	2:B:209:PRO:HD2	0.62	1.72	6	16
2:B:208:LEU:N	2:B:208:LEU:CD1	0.62	2.63	10	2
1:A:60:LEU:HD11	2:B:63:ASP:HB3	0.62	0.64	12	1
1:A:57:ASN:ND2	1:A:68:TYR:CE2	0.62	2.68	7	1
1:A:42:ILE:HG13	1:A:83:THR:HG1	0.62	1.53	11	1
1:A:12:TYR:CE2	2:B:3:PHE:CB	0.62	2.82	20	1
2:B:1:TYR:HD2	2:B:3:PHE:CD2	0.62	2.13	20	1
2:B:162:TYR:OH	2:B:168:SER:HB2	0.62	1.92	6	1
1:A:12:TYR:CE2	2:B:3:PHE:C	0.62	2.78	19	1
1:A:37:GLY:O	4:B:250:HEC:O1D	0.62	2.17	20	2
1:A:60:LEU:HD13	2:B:61:GLN:HG3	0.62	1.70	12	1
2:B:187:ASN:CB	2:B:189:PHE:CD1	0.62	2.83	18	3
2:B:32:GLU:HA	2:B:239:MET:HE1	0.61	1.72	1	20
2:B:70:ASN:HB2	4:B:250:HEC:CGA	0.61	2.24	15	16
1:A:62:ILE:HD12	2:B:70:ASN:HD21	0.61	1.53	7	1
2:B:61:GLN:HG3	2:B:62:ALA:N	0.61	2.09	16	1
2:B:8:ASN:ND2	2:B:9:TYR:CE1	0.61	2.68	18	1
2:B:100:PHE:CE2	2:B:101:TYR:HD1	0.61	2.13	1	11
1:A:36:VAL:O	1:A:36:VAL:CG2	0.61	2.48	6	2
1:A:7:MET:HB3	1:A:90:MET:HE1	0.61	1.71	4	20
2:B:41:PRO:O	2:B:134:SER:HB2	0.61	1.96	1	20
2:B:102:TYR:CD2	2:B:103:LEU:HD12	0.61	2.30	2	2
2:B:31:VAL:HG11	2:B:237:GLY:O	0.61	1.95	1	20
1:A:52:ALA:HB3	1:A:53:PRO:HD3	0.61	1.73	12	20
1:A:38:PRO:CD	2:B:70:ASN:CG	0.61	2.73	13	2
1:A:84:PRO:O	2:B:163:PRO:HG2	0.61	1.95	16	1
1:A:84:PRO:HB2	2:B:162:TYR:CE2	0.61	2.31	15	1
1:A:86:ARG:NH1	1:A:91:VAL:HG11	0.61	1.99	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:TYR:HB3	2:B:4:TYR:HE1	0.61	1.45	19	1
1:A:9:THR:O	1:A:35:LYS:HD3	0.61	1.96	8	3
1:A:62:ILE:CG1	2:B:121:PRO:HB3	0.61	2.25	13	1
2:B:104:VAL:HG13	2:B:115:LEU:HD12	0.61	1.60	17	1
2:B:3:PHE:CE2	2:B:4:TYR:CE1	0.60	2.89	3	2
1:A:86:ARG:CZ	1:A:87:GLY:H	0.60	2.07	10	1
1:A:40:ASN:ND2	1:A:42:ILE:HG12	0.60	2.11	16	1
2:B:170:ASN:CB	2:B:170:ASN:N	0.60	2.61	1	6
1:A:60:LEU:HD21	2:B:61:GLN:CB	0.60	2.25	8	1
1:A:9:THR:OG1	1:A:13:ALA:HB3	0.60	1.97	6	15
2:B:19:ILE:HG12	2:B:238:GLN:OE1	0.60	1.96	1	20
1:A:38:PRO:CD	2:B:1:TYR:CZ	0.60	2.84	18	2
1:A:62:ILE:HG23	2:B:70:ASN:OD1	0.60	1.95	11	1
2:B:162:TYR:CD1	2:B:163:PRO:HD2	0.60	2.30	9	1
1:A:84:PRO:HB3	2:B:62:ALA:O	0.60	1.97	19	2
1:A:36:VAL:HG23	2:B:119:PRO:CG	0.60	2.26	13	1
2:B:120:LEU:HD22	2:B:125:TYR:HE2	0.60	1.56	9	1
2:B:1:TYR:CD1	2:B:4:TYR:CD2	0.59	2.90	11	1
1:A:38:PRO:HG2	2:B:62:ALA:HB2	0.59	1.72	15	1
1:A:12:TYR:CD2	2:B:3:PHE:CE1	0.59	2.88	16	1
1:A:60:LEU:CD2	2:B:63:ASP:N	0.59	2.66	12	1
2:B:86:PRO:HD3	2:B:101:TYR:CE1	0.59	2.32	1	11
2:B:192:ASP:CB	2:B:204:VAL:HG22	0.59	2.26	1	20
2:B:86:PRO:HD3	2:B:101:TYR:CE2	0.59	2.32	2	9
1:A:15:LEU:C	1:A:15:LEU:HD12	0.59	2.22	3	3
2:B:24:CYS:HA	2:B:161:VAL:CG1	0.59	2.27	4	10
2:B:162:TYR:CE1	2:B:168:SER:HB3	0.59	2.32	2	2
2:B:29:LYS:HD2	2:B:234:GLY:C	0.59	2.21	1	20
1:A:14:PRO:HB2	1:A:85:HIS:CD2	0.59	2.33	4	1
2:B:162:TYR:CD2	2:B:164:THR:HG22	0.59	2.33	9	1
1:A:87:GLY:HA2	2:B:164:THR:CG2	0.59	2.26	3	1
1:A:37:GLY:HA2	1:A:39:HIS:CD2	0.59	2.33	14	20
1:A:87:GLY:HA3	2:B:162:TYR:CE2	0.59	2.31	17	1
2:B:156:ARG:HD2	2:B:235:GLY:O	0.59	1.97	1	20
1:A:83:THR:C	1:A:86:ARG:HG2	0.58	2.23	11	2
1:A:83:THR:O	1:A:86:ARG:HG3	0.58	1.97	16	1
1:A:82:CYS:O	1:A:86:ARG:CG	0.58	2.50	16	1
2:B:107:TYR:HA	2:B:116:LEU:CD1	0.58	2.27	1	1
2:B:1:TYR:CE1	2:B:4:TYR:CD2	0.58	2.92	11	1
2:B:83:LEU:HD11	2:B:131:PRO:CD	0.58	2.28	17	20
2:B:86:PRO:HG3	2:B:101:TYR:HE2	0.58	1.57	2	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:59:GLN:HB2	2:B:233:VAL:CG2	0.58	2.28	10	2
2:B:83:LEU:CD2	2:B:104:VAL:HB	0.58	2.29	14	20
1:A:83:THR:CG2	2:B:62:ALA:HB2	0.58	2.27	1	1
1:A:33:MET:HE2	1:A:64:PRO:HB3	0.58	1.76	3	6
2:B:187:ASN:CB	2:B:189:PHE:HD1	0.58	2.11	18	3
1:A:39:HIS:N	1:A:60:LEU:HD11	0.58	2.14	15	1
2:B:86:PRO:HG3	2:B:101:TYR:HE1	0.58	1.57	1	11
2:B:90:ASP:CG	2:B:93:LEU:HD13	0.58	2.23	1	20
2:B:1:TYR:CD2	2:B:119:PRO:CG	0.58	2.86	16	2
2:B:107:TYR:CD1	2:B:116:LEU:HD11	0.58	2.34	19	4
1:A:40:ASN:C	1:A:40:ASN:ND2	0.58	2.58	16	1
1:A:60:LEU:HG	1:A:60:LEU:O	0.58	1.99	17	3
2:B:4:TYR:OH	2:B:162:TYR:HD1	0.58	1.82	20	1
2:B:4:TYR:CE1	2:B:163:PRO:HG3	0.58	2.34	3	1
1:A:60:LEU:CD1	2:B:61:GLN:HB2	0.58	2.29	11	1
1:A:62:ILE:HD13	1:A:63:ALA:H	0.58	1.57	15	1
2:B:208:LEU:N	2:B:208:LEU:CD2	0.57	2.67	13	5
2:B:1:TYR:N	2:B:1:TYR:HD1	0.57	1.95	10	1
