Full wwPDB NMR Structure Validation Report (i)

Dec 17, 2023 – 01:03 PM EST

PDB ID	:	1CKK
Title	:	CALMODULIN/RAT CA2+/CALMODULIN DEPENDENT PROTEIN KINASE FRAGMENT
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Deposited on	:	1998-11-20

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

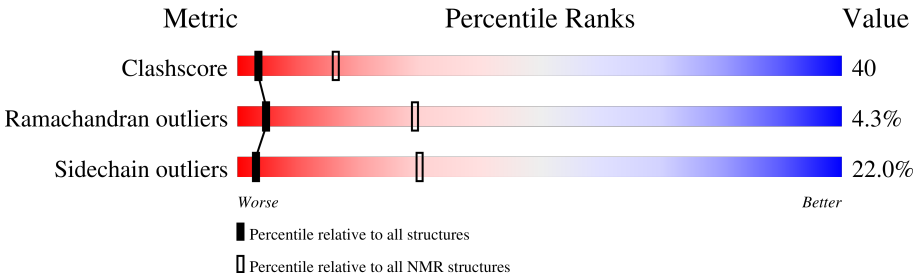
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	148	23% 61% 6% 10%
2	B	26	12% 58% 12% 8% 12%

2 Ensemble composition and analysis (i)

This entry contains 30 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:8-A:75, A:82-A:146, B:4-B:26 (156)	0.97	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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 11, 12, 13, 14, 15, 16, 18, 19, 21, 22, 23, 30
2	10, 20, 25
3	24, 28
4	17, 27
Single-model clusters	26; 29

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2717 atoms, of which 1334 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	148	2262	714	1096	188	255	9	0

- Molecule 2 is a protein called Calcium/calmodulin-dependent protein kinase kinase 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	26	451	142	238	37	33	1	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
3	A	4	4	4

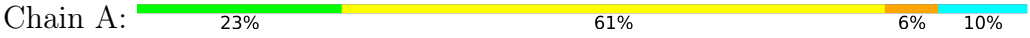
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

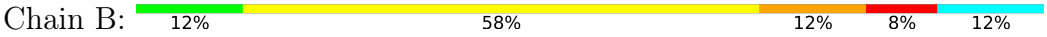
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

Chain B:



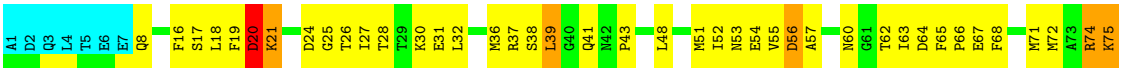
4.2 Scores per residue for each member of the ensemble

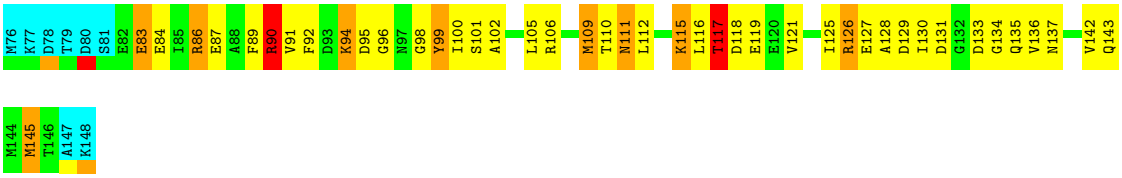
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Calmodulin-1

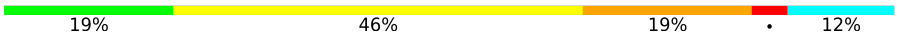
Chain A:

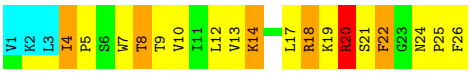




• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

Chain B:

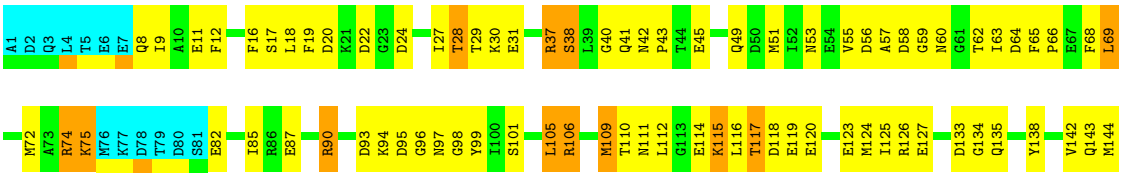




4.2.2 Score per residue for model 2

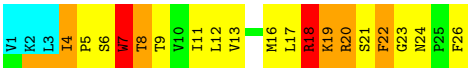
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

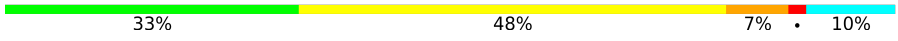
Chain B:



4.2.3 Score per residue for model 3

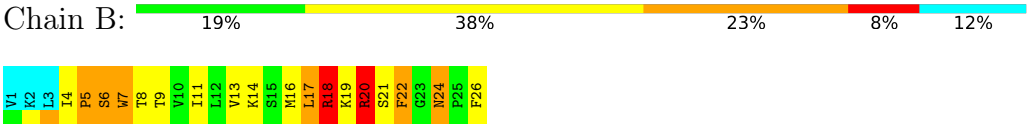
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

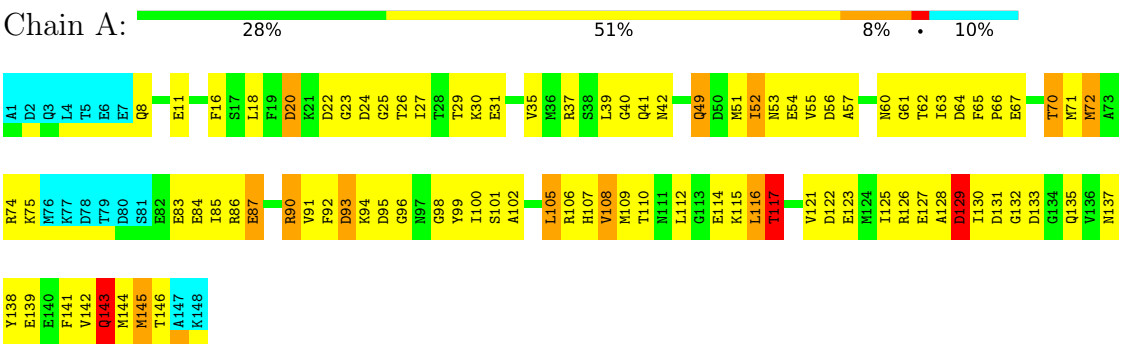
Chain B:



4.2.4 Score per residue for model 4

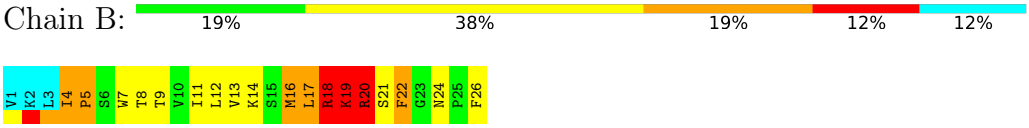
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

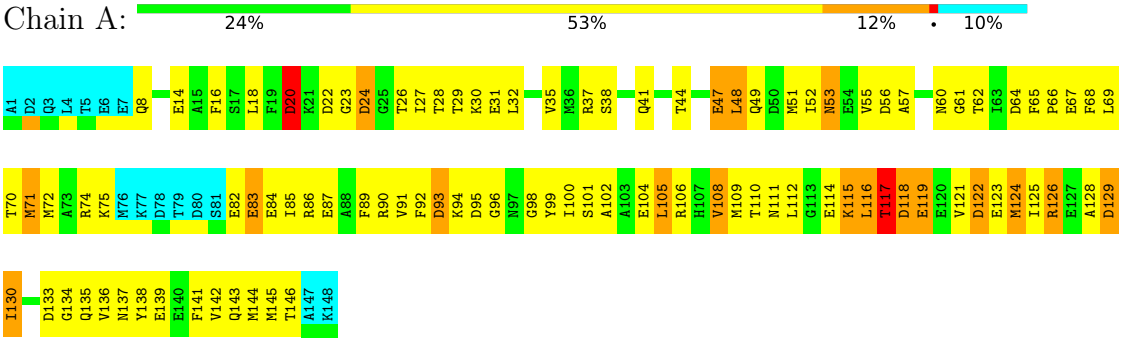
Chain B:



4.2.5 Score per residue for model 5

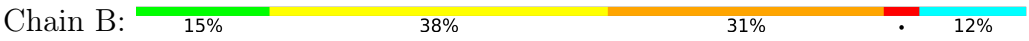
• Molecule 1: Calmodulin-1

Chain A:



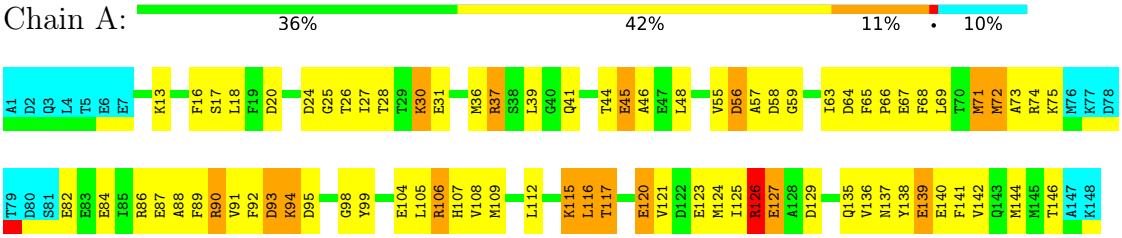
• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