1:A:86:ARG:HA	1:A:86:ARG:NH1	0.57	2.13	16	1
2:B:85:PRO:HG2	2:B:88:ARG:CG	0.57	2.29	1	20
1:A:62:ILE:HD13	2:B:121:PRO:CB	0.57	2.28	13	1
2:B:46:LYS:HD2	2:B:93:LEU:HD23	0.57	1.75	1	20
1:A:64:PRO:HG3	2:B:102:TYR:CE1	0.57	2.34	2	1
2:B:162:TYR:CE1	4:B:250:HEC:HMD3	0.57	2.34	3	2
1:A:38:PRO:HD2	2:B:62:ALA:CB	0.57	2.14	20	2
2:B:222:GLU:HB3	2:B:225:GLN:HG3	0.57	1.77	1	20
1:A:36:VAL:CA	2:B:119:PRO:HD2	0.57	2.29	13	1
1:A:81:TYR:CD1	1:A:86:ARG:NE	0.57	2.72	16	1
1:A:58:THR:HG22	2:B:63:ASP:OD1	0.57	1.99	19	1
1:A:60:LEU:HD11	2:B:63:ASP:CA	0.57	2.25	12	1
1:A:14:PRO:HB3	1:A:36:VAL:CG2	0.57	2.29	6	3
2:B:62:ALA:HA	2:B:158:ARG:HH22	0.57	1.59	15	1
2:B:3:PHE:C	2:B:6:GLN:HG3	0.57	2.24	8	1
1:A:60:LEU:N	1:A:60:LEU:HD23	0.57	2.14	16	1
1:A:39:HIS:N	1:A:60:LEU:CD1	0.57	2.68	15	1
2:B:54:ASP:O	2:B:57:ILE:HG22	0.56	1.99	1	20
2:B:85:PRO:HG2	2:B:88:ARG:HG2	0.56	1.75	1	20
2:B:97:VAL:HA	2:B:129:ILE:HG23	0.56	1.76	1	20
2:B:105:THR:CG2	2:B:116:LEU:HB2	0.56	2.30	20	5
1:A:62:ILE:HD11	2:B:61:GLN:NE2	0.56	2.15	12	1
1:A:83:THR:CG2	2:B:62:ALA:CB	0.56	2.82	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:PRO:HB2	2:B:1:TYR:HE2	0.56	1.60	1	2
1:A:86:ARG:HH12	2:B:166:GLU:HB2	0.56	1.60	12	1
1:A:46:VAL:CG1	1:A:78:TYR:CD2	0.56	2.89	1	20
1:A:85:HIS:CD2	2:B:3:PHE:CE2	0.56	2.94	3	1
1:A:86:ARG:HA	1:A:86:ARG:CZ	0.56	2.30	3	1
2:B:1:TYR:CD1	2:B:119:PRO:CG	0.56	2.88	18	4
2:B:205:THR:HG21	2:B:227:LEU:HD11	0.56	1.78	1	18
2:B:100:PHE:CE2	2:B:101:TYR:CD2	0.56	2.93	2	9
1:A:62:ILE:CG2	2:B:121:PRO:HB3	0.56	2.28	11	1
1:A:84:PRO:CB	2:B:162:TYR:CE2	0.56	2.89	15	1
2:B:12:PRO:O	2:B:20:VAL:HG23	0.56	2.00	1	20
1:A:86:ARG:HG3	2:B:164:THR:HB	0.56	1.75	16	1
2:B:1:TYR:CD2	2:B:3:PHE:CD2	0.56	2.94	20	1
2:B:96:GLU:O	2:B:129:ILE:HG21	0.56	1.99	1	20
1:A:58:THR:HG21	2:B:63:ASP:OD2	0.56	2.00	3	1
1:A:86:ARG:CZ	1:A:86:ARG:CB	0.56	2.83	11	1
2:B:4:TYR:OH	2:B:162:TYR:CD1	0.56	2.59	20	1
2:B:59:GLN:HG2	2:B:60:VAL:N	0.56	2.15	16	6
1:A:37:GLY:O	2:B:119:PRO:CD	0.56	2.54	9	2
1:A:86:ARG:HH11	1:A:87:GLY:N	0.56	1.99	9	1
1:A:86:ARG:CZ	1:A:87:GLY:CA	0.56	2.80	10	1
1:A:57:ASN:OD1	1:A:68:TYR:CZ	0.56	2.57	11	1
1:A:62:ILE:CG2	2:B:121:PRO:CB	0.56	2.79	13	2
1:A:38:PRO:HG3	2:B:62:ALA:HB2	0.56	1.76	15	1
1:A:24:SER:CA	1:A:97:GLU:OXT	0.56	2.54	15	20
1:A:36:VAL:HB	2:B:3:PHE:CE2	0.56	2.35	18	1
2:B:8:ASN:CG	2:B:9:TYR:CE1	0.56	2.84	18	1
2:B:164:THR:HG21	2:B:166:GLU:HB2	0.55	1.77	1	1
1:A:36:VAL:HG23	2:B:3:PHE:CB	0.55	2.32	3	2
1:A:38:PRO:N	2:B:1:TYR:CE1	0.55	2.73	4	1
1:A:62:ILE:H	1:A:62:ILE:CD1	0.55	2.06	10	1
1:A:42:ILE:O	1:A:81:TYR:CD1	0.55	2.60	18	1
2:B:24:CYS:CB	4:B:250:HEC:HAC	0.55	2.31	20	20
2:B:102:TYR:CD1	2:B:102:TYR:C	0.55	2.84	14	3
2:B:170:ASN:OD1	2:B:170:ASN:C	0.55	2.46	15	1
1:A:14:PRO:CG	2:B:3:PHE:CE2	0.55	2.85	18	1
1:A:41:VAL:O	1:A:42:ILE:HD13	0.55	2.02	3	9
2:B:97:VAL:CG1	2:B:131:PRO:HD3	0.55	2.31	1	20
2:B:162:TYR:CE1	2:B:168:SER:CB	0.55	2.89	6	1
1:A:42:ILE:HG22	1:A:81:TYR:CZ	0.55	2.37	16	2
1:A:86:ARG:CZ	1:A:91:VAL:HG13	0.55	2.31	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:8:ASN:HB3	2:B:9:TYR:CD1	0.55	2.37	18	1
1:A:60:LEU:HD13	2:B:63:ASP:H	0.55	1.61	12	1
1:A:58:THR:HG23	2:B:63:ASP:HA	0.55	1.77	18	1
2:B:167:LEU:N	2:B:167:LEU:CD2	0.55	2.69	10	11
2:B:162:TYR:CZ	2:B:168:SER:HB3	0.55	2.35	6	1
1:A:83:THR:HG22	2:B:62:ALA:HB1	0.55	1.77	11	2
2:B:100:PHE:CE2	2:B:101:TYR:CD1	0.55	2.95	1	11
2:B:86:PRO:CG	2:B:101:TYR:HE2	0.55	2.15	2	9
2:B:3:PHE:HE2	2:B:4:TYR:CZ	0.55	2.20	3	1
1:A:84:PRO:O	1:A:86:ARG:HG3	0.55	2.00	11	2
1:A:40:ASN:CB	2:B:63:ASP:OD2	0.55	2.54	20	1
2:B:86:PRO:CG	2:B:101:TYR:HE1	0.55	2.15	1	11
2:B:208:LEU:H	2:B:208:LEU:CD2	0.55	2.13	3	5
1:A:14:PRO:HD3	2:B:3:PHE:CZ	0.55	2.37	18	2
1:A:36:VAL:HG23	2:B:3:PHE:HB2	0.55	1.78	14	1
1:A:60:LEU:HG	2:B:61:GLN:NE2	0.55	2.13	20	1
2:B:1:TYR:CE1	2:B:119:PRO:CG	0.55	2.89	4	2
1:A:14:PRO:HB3	1:A:36:VAL:HG13	0.55	1.79	19	4
2:B:75:LEU:HD22	2:B:130:PHE:HD2	0.55	1.62	1	20
2:B:162:TYR:HE1	2:B:168:SER:CB	0.55	2.15	2	3
1:A:40:ASN:HD21	1:A:84:PRO:CD	0.55	2.15	20	1
1:A:29:VAL:HG11	1:A:94:ILE:HD13	0.54	1.79	4	20
2:B:118:GLY:HA2	2:B:120:LEU:HG	0.54	1.80	8	3
2:B:1:TYR:CZ	4:B:250:HEC:HBD1	0.54	2.37	11	2
1:A:86:ARG:HB2	2:B:62:ALA:CB	0.54	2.32	13	2
1:A:40:ASN:OD1	1:A:42:ILE:HG12	0.54	2.02	20	1
1:A:32:VAL:HG23	1:A:66:SER:HA	0.54	1.79	11	20
2:B:104:VAL:CG2	2:B:115:LEU:HD11	0.54	2.33	5	12
2:B:23:ASN:CB	2:B:23:ASN:C	0.54	2.76	16	1
2:B:98:GLY:H	2:B:129:ILE:HG23	0.54	1.61	1	20
1:A:12:TYR:CE2	2:B:3:PHE:HB3	0.54	2.38	20	1
2:B:29:LYS:HD3	2:B:156:ARG:HD3	0.54	1.80	1	20
1:A:62:ILE:HD12	1:A:62:ILE:N	0.54	2.11	10	1
1:A:86:ARG:NH2	1:A:91:VAL:HG13	0.54	2.17	18	1
2:B:187:ASN:O	2:B:189:PHE:HD1	0.54	1.83	20	1
2:B:162:TYR:HE1	2:B:168:SER:CA	0.54	2.15	1	1
2:B:59:GLN:CG	2:B:233:VAL:CG2	0.54	2.79	12	2
2:B:40:LEU:O	2:B:43:THR:HG22	0.54	2.03	1	20
2:B:53:TYR:CE2	2:B:55:LEU:HD13	0.54	2.38	13	20
2:B:189:PHE:CZ	2:B:209:PRO:HG3	0.54	2.38	4	3
1:A:86:ARG:HH22	2:B:166:GLU:CD	0.54	2.11	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:59:GLN:CG	2:B:233:VAL:HG22	0.54	2.28	15	1
1:A:14:PRO:CB	1:A:36:VAL:CG1	0.54	2.81	19	1
1:A:84:PRO:CG	2:B:62:ALA:HB1	0.54	2.33	19	2
2:B:203:VAL:HG22	2:B:204:VAL:N	0.53	2.18	1	20
2:B:161:VAL:HG22	2:B:162:TYR:N	0.53	2.17	13	6
2:B:162:TYR:HH	2:B:168:SER:CA	0.53	1.88	6	1
1:A:64:PRO:HD3	2:B:121:PRO:CG	0.53	2.31	11	1
1:A:86:ARG:NH1	2:B:162:TYR:CE2	0.53	2.75	9	1
1:A:42:ILE:CG1	1:A:83:THR:OG1	0.53	2.53	11	1
2:B:173:PHE:H	2:B:228:THR:CG2	0.53	2.17	1	20
2:B:4:TYR:CZ	2:B:163:PRO:HG3	0.53	2.27	4	1
1:A:60:LEU:CD1	2:B:63:ASP:N	0.53	2.71	12	1
1:A:36:VAL:CG2	2:B:3:PHE:CG	0.53	2.90	3	1
1:A:39:HIS:C	1:A:40:ASN:CG	0.53	2.76	10	9
1:A:85:HIS:N	1:A:85:HIS:CD2	0.53	2.75	10	1
2:B:160:GLN:HE21	2:B:170:ASN:HD22	0.53	1.47	18	1
1:A:12:TYR:HH	2:B:3:PHE:CB	0.53	2.15	19	1
1:A:38:PRO:CD	4:B:250:HEC:O2D	0.53	2.56	20	2
1:A:80:PHE:CD1	1:A:80:PHE:N	0.53	2.77	19	20
2:B:177:ILE:HG22	2:B:203:VAL:HG11	0.53	1.80	1	20
2:B:197:PRO:HD2	2:B:201:ASP:O	0.53	2.03	1	20
1:A:9:THR:HG21	1:A:15:LEU:HD11	0.53	1.80	9	6
1:A:62:ILE:CD1	2:B:120:LEU:HA	0.53	2.22	2	1
1:A:38:PRO:CD	2:B:62:ALA:CB	0.53	2.81	20	2
2:B:51:VAL:HG13	2:B:51:VAL:O	0.53	2.04	1	20
2:B:3:PHE:CE2	2:B:4:TYR:CZ	0.53	2.96	3	1
2:B:3:PHE:HE2	2:B:4:TYR:CE1	0.53	2.22	6	1
1:A:36:VAL:HB	2:B:3:PHE:CD2	0.53	2.38	18	1
1:A:35:LYS:O	1:A:36:VAL:HG12	0.53	2.04	15	11
2:B:29:LYS:O	2:B:237:GLY:HA3	0.53	2.03	1	20
2:B:187:ASN:CB	2:B:189:PHE:CE2	0.53	2.92	15	1
2:B:67:SER:OG	2:B:68:GLY:N	0.52	2.42	6	3
1:A:84:PRO:CB	2:B:1:TYR:OH	0.52	2.56	10	1
1:A:58:THR:O	2:B:62:ALA:HB1	0.52	2.02	18	1
2:B:193:VAL:HB	2:B:205:THR:HG23	0.52	1.80	19	2
1:A:12:TYR:CG	2:B:4:TYR:CD1	0.52	2.98	19	1
2:B:3:PHE:CD2	2:B:4:TYR:CE2	0.52	2.97	19	1
1:A:14:PRO:C	1:A:90:MET:SD	0.52	2.92	14	16
1:A:52:ALA:N	1:A:53:PRO:CD	0.52	2.73	4	20
1:A:60:LEU:HD22	2:B:61:GLN:HB2	0.52	1.81	8	1
2:B:69:LEU:HD21	2:B:233:VAL:HG23	0.52	1.80	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:ARG:NH1	1:A:87:GLY:HA3	0.52	1.95	10	1
2:B:182:ALA:HB3	2:B:194:THR:CG2	0.52	2.35	1	20
2:B:193:VAL:HB	2:B:205:THR:CG2	0.52	2.35	1	18
1:A:86:ARG:HH11	1:A:86:ARG:HG3	0.52	1.65	20	1
2:B:208:LEU:N	2:B:208:LEU:HD13	0.52	2.20	7	3
1:A:38:PRO:HG2	1:A:60:LEU:CD2	0.52	2.30	15	1
2:B:4:TYR:CD1	2:B:163:PRO:CB	0.52	2.56	20	1
1:A:81:TYR:CD1	1:A:81:TYR:C	0.52	2.88	6	15
2:B:97:VAL:HG12	2:B:98:GLY:N	0.52	2.20	1	20
1:A:35:LYS:C	1:A:36:VAL:CG1	0.52	2.83	13	5
1:A:62:ILE:CD1	2:B:70:ASN:HD21	0.52	2.18	11	2
1:A:38:PRO:CD	4:B:250:HEC:O1D	0.52	2.58	15	1
2:B:6:GLN:HE21	2:B:116:LEU:CD1	0.52	2.18	19	1
2:B:29:LYS:HE2	2:B:233:VAL:O	0.52	2.04	1	20
1:A:42:ILE:HB	1:A:81:TYR:CE1	0.52	2.39	6	1
2:B:70:ASN:ND2	4:B:250:HEC:O2A	0.52	2.42	14	2
1:A:80:PHE:CE1	1:A:92:GLY:C	0.51	2.89	9	20
2:B:40:LEU:HD12	2:B:40:LEU:N	0.51	2.20	1	20
1:A:6:LYS:CG	1:A:32:VAL:CG1	0.51	2.89	20	20
2:B:129:ILE:HG23	2:B:129:ILE:O	0.51	2.05	1	20
2:B:120:LEU:HD22	2:B:125:TYR:CE1	0.51	2.40	4	1
2:B:9:TYR:CD1	2:B:20:VAL:CG1	0.51	2.91	16	20
2:B:29:LYS:CD	2:B:156:ARG:HD3	0.51	2.36	1	20
2:B:1:TYR:CE2	4:B:250:HEC:HBD1	0.51	2.40	18	2
2:B:158:ARG:HH12	2:B:169:ASN:HD21	0.51	1.49	2	1
2:B:187:ASN:CG	2:B:191:PHE:HE1	0.51	2.13	4	14
2:B:19:ILE:H	2:B:238:GLN:NE2	0.51	2.04	1	20
2:B:155:ASN:HB2	2:B:236:PHE:HD1	0.51	1.64	1	20