Chain B:

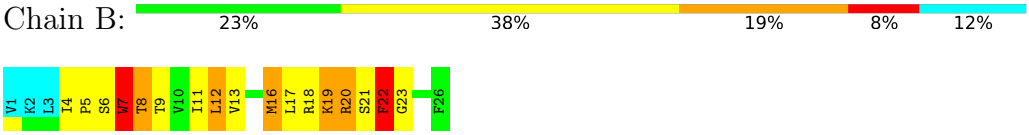


4.2.6 Score per residue for model 6

• Molecule 1: Calmodulin-1

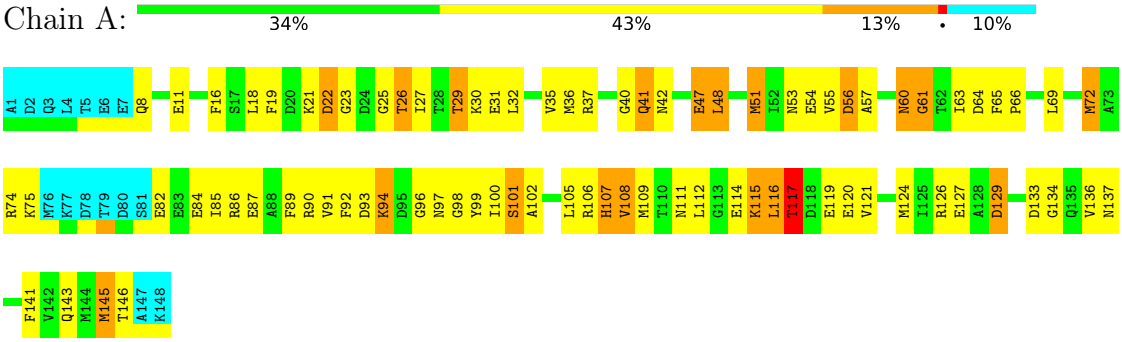


• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1



4.2.7 Score per residue for model 7

• Molecule 1: Calmodulin-1

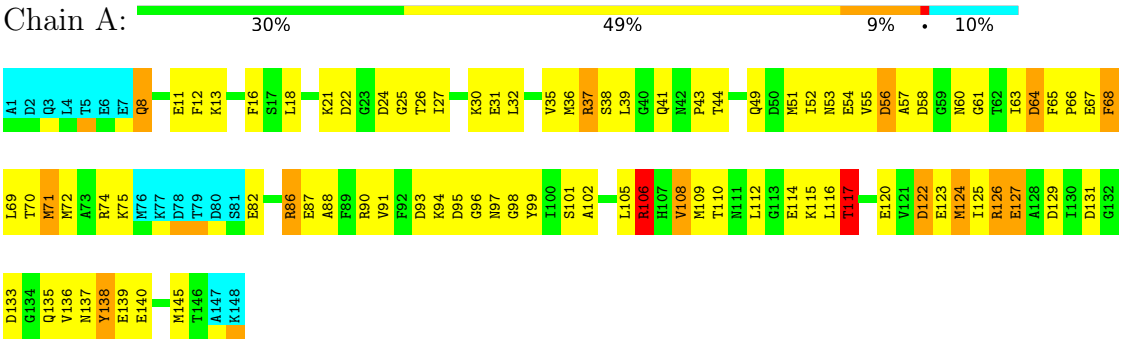


• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

4.2.8 Score per residue for model 8

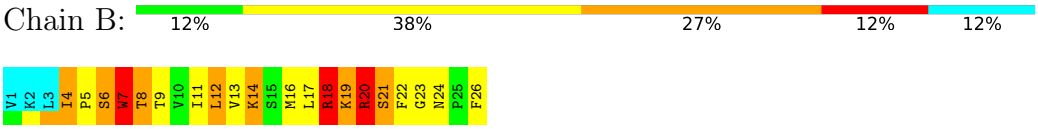
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