2:B:208:LEU:O	2:B:211:PRO:HD2	0.51	2.05	13	7
1:A:38:PRO:CD	2:B:119:PRO:C	0.51	2.72	2	1
1:A:36:VAL:O	1:A:85:HIS:HE1	0.51	1.84	4	1
2:B:4:TYR:O	2:B:8:ASN:ND2	0.51	2.43	14	1
2:B:191:PHE:C	2:B:192:ASP:CG	0.51	2.76	20	1
1:A:14:PRO:CG	2:B:3:PHE:CZ	0.51	2.92	6	3
1:A:57:ASN:HB2	1:A:68:TYR:OH	0.51	2.06	14	8
1:A:85:HIS:HD2	2:B:3:PHE:CE2	0.51	2.23	3	1
2:B:98:GLY:N	2:B:129:ILE:HG23	0.51	2.21	1	20
1:A:83:THR:HG21	2:B:62:ALA:HB1	0.51	1.83	5	1
1:A:24:SER:CB	1:A:97:GLU:OXT	0.51	2.59	1	20
1:A:96:VAL:O	1:A:96:VAL:CG1	0.51	2.59	7	19
2:B:162:TYR:HB2	2:B:164:THR:OG1	0.51	2.06	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:ARG:HD2	1:A:86:ARG:O	0.51	2.01	9	2
1:A:84:PRO:HG3	2:B:62:ALA:HB1	0.51	1.83	19	2
2:B:1:TYR:HD1	4:B:250:HEC:C1A	0.51	2.19	3	2
1:A:62:ILE:HG21	2:B:70:ASN:CG	0.51	2.31	5	1
2:B:100:PHE:CD2	2:B:101:TYR:CD2	0.50	2.98	2	9
2:B:115:LEU:O	2:B:115:LEU:CD2	0.50	2.49	14	1
2:B:8:ASN:HB3	2:B:9:TYR:CE1	0.50	2.42	16	17
2:B:182:ALA:HB3	2:B:194:THR:HG23	0.50	1.83	1	20
2:B:198:GLU:CD	2:B:198:GLU:H	0.50	2.14	1	20
2:B:1:TYR:HB3	2:B:3:PHE:HD2	0.50	1.64	20	1
1:A:83:THR:N	1:A:84:PRO:CD	0.50	2.75	14	20
2:B:59:GLN:HE22	2:B:157:GLY:HA2	0.50	1.66	1	2
1:A:38:PRO:HB3	1:A:62:ILE:HD13	0.50	1.82	2	1
1:A:86:ARG:NH1	1:A:86:ARG:C	0.50	2.66	10	1
1:A:40:ASN:ND2	1:A:42:ILE:CG1	0.50	2.74	16	1
1:A:62:ILE:HG21	2:B:124:ASP:HB2	0.50	1.84	17	1
1:A:35:LYS:O	1:A:36:VAL:CG1	0.50	2.59	3	15
2:B:222:GLU:H	2:B:225:GLN:HE21	0.50	1.46	1	20
2:B:59:GLN:NE2	2:B:158:ARG:H	0.50	2.04	15	6
1:A:86:ARG:O	1:A:86:ARG:CZ	0.50	2.59	18	1
2:B:1:TYR:HE1	4:B:250:HEC:HBD1	0.50	1.66	16	2
1:A:32:VAL:CG2	1:A:65:GLY:O	0.50	2.60	8	20
1:A:83:THR:HB	1:A:84:PRO:HD3	0.50	1.84	11	5
2:B:158:ARG:HH12	2:B:169:ASN:ND2	0.50	2.05	2	1
1:A:38:PRO:CG	2:B:1:TYR:CZ	0.50	2.95	18	1
1:A:85:HIS:HD2	2:B:3:PHE:HE2	0.50	1.49	3	1
2:B:1:TYR:CE1	2:B:119:PRO:CD	0.50	2.95	4	1
1:A:38:PRO:HG3	1:A:62:ILE:HD12	0.50	1.84	19	1
2:B:1:TYR:CD1	4:B:250:HEC:C1A	0.49	2.95	3	1
2:B:3:PHE:HA	2:B:6:GLN:CD	0.49	2.32	8	1
1:A:62:ILE:HB	2:B:121:PRO:CG	0.49	2.36	10	1
1:A:62:ILE:CG1	2:B:121:PRO:CB	0.49	2.90	13	1
1:A:62:ILE:CG2	2:B:119:PRO:O	0.49	2.61	6	2
1:A:86:ARG:HH22	1:A:87:GLY:HA3	0.49	1.66	10	1
2:B:3:PHE:HA	2:B:6:GLN:OE1	0.49	2.07	8	1
2:B:61:GLN:NE2	2:B:67:SER:OG	0.49	2.45	11	2
1:A:21:LEU:HD12	1:A:22:SER:N	0.49	2.23	10	20
2:B:100:PHE:CD2	2:B:101:TYR:CD1	0.49	3.00	1	11
1:A:10:ASP:HA	1:A:35:LYS:HE2	0.49	1.83	13	1
1:A:83:THR:HG22	1:A:84:PRO:CD	0.49	2.38	1	1
1:A:86:ARG:NH2	2:B:166:GLU:CD	0.49	2.71	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:TYR:CE2	2:B:3:PHE:HB2	0.49	2.34	19	1
1:A:32:VAL:HG23	1:A:65:GLY:O	0.49	2.08	2	20
1:A:35:LYS:C	1:A:36:VAL:HG12	0.49	2.33	3	10
1:A:35:LYS:O	1:A:36:VAL:HG22	0.49	2.08	18	1
2:B:59:GLN:HE22	2:B:158:ARG:HG3	0.49	1.66	4	2
1:A:81:TYR:HB2	1:A:86:ARG:HH12	0.49	1.67	1	1
1:A:37:GLY:O	2:B:119:PRO:CG	0.49	2.61	10	2
1:A:60:LEU:HD12	1:A:62:ILE:CD1	0.49	2.38	18	2
1:A:36:VAL:HB	2:B:119:PRO:HD2	0.49	1.84	13	1
1:A:83:THR:HG21	2:B:61:GLN:CD	0.49	2.31	17	1
1:A:40:ASN:HD21	1:A:84:PRO:HD3	0.49	1.66	20	1
1:A:39:HIS:C	1:A:40:ASN:ND2	0.48	2.71	11	2
1:A:62:ILE:CD1	2:B:121:PRO:CB	0.48	2.91	13	1
2:B:187:ASN:HB3	2:B:189:PHE:CE2	0.48	2.43	15	1
1:A:86:ARG:NE	1:A:86:ARG:C	0.48	2.42	18	1
2:B:55:LEU:N	2:B:55:LEU:HD22	0.48	2.23	13	20
2:B:221:VAL:CG2	2:B:225:GLN:HB2	0.48	2.38	1	20
2:B:1:TYR:CE1	4:B:250:HEC:HBD1	0.48	2.42	12	2
1:A:38:PRO:N	2:B:1:TYR:CZ	0.48	2.70	4	1
2:B:102:TYR:CE2	2:B:103:LEU:HD23	0.48	2.43	6	1
2:B:1:TYR:CE2	2:B:119:PRO:CD	0.48	2.96	20	1
1:A:84:PRO:HB2	2:B:1:TYR:CE2	0.48	2.41	1	1
2:B:162:TYR:HE1	2:B:168:SER:HB3	0.48	1.67	2	2
1:A:36:VAL:HG22	1:A:85:HIS:NE2	0.48	2.22	4	1
1:A:86:ARG:NH2	1:A:87:GLY:HA3	0.48	2.24	10	1
2:B:189:PHE:CD2	2:B:209:PRO:HG3	0.48	2.44	19	4
1:A:35:LYS:O	1:A:36:VAL:CG2	0.48	2.62	18	1
1:A:17:GLU:HA	1:A:18:PRO:C	0.48	2.34	8	20
1:A:58:THR:O	1:A:60:LEU:HD23	0.48	2.08	7	2
2:B:156:ARG:O	2:B:156:ARG:HG2	0.48	2.08	5	20
1:A:14:PRO:CA	1:A:36:VAL:HG11	0.48	2.37	19	9
2:B:1:TYR:HD2	2:B:4:TYR:CD2	0.48	2.23	9	1
1:A:11:LYS:C	1:A:13:ALA:N	0.48	2.72	19	20
2:B:29:LYS:HD2	2:B:235:GLY:N	0.48	2.24	1	20
2:B:61:GLN:NE2	2:B:67:SER:HB3	0.48	2.23	8	2
2:B:189:PHE:CD2	2:B:209:PRO:CG	0.48	2.96	13	4
2:B:160:GLN:HE21	2:B:170:ASN:ND2	0.48	2.06	18	3
1:A:12:TYR:OH	2:B:3:PHE:CD2	0.48	2.67	20	1
1:A:57:ASN:ND2	1:A:68:TYR:CZ	0.48	2.82	7	1
1:A:8:GLY:C	1:A:34:ASN:HD22	0.48	2.11	14	1
1:A:83:THR:HG22	1:A:84:PRO:N	0.48	2.23	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:48:VAL:HG13	2:B:127:GLU:HG2	0.48	1.84	1	20
2:B:158:ARG:NE	4:B:250:HEC:O2D	0.48	2.47	17	1
2:B:191:PHE:O	2:B:192:ASP:CG	0.48	2.57	19	1
2:B:158:ARG:NE	4:B:250:HEC:CGD	0.48	2.71	17	1
1:A:61:ALA:HB3	1:A:67:PHE:CE1	0.47	2.44	2	3
1:A:86:ARG:HB2	2:B:62:ALA:HB1	0.47	1.86	13	1
1:A:85:HIS:HE2	2:B:4:TYR:HE1	0.47	1.51	16	1
1:A:83:THR:HG22	1:A:84:PRO:HD3	0.47	1.86	1	1
1:A:22:SER:C	1:A:23:ILE:HG23	0.47	2.35	4	20
2:B:161:VAL:CA	2:B:162:TYR:CD1	0.47	2.96	12	1
1:A:34:ASN:CG	1:A:35:LYS:HD3	0.47	2.34	13	1
2:B:1:TYR:CD1	4:B:250:HEC:CHA	0.47	2.97	19	1
1:A:22:SER:O	1:A:23:ILE:CG2	0.47	2.63	6	20
2:B:226:LEU:N	2:B:226:LEU:HD12	0.47	2.24	1	20
1:A:14:PRO:HB3	1:A:36:VAL:HG11	0.47	1.86	20	5
1:A:86:ARG:NH1	1:A:87:GLY:HA2	0.47	2.08	10	1
1:A:38:PRO:HG3	2:B:121:PRO:HB3	0.47	1.86	17	1
1:A:23:ILE:HD12	1:A:27:ASP:HB2	0.47	1.87	16	20
1:A:60:LEU:HD13	1:A:60:LEU:N	0.47	2.24	20	1
1:A:60:LEU:HD21	2:B:61:GLN:CD	0.47	2.35	7	1
1:A:83:THR:HG21	2:B:61:GLN:HE21	0.47	1.59	17	1
2:B:195:ILE:O	2:B:197:PRO:HD3	0.47	2.10	1	20
1:A:60:LEU:HD23	1:A:60:LEU:H	0.47	1.70	7	1
2:B:123:GLU:HG2	2:B:124:ASP:N	0.47	2.24	10	1
2:B:61:GLN:NE2	2:B:63:ASP:HB3	0.47	2.23	18	1
1:A:9:THR:OG1	1:A:15:LEU:HD21	0.47	2.10	4	1
2:B:75:LEU:CB	2:B:115:LEU:HD22	0.47	2.36	9	1
2:B:1:TYR:HE1	2:B:4:TYR:CE2	0.47	2.22	11	1
2:B:6:GLN:NE2	2:B:116:LEU:CD1	0.47	2.78	19	1
2:B:62:ALA:CA	2:B:158:ARG:NH2	0.47	2.74	15	1
1:A:88:ALA:CB	2:B:7:TYR:CD2	0.47	2.98	16	1
1:A:29:VAL:HG12	1:A:31:PHE:CE1	0.46	2.46	9	20
1:A:41:VAL:C	1:A:42:ILE:HD13	0.46	2.35	7	3
2:B:103:LEU:CD2	2:B:120:LEU:HD11	0.46	2.40	9	1
2:B:99:ASP:HB2	2:B:103:LEU:HD12	0.46	1.86	11	1
1:A:86:ARG:CZ	1:A:86:ARG:CA	0.46	2.81	16	1
1:A:83:THR:HG22	2:B:62:ALA:CB	0.46	2.40	11	1
2:B:118:GLY:HA2	2:B:119:PRO:C	0.46	2.36	1	20
2:B:187:ASN:C	2:B:189:PHE:H	0.46	2.18	1	20
2:B:59:GLN:CG	2:B:60:VAL:N	0.46	2.78	16	3
2:B:104:VAL:HG21	2:B:115:LEU:HD11	0.46	1.86	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:61:GLN:NE2	2:B:67:SER:HB2	0.46	2.25	13	1
1:A:60:LEU:CD1	1:A:62:ILE:CD1	0.46	2.93	18	1
1:A:44:ASP:O	1:A:45:LYS:CB	0.46	2.64	8	20
2:B:61:GLN:NE2	2:B:67:SER:CB	0.46	2.79	20	2
2:B:169:ASN:N	2:B:169:ASN:OD1	0.46	2.48	20	1
1:A:23:ILE:O	1:A:97:GLU:N	0.46	2.49	11	20
1:A:83:THR:N	1:A:84:PRO:HD2	0.46	2.26	12	9
1:A:35:LYS:NZ	1:A:35:LYS:CB	0.46	2.79	4	1
2:B:102:TYR:CD2	2:B:103:LEU:HD23	0.46	2.46	4	2
1:A:60:LEU:HD11	2:B:61:GLN:HB2	0.46	1.88	11	1
1:A:86:ARG:NH1	2:B:166:GLU:HB2	0.46	2.25	12	1
2:B:189:PHE:CD1	2:B:189:PHE:N	0.46	2.84	15	2
1:A:40:ASN:HD22	1:A:60:LEU:HD22	0.46	1.70	3	1
2:B:70:ASN:HD22	4:B:250:HEC:CGA	0.46	2.23	11	1
1:A:38:PRO:HD2	2:B:70:ASN:OD1	0.46	2.04	17	1
1:A:5:ILE:N	1:A:30:GLU:O	0.46	2.50	7	20
1:A:21:LEU:HD12	1:A:22:SER:H	0.46	1.71	7	20
1:A:23:ILE:N	1:A:95:THR:O	0.46	2.50	13	20
2:B:19:ILE:HG12	2:B:238:GLN:CD	0.46	2.36	1	20
1:A:81:TYR:HB3	1:A:86:ARG:HH22	0.46	1.69	4	1
2:B:61:GLN:OE1	2:B:67:SER:HB2	0.46	2.11	15	1
2:B:166:GLU:OE1	2:B:166:GLU:HA	0.46	2.11	15	1
1:A:18:PRO:O	1:A:19:LYS:C	0.45	2.60	3	20
1:A:47:PRO:O	1:A:48:ALA:C	0.45	2.60	2	20
2:B:193:VAL:HB	2:B:205:THR:HG22	0.45	1.87	1	18
1:A:37:GLY:C	2:B:1:TYR:HE1	0.45	2.05	4	1
1:A:84:PRO:HA	2:B:163:PRO:HD2	0.45	1.88	16	1
1:A:83:THR:CG2	2:B:61:GLN:NE2	0.45	2.62	17	1
2:B:74:VAL:O	2:B:74:VAL:HG13	0.45	2.11	1	20
1:A:39:HIS:CE1	1:A:85:HIS:CE1	0.45	3.04	4	1
2:B:162:TYR:CD1	2:B:163:PRO:CD	0.45	2.97	9	1
1:A:42:ILE:O	1:A:81:TYR:CE1	0.45	2.69	18	1
1:A:11:LYS:O	1:A:13:ALA:N	0.45	2.50	16	20
2:B:51:VAL:CG2	2:B:156:ARG:CZ	0.45	2.95	1	20
2:B:86:PRO:HD3	2:B:101:TYR:CZ	0.45	2.46	1	20
1:A:14:PRO:HG2	2:B:3:PHE:CZ	0.45	2.46	3	1
2:B:189:PHE:CD1	2:B:209:PRO:HD3	0.45	2.46	3	1
2:B:59:GLN:HE22	2:B:158:ARG:H	0.45	1.52	20	4
2:B:75:LEU:HB3	2:B:115:LEU:CD2	0.45	2.41	17	1