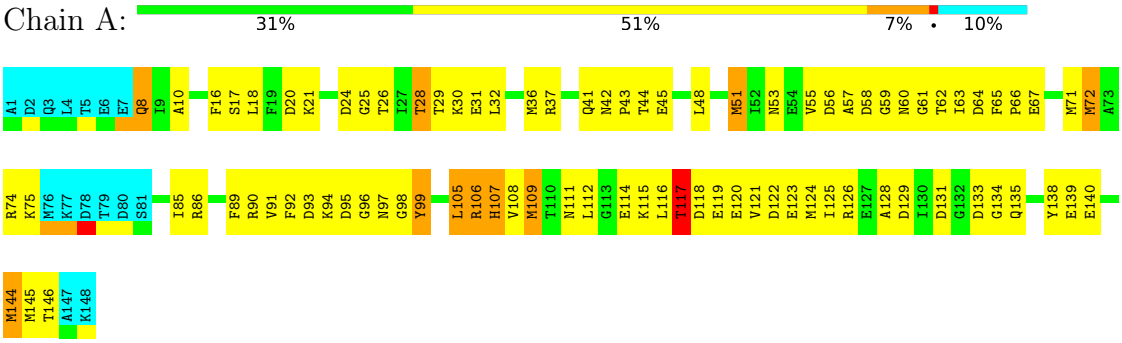
Chain B:



4.2.9 Score per residue for model 9

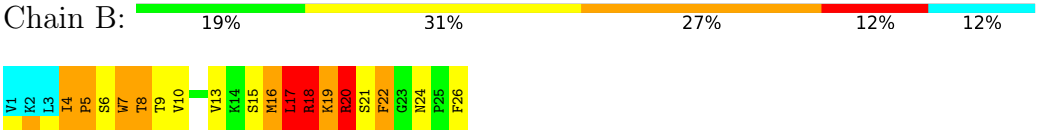
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

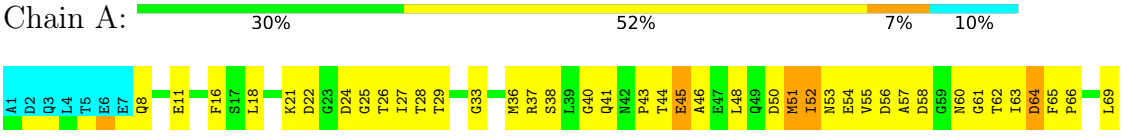
Chain B:

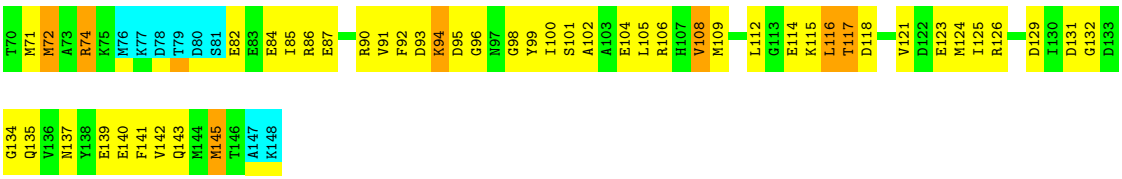


4.2.10 Score per residue for model 10

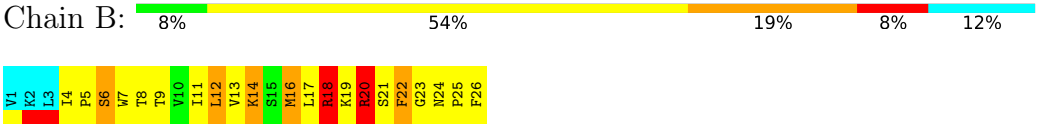
• Molecule 1: Calmodulin-1

Chain A:



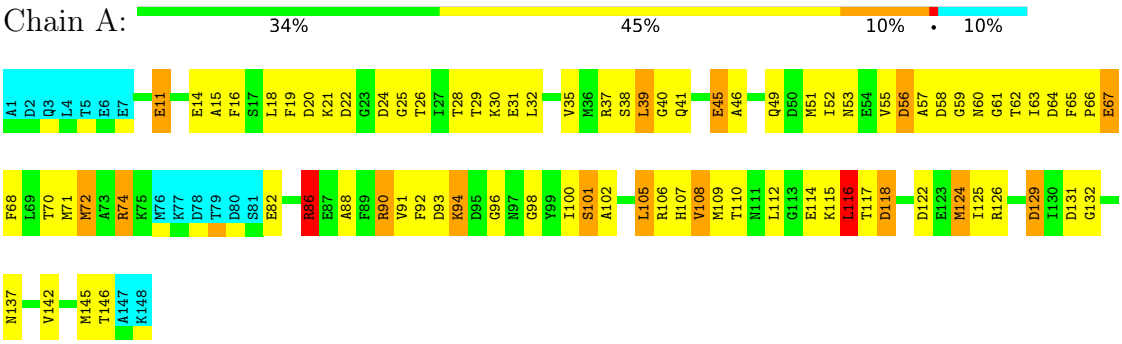


• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

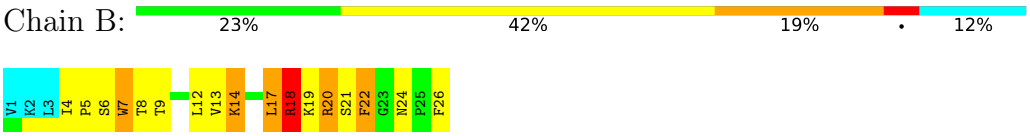


4.2.11 Score per residue for model 11

• Molecule 1: Calmodulin-1

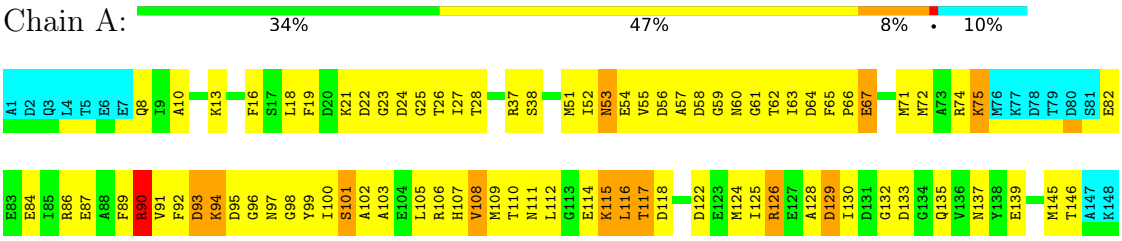


• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1



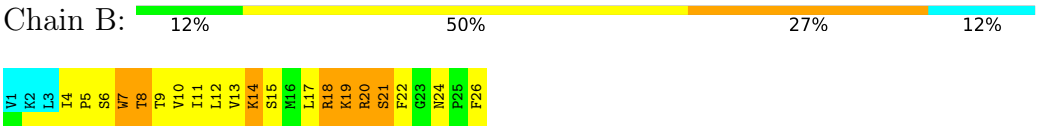
4.2.12 Score per residue for model 12

• Molecule 1: Calmodulin-1



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

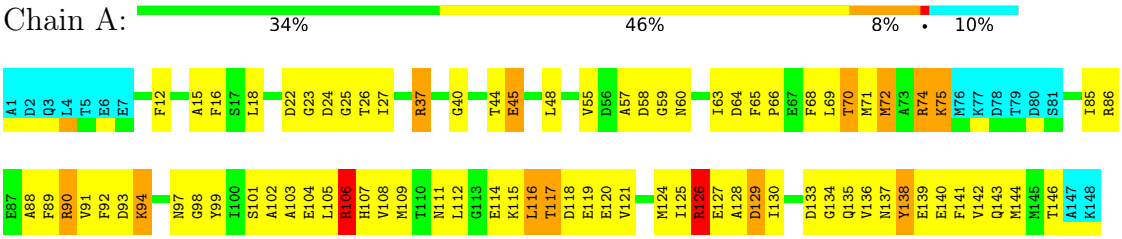
Chain B:



4.2.13 Score per residue for model 13

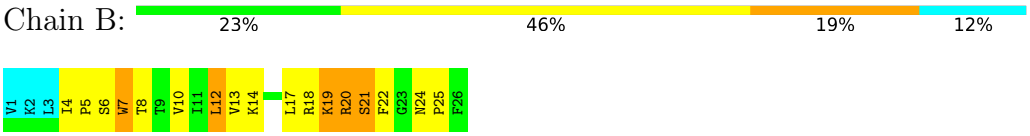
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

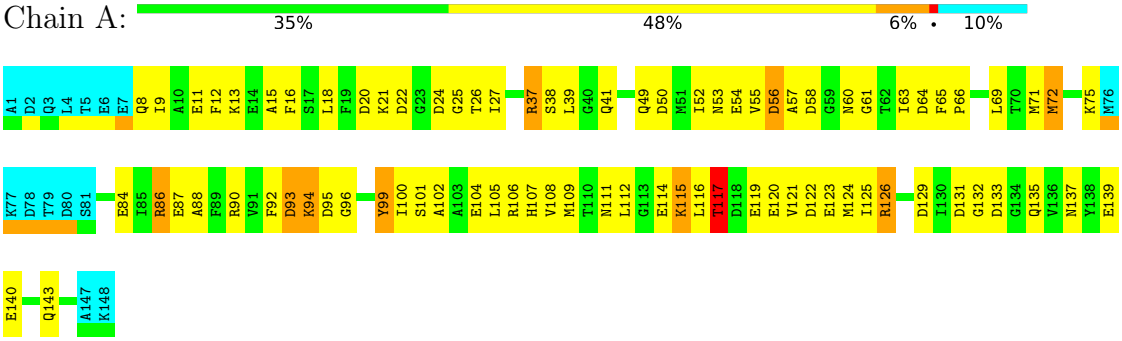
Chain B:



4.2.14 Score per residue for model 14

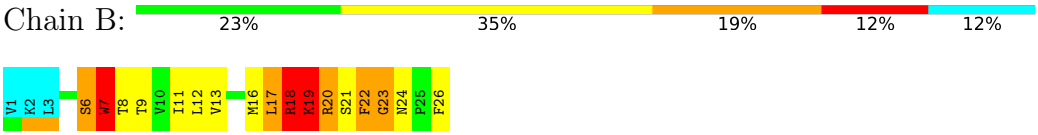
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

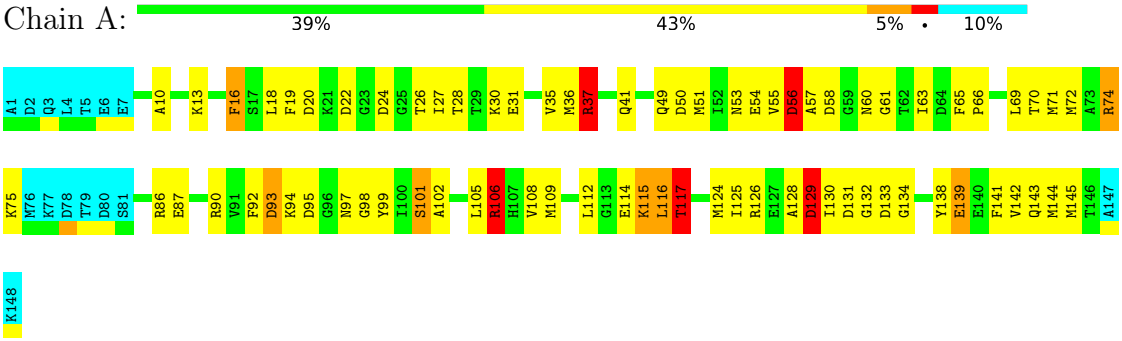
Chain B:



4.2.15 Score per residue for model 15

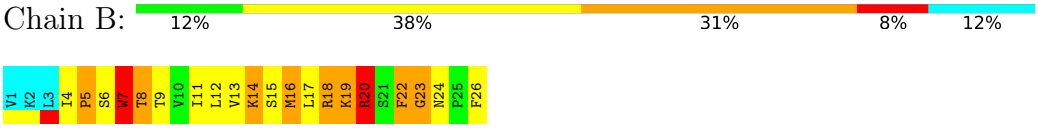
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

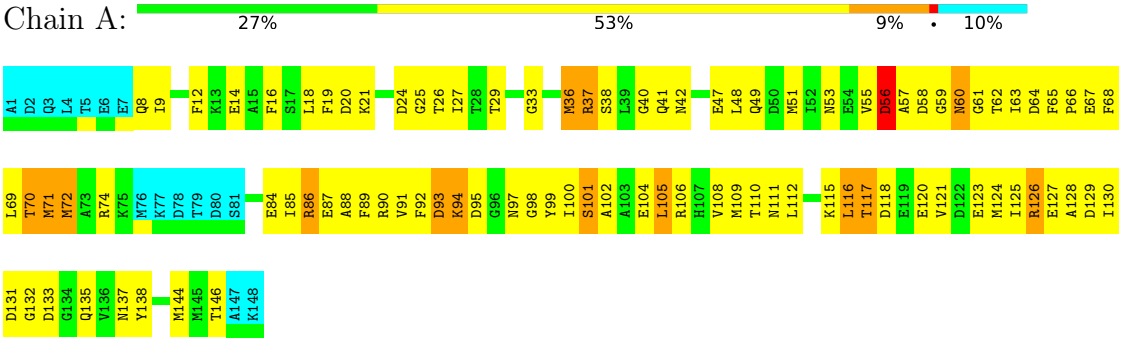
Chain B:



4.2.16 Score per residue for model 16

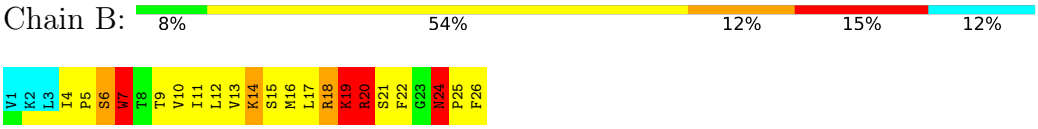
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

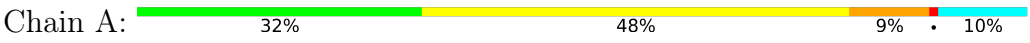
Chain B:

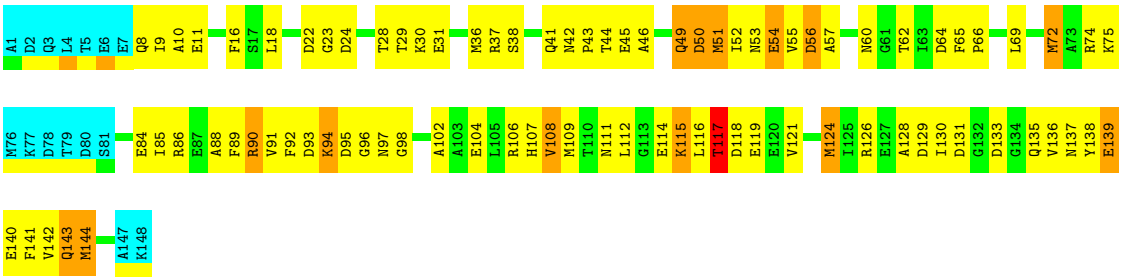


4.2.17 Score per residue for model 17

• Molecule 1: Calmodulin-1

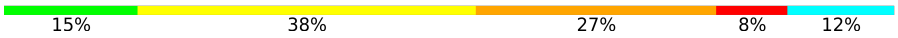
Chain A:

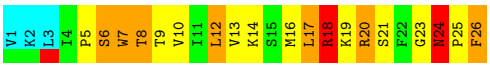




• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

Chain B:

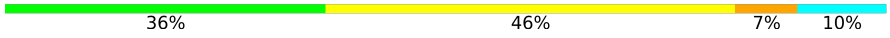


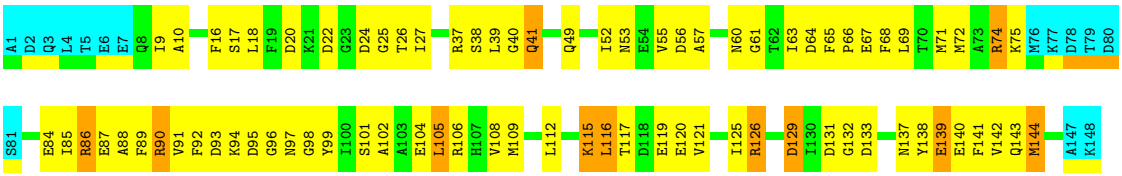


4.2.18 Score per residue for model 18

• Molecule 1: Calmodulin-1

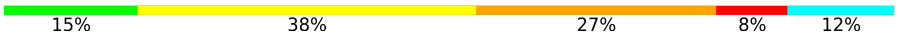
Chain A:

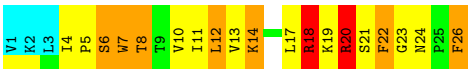




• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

Chain B:

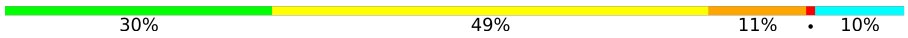




4.2.19 Score per residue for model 19

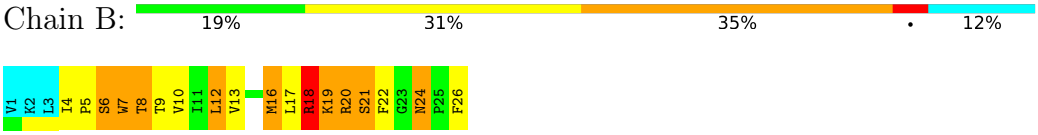
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

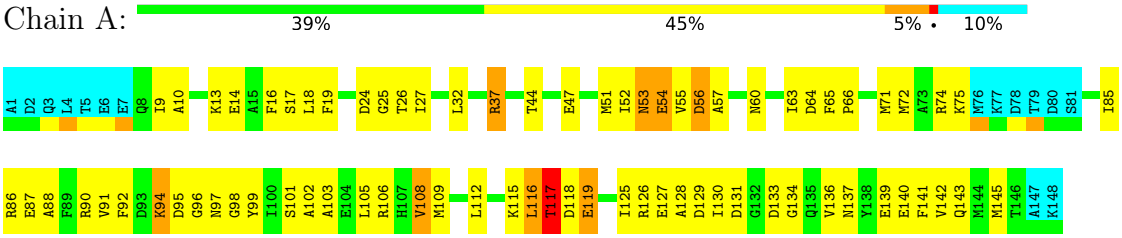
Chain B:



4.2.20 Score per residue for model 20

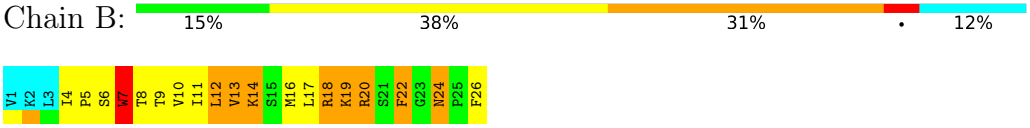
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

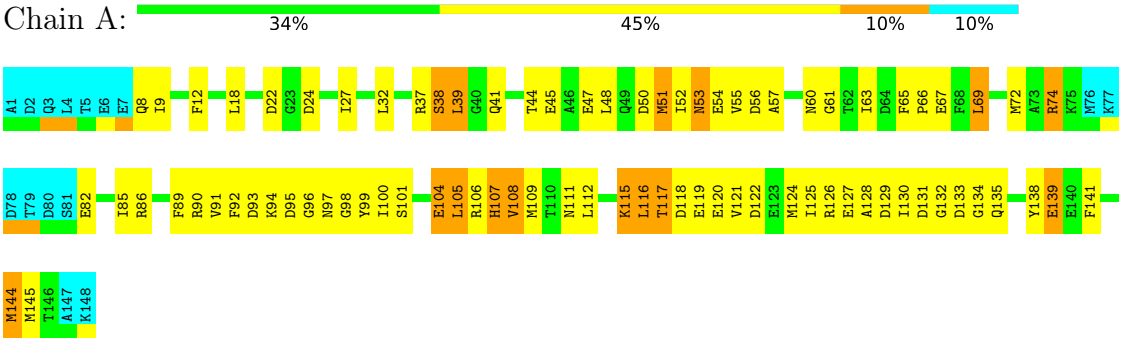
Chain B:



4.2.21 Score per residue for model 21

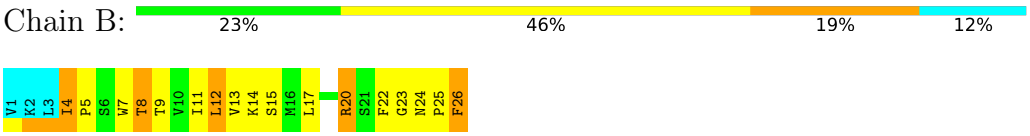
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

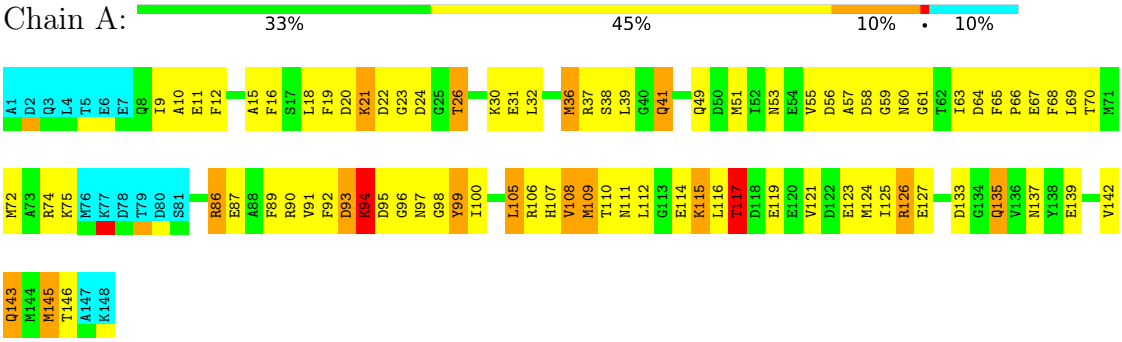
Chain B:



4.2.22 Score per residue for model 22

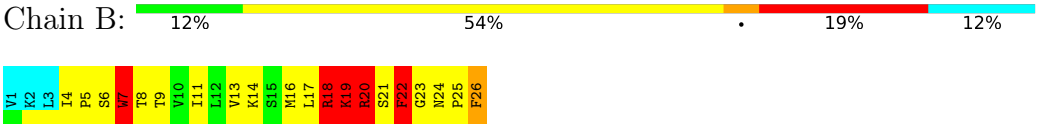
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

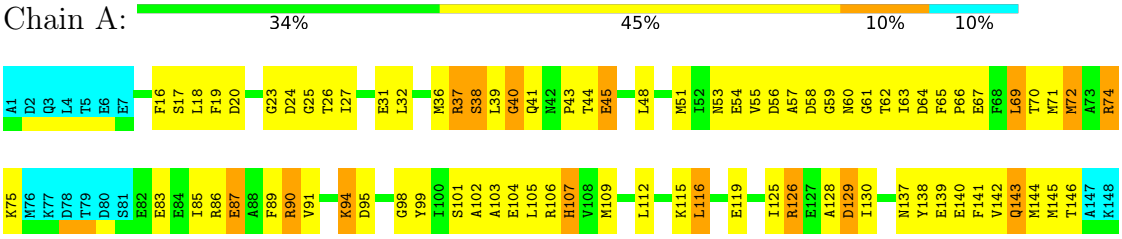
Chain B:



4.2.23 Score per residue for model 23