1:A:59:LYS:O	1:A:60:LEU:C	0.45	2.60	2	20
1:A:50:GLU:OE1	1:A:55:LEU:HD12	0.45	2.12	3	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:THR:HG23	2:B:61:GLN:NE2	0.45	2.27	4	1
1:A:82:CYS:C	1:A:86:ARG:NE	0.45	2.32	16	1
1:A:17:GLU:CG	1:A:18:PRO:HA	0.45	2.42	13	20
2:B:78:PRO:HB2	2:B:81:PHE:CE1	0.45	2.47	1	20
1:A:64:PRO:HD3	2:B:102:TYR:CE2	0.45	2.46	2	1
2:B:70:ASN:OD1	2:B:70:ASN:N	0.45	2.49	5	3
1:A:61:ALA:HB3	1:A:67:PHE:CE2	0.45	2.45	13	1
1:A:60:LEU:O	1:A:60:LEU:CG	0.45	2.64	18	1
1:A:62:ILE:HD11	2:B:61:GLN:HE21	0.45	1.71	12	1
1:A:81:TYR:CD1	1:A:86:ARG:CD	0.45	2.99	16	1
2:B:39:VAL:HG13	2:B:243:ILE:HD11	0.45	1.88	1	20
1:A:86:ARG:HH11	1:A:86:ARG:HB3	0.45	1.72	9	1
1:A:34:ASN:HB3	1:A:35:LYS:HD3	0.45	1.87	16	1
2:B:6:GLN:HE21	2:B:116:LEU:HD12	0.45	1.66	19	1
1:A:66:SER:O	1:A:67:PHE:C	0.45	2.60	1	20
2:B:189:PHE:CG	2:B:209:PRO:CD	0.45	2.96	2	4
1:A:86:ARG:CD	1:A:86:ARG:O	0.45	2.65	9	1
1:A:62:ILE:HG13	2:B:70:ASN:OD1	0.45	2.12	14	1
1:A:14:PRO:CD	2:B:7:TYR:CE2	0.45	2.89	16	1
1:A:35:LYS:C	1:A:36:VAL:HG22	0.45	2.37	18	1
2:B:1:TYR:CD2	2:B:3:PHE:CE2	0.45	3.04	20	2
2:B:205:THR:O	2:B:205:THR:HG23	0.45	2.12	1	18
1:A:37:GLY:HA2	2:B:1:TYR:OH	0.45	2.10	4	1
1:A:39:HIS:C	1:A:40:ASN:HD22	0.45	2.19	11	1
1:A:60:LEU:HG	2:B:61:GLN:HG3	0.45	1.89	20	1
1:A:11:LYS:O	1:A:12:TYR:C	0.44	2.61	20	20
2:B:61:GLN:HB3	2:B:67:SER:OG	0.44	2.12	11	1
1:A:36:VAL:CG2	1:A:36:VAL:O	0.44	2.57	16	1
1:A:60:LEU:HD22	4:B:250:HEC:O2D	0.44	2.12	18	1
1:A:5:ILE:HG21	1:A:31:PHE:CE2	0.44	2.48	18	20
1:A:15:LEU:N	1:A:90:MET:SD	0.44	2.90	14	7
1:A:86:ARG:NH1	1:A:86:ARG:HB3	0.44	2.27	9	1
1:A:69:SER:O	1:A:70:VAL:HG13	0.44	2.13	2	20
2:B:20:VAL:O	2:B:20:VAL:HG12	0.44	2.13	1	20
2:B:177:ILE:HG12	2:B:178:ALA:N	0.44	2.28	1	20
1:A:40:ASN:HB3	1:A:60:LEU:HD23	0.44	1.88	11	1
1:A:62:ILE:CD1	1:A:63:ALA:N	0.44	2.80	15	1
1:A:14:PRO:CG	1:A:36:VAL:HG11	0.44	2.41	19	1
2:B:100:PHE:CD2	2:B:101:TYR:N	0.44	2.86	1	20
1:A:83:THR:CG2	2:B:62:ALA:HB1	0.44	2.43	3	1
1:A:40:ASN:ND2	1:A:60:LEU:HD22	0.44	2.27	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:PRO:CG	1:A:60:LEU:HD21	0.44	2.33	15	1
1:A:86:ARG:HH21	1:A:91:VAL:CG1	0.44	2.25	15	1
2:B:162:TYR:CB	2:B:164:THR:OG1	0.44	2.66	18	1
2:B:1:TYR:CD1	2:B:119:PRO:HD3	0.44	2.48	4	1
1:A:60:LEU:H	1:A:60:LEU:HD23	0.44	1.72	6	1
1:A:88:ALA:HB1	2:B:7:TYR:CD2	0.44	2.48	16	1
2:B:1:TYR:HE2	4:B:250:HEC:HBD1	0.44	1.73	18	1
1:A:6:LYS:HG3	1:A:32:VAL:CG1	0.44	2.43	13	20
2:B:48:VAL:CG1	2:B:127:GLU:CG	0.44	2.95	1	20
1:A:6:LYS:HG2	1:A:32:VAL:CG1	0.44	2.43	8	20
2:B:86:PRO:HG3	2:B:101:TYR:CE1	0.44	2.44	1	11
2:B:86:PRO:HG3	2:B:101:TYR:CE2	0.44	2.44	2	9
2:B:63:ASP:OD1	2:B:63:ASP:C	0.44	2.60	14	1
1:A:86:ARG:HH22	1:A:91:VAL:HG13	0.44	1.73	18	1
2:B:177:ILE:CG2	2:B:203:VAL:HG11	0.44	2.43	1	20
2:B:1:TYR:HB3	2:B:2:PRO:HD2	0.44	1.90	6	3
1:A:35:LYS:O	1:A:36:VAL:HG13	0.43	2.12	13	2
1:A:12:TYR:HA	1:A:35:LYS:HE3	0.43	1.89	9	1
2:B:187:ASN:O	2:B:189:PHE:CE1	0.43	2.71	12	1
2:B:2:PRO:O	2:B:6:GLN:HG3	0.43	2.13	19	1
1:A:58:THR:CG2	2:B:63:ASP:HA	0.43	2.42	18	1
2:B:61:GLN:HE21	2:B:63:ASP:H	0.43	1.56	18	1
1:A:60:LEU:HD13	2:B:61:GLN:HE21	0.43	1.67	19	1
2:B:1:TYR:HD2	2:B:3:PHE:CE1	0.43	2.28	19	1
2:B:40:LEU:HB3	2:B:41:PRO:CD	0.43	2.36	1	20
2:B:187:ASN:CB	2:B:189:PHE:CD2	0.43	2.99	15	1
1:A:60:LEU:CD1	2:B:61:GLN:CG	0.43	2.92	19	1
2:B:51:VAL:HG23	2:B:156:ARG:CZ	0.43	2.43	1	20
2:B:114:ILE:HD12	2:B:114:ILE:N	0.43	2.28	1	20
2:B:104:VAL:CG1	2:B:115:LEU:CG	0.43	2.85	4	4
1:A:34:ASN:ND2	1:A:35:LYS:CD	0.43	2.81	10	1
1:A:38:PRO:CG	2:B:119:PRO:HG2	0.43	2.43	14	1
2:B:69:LEU:N	2:B:69:LEU:HD12	0.43	2.29	10	2
1:A:40:ASN:OD1	1:A:42:ILE:CD1	0.43	2.66	20	1
1:A:40:ASN:OD1	1:A:42:ILE:HD11	0.43	2.14	20	1
1:A:85:HIS:CD2	1:A:85:HIS:N	0.43	2.87	2	1
1:A:81:TYR:HB2	1:A:86:ARG:HH21	0.43	0.63	3	1
1:A:14:PRO:HB3	1:A:36:VAL:HG21	0.43	1.90	6	1
2:B:61:GLN:C	2:B:158:ARG:HH11	0.43	2.21	7	1
2:B:97:VAL:CG1	2:B:98:GLY:N	0.43	2.81	1	20
2:B:104:VAL:HG22	2:B:115:LEU:HD21	0.43	1.89	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:TYR:OH	2:B:105:THR:HG21	0.43	2.14	5	1
1:A:86:ARG:NH2	1:A:90:MET:H	0.43	2.12	18	1
1:A:6:LYS:HG3	1:A:32:VAL:HG12	0.43	1.91	18	19
1:A:61:ALA:CB	1:A:67:PHE:CE2	0.43	3.02	13	1
1:A:38:PRO:HB3	1:A:62:ILE:CD1	0.43	2.44	19	1
2:B:8:ASN:CB	2:B:9:TYR:CD1	0.43	3.02	2	12
1:A:14:PRO:CG	1:A:85:HIS:CD2	0.43	3.02	4	1
1:A:36:VAL:HG23	2:B:119:PRO:CD	0.43	2.44	13	1
2:B:6:GLN:HE21	2:B:107:TYR:HA	0.43	1.74	15	1
1:A:85:HIS:O	1:A:86:ARG:NH2	0.43	2.52	16	1
1:A:14:PRO:HB2	1:A:85:HIS:CG	0.42	2.49	4	1
2:B:69:LEU:HD21	2:B:233:VAL:CG2	0.42	2.44	8	1
2:B:71:VAL:CG2	2:B:128:MET:CE	0.42	2.97	12	5
1:A:1:ALA:N	1:A:27:ASP:OD2	0.42	2.50	18	1
1:A:36:VAL:O	1:A:36:VAL:HG23	0.42	2.13	18	1
2:B:192:ASP:CB	2:B:204:VAL:CG2	0.42	2.94	1	18
2:B:161:VAL:CG2	2:B:162:TYR:N	0.42	2.81	11	6
2:B:126:GLN:OE1	2:B:126:GLN:HA	0.42	2.13	13	2
1:A:86:ARG:HD3	1:A:86:ARG:HA	0.42	1.47	19	1
1:A:22:SER:C	1:A:23:ILE:CG2	0.42	2.93	15	20
1:A:38:PRO:HD3	2:B:1:TYR:HE1	0.42	1.73	4	1
2:B:189:PHE:CZ	2:B:209:PRO:CG	0.42	3.03	4	3
1:A:86:ARG:CZ	1:A:87:GLY:HA3	0.42	2.42	10	1
2:B:207:ILE:C	2:B:208:LEU:HD13	0.42	2.39	10	1
1:A:12:TYR:CD2	2:B:105:THR:CG2	0.42	3.01	13	1
2:B:211:PRO:HA	2:B:231:PRO:HG3	0.42	1.92	17	1
2:B:212:GLU:CG	2:B:229:THR:HG22	0.42	2.41	1	20
2:B:99:ASP:HB2	2:B:103:LEU:CD1	0.42	2.44	11	1
1:A:60:LEU:CD1	2:B:63:ASP:CA	0.42	2.92	12	1
2:B:164:THR:HG23	2:B:165:GLY:N	0.42	2.29	14	1
1:A:38:PRO:HD2	2:B:1:TYR:CD2	0.42	2.50	18	1
2:B:46:LYS:CD	2:B:93:LEU:HD23	0.42	2.45	1	20
2:B:184:ILE:HG22	2:B:193:VAL:HA	0.42	1.92	19	20
2:B:212:GLU:CG	2:B:229:THR:CG2	0.42	2.95	1	20
1:A:40:ASN:HB2	1:A:42:ILE:HD11	0.42	1.91	7	1
2:B:63:ASP:O	2:B:63:ASP:CG	0.42	2.63	12	1
1:A:83:THR:O	2:B:62:ALA:HB2	0.42	2.06	17	1
1:A:29:VAL:HG11	1:A:94:ILE:CD1	0.42	2.45	20	18
2:B:3:PHE:HA	2:B:6:GLN:CG	0.42	2.44	8	1
2:B:65:SER:OG	2:B:66:PRO:HD2	0.42	2.15	11	1
2:B:162:TYR:HB2	2:B:164:THR:HG23	0.42	1.89	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:162:TYR:CZ	4:B:250:HEC:CMD	0.42	3.02	12	1
2:B:1:TYR:CE2	2:B:119:PRO:HG3	0.42	2.48	16	1
2:B:77:LEU:HD11	2:B:132:ILE:HD13	0.42	1.91	1	20
2:B:93:LEU:HD12	2:B:93:LEU:N	0.42	2.30	1	20
2:B:49:VAL:HG21	2:B:130:PHE:CE2	0.42	2.50	13	1
2:B:189:PHE:HD1	2:B:209:PRO:CD	0.42	2.25	15	1
1:A:62:ILE:N	1:A:62:ILE:HD13	0.42	2.30	19	1
1:A:12:TYR:O	2:B:3:PHE:CD1	0.42	2.73	8	1
2:B:208:LEU:CD2	2:B:208:LEU:H	0.42	2.27	13	1
2:B:8:ASN:ND2	2:B:9:TYR:CZ	0.42	2.88	18	1
2:B:97:VAL:HG11	2:B:131:PRO:CD	0.41	2.45	1	20
1:A:64:PRO:HG3	2:B:102:TYR:CD2	0.41	2.49	2	1
1:A:46:VAL:HG11	1:A:78:TYR:HD2	0.41	1.70	6	4
2:B:158:ARG:NH2	2:B:158:ARG:HB3	0.41	2.30	14	1
2:B:162:TYR:HB3	2:B:164:THR:OG1	0.41	2.14	18	1
2:B:44:VAL:HA	2:B:132:ILE:O	0.41	2.16	1	20
2:B:3:PHE:CD1	2:B:3:PHE:O	0.41	2.73	3	1
1:A:36:VAL:HA	2:B:119:PRO:CD	0.41	2.40	13	1
2:B:187:ASN:C	2:B:189:PHE:HD1	0.41	2.23	20	1
2:B:194:THR:HG23	2:B:194:THR:O	0.41	2.15	1	20
1:A:14:PRO:HB3	1:A:85:HIS:NE2	0.41	2.30	4	1
2:B:169:ASN:OD1	2:B:169:ASN:N	0.41	2.54	15	3
1:A:52:ALA:N	1:A:53:PRO:HD2	0.41	2.31	4	14
2:B:71:VAL:HG23	2:B:128:MET:CE	0.41	2.45	9	1
1:A:12:TYR:HB3	2:B:3:PHE:CE1	0.41	2.50	15	1
2:B:189:PHE:CD1	2:B:209:PRO:CD	0.41	3.02	15	1
1:A:10:ASP:HA	1:A:35:LYS:NZ	0.41	2.30	17	1
2:B:74:VAL:HA	2:B:116:LEU:HD23	0.41	1.93	8	1
1:A:38:PRO:C	1:A:60:LEU:HD11	0.41	2.40	15	1
1:A:61:ALA:CB	1:A:67:PHE:CE1	0.41	3.04	16	1
1:A:86:ARG:NH2	1:A:87:GLY:N	0.41	2.68	10	1
2:B:208:LEU:CB	2:B:209:PRO:HD2	0.41	2.45	10	1
2:B:65:SER:OG	2:B:66:PRO:CD	0.41	2.68	11	1
1:A:39:HIS:O	1:A:40:ASN:ND2	0.41	2.53	17	1
1:A:83:THR:OG1	2:B:62:ALA:HB1	0.41	2.15	1	1
2:B:86:PRO:CD	2:B:101:TYR:CE1	0.41	3.03	1	11
2:B:183:ALA:H	2:B:194:THR:HG22	0.41	1.76	1	20
2:B:187:ASN:C	2:B:189:PHE:N	0.41	2.79	1	20
2:B:86:PRO:CD	2:B:101:TYR:CE2	0.41	3.03	2	9
1:A:46:VAL:HG22	1:A:52:ALA:H	0.41	1.76	5	5
2:B:59:GLN:HB2	2:B:69:LEU:HD11	0.41	1.91	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:4:TYR:OH	2:B:162:TYR:CA	0.41	2.68	20	1
2:B:57:ILE:O	2:B:57:ILE:HG23	0.41	2.16	1	20
2:B:107:TYR:CA	2:B:116:LEU:HD11	0.41	2.38	1	1
2:B:108:SER:N	2:B:111:ASP:HB2	0.41	2.31	1	20
1:A:86:ARG:HD3	1:A:87:GLY:H	0.41	1.74	12	1
1:A:36:VAL:HB	2:B:4:TYR:OH	0.41	2.15	19	1
2:B:18:LYS:NZ	2:B:22:ALA:HB3	0.41	2.31	1	20
2:B:33:ILE:O	2:B:33:ILE:HG23	0.41	2.16	1	20
2:B:46:LYS:CB	2:B:129:ILE:HD11	0.41	2.44	1	20
1:A:62:ILE:HD13	1:A:62:ILE:HA	0.41	1.73	2	1
2:B:4:TYR:CZ	2:B:163:PRO:HB2	0.41	2.47	4	1
1:A:86:ARG:HG3	1:A:87:GLY:N	0.41	2.31	5	1
1:A:86:ARG:NH2	1:A:87:GLY:H	0.41	2.13	10	1
1:A:14:PRO:HD3	2:B:3:PHE:HZ	0.41	1.71	18	1
1:A:12:TYR:HB3	2:B:4:TYR:CD1	0.41	2.48	19	1
2:B:31:VAL:CG2	2:B:238:GLN:C	0.41	2.94	1	20
1:A:62:ILE:H	1:A:62:ILE:HG12	0.41	1.48	5	1
1:A:21:LEU:HD23	1:A:94:ILE:HG12	0.41	1.93	17	7
2:B:185:GLU:O	2:B:190:GLY:HA2	0.40	2.16	1	20
1:A:85:HIS:HA	2:B:4:TYR:HH	0.40	1.75	6	1
2:B:3:PHE:CD1	2:B:6:GLN:OE1	0.40	2.74	8	1
2:B:186:ASP:HA	2:B:189:PHE:O	0.40	2.16	19	1
1:A:12:TYR:CE2	2:B:105:THR:HG21	0.40	2.51	11	1
1:A:38:PRO:HD3	2:B:119:PRO:HG3	0.40	1.82	14	1
2:B:192:ASP:OD1	2:B:204:VAL:CG1	0.40	2.68	19	1
1:A:36:VAL:O	1:A:36:VAL:HG13	0.40	2.16	1	1
2:B:29:LYS:HB2	2:B:156:ARG:NH1	0.40	2.31	1	20
2:B:4:TYR:OH	2:B:162:TYR:CB	0.40	2.69	20	1
2:B:20:VAL:HG13	2:B:23:ASN:HD22	0.40	1.76	1	20
1:A:86:ARG:CZ	1:A:91:VAL:HG11	0.40	2.31	19	1
2:B:211:PRO:HB2	2:B:228:THR:OG1	0.40	2.16	20	1
1:A:7:MET:CB	1:A:90:MET:HE1	0.40	2.43	4	1
1:A:9:THR:OG1	1:A:15:LEU:CD2	0.40	2.69	4	1
2:B:1:TYR:HE2	2:B:119:PRO:HG2	0.40	1.75	16	1
2:B:8:ASN:HD22	2:B:8:ASN:N	0.40	2.14	16	1

6.3 Torsion angles

6.3.1 Protein backbone

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	95/97 (98%)	67±0 (71±0%)	21±0 (22±0%)	7±0 (7±0%)	1	15
2	B	247/249 (99%)	241±0 (98±0%)	5±0 (2±0%)	1±0 (0±0%)	31	76
All	All	6840/6920 (99%)	6160 (90%)	520 (8%)	160 (2%)	7	45

All 8 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	12	TYR	20
1	A	45	LYS	20
1	A	60	LEU	20
1	A	66	SER	20
1	A	67	PHE	20
1	A	73	GLY	20
1	A	84	PRO	20
2	B	41	PRO	20

6.3.2 Protein sidechains

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	77/77 (100%)	63±1 (82±2%)	14±1 (18±2%)	3	36
2	B	204/204 (100%)	194±2 (95±1%)	10±2 (5±1%)	25	75
All	All	5620/5620 (100%)	5151 (92%)	469 (8%)	12	59

All 61 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	7	MET	20
1	A	35	LYS	20
1	A	50	GLU	20
1	A	69	SER	20
1	A	74	THR	20
1	A	97	GLU	20
2	B	28	LYS	20
2	B	46	LYS	20
2	B	204	VAL	20
1	A	82	CYS	19
1	A	86	ARG	18
1	A	60	LEU	16
1	A	83	THR	16
2	B	208	LEU	14
1	A	9	THR	12
1	A	40	ASN	12
2	B	63	ASP	12
1	A	42	ILE	12
2	B	105	THR	11
1	A	62	ILE	11
2	B	7	TYR	10
2	B	67	SER	10
1	A	15	LEU	9
1	A	12	TYR	8
2	B	115	LEU	8
2	B	103	LEU	7
1	A	57	ASN	7
2	B	158	ARG	6
2	B	164	THR	5
1	A	34	ASN	5
2	B	1	TYR	4
2	B	65	SER	4
2	B	189	PHE	4
2	B	170	ASN	4
2	B	162	TYR	3
1	A	45	LYS	3
1	A	36	VAL	3
2	B	61	GLN	3
1	A	59	LYS	3
1	A	33	MET	3
2	B	8	ASN	3
2	B	171	ASN	2
2	B	3	PHE	2

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Mol	Chain	Res	Type	Models (Total)
2	B	4	TYR	2
2	B	205	THR	2
2	B	120	LEU	1
2	B	70	ASN	1
2	B	116	LEU	1
1	A	11	LYS	1
2	B	6	GLN	1
2	B	99	ASP	1
2	B	102	TYR	1
2	B	168	SER	1
2	B	59	GLN	1
2	B	161	VAL	1
2	B	166	GLU	1
1	A	58	THR	1
2	B	186	ASP	1
2	B	169	ASN	1
2	B	192	ASP	1
2	B	206	SER	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 oligosaccharides 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	250	2	46,50,50	1.28±0.00	6±0 (13±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	250	2	58,82,82	1.36±0.00	4±0 (6±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	250	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	250	HEC	CAB-C3B	3.09	1.45	1.35	1	20
4	B	250	HEC	CAC-C3C	2.93	1.44	1.35	1	20
4	B	250	HEC	CMD-C2D	2.60	1.56	1.50	1	20
4	B	250	HEC	C1B-C2B	2.32	1.48	1.43	1	20
4	B	250	HEC	CBC-CAC	2.06	1.57	1.49	1	20
4	B	250	HEC	C3C-C2C	2.05	1.34	1.41	1	20

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

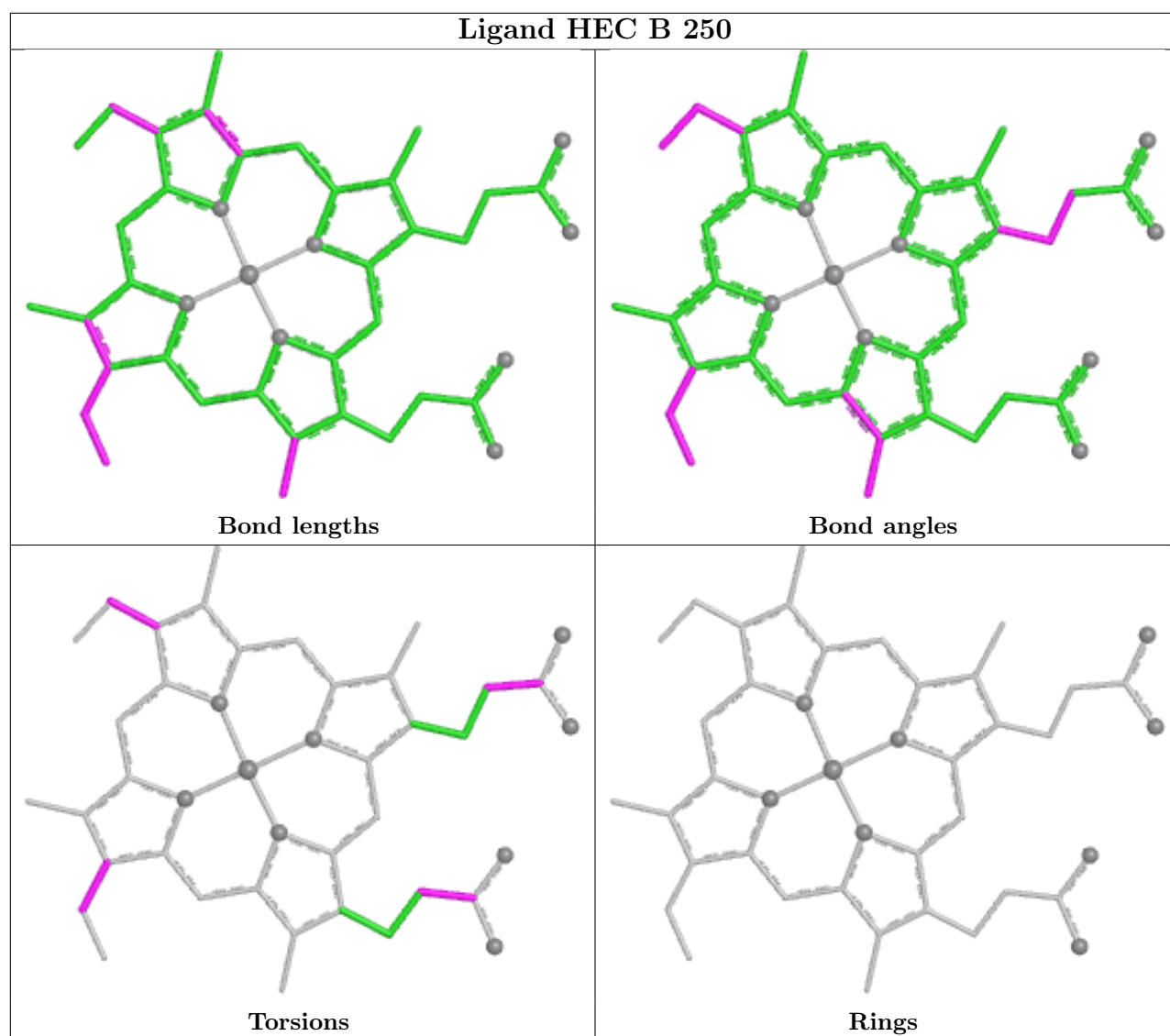
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	B	250	HEC	CBB-CAB-C3B	5.63	116.18	127.43	1	20
4	B	250	HEC	CBC-CAC-C3C	4.82	117.80	127.43	1	20
4	B	250	HEC	CBA-CAA-C2A	2.61	105.33	112.53	1	20
4	B	250	HEC	CMD-C2D-C1D	2.46	129.16	125.42	1	20

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 than 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.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided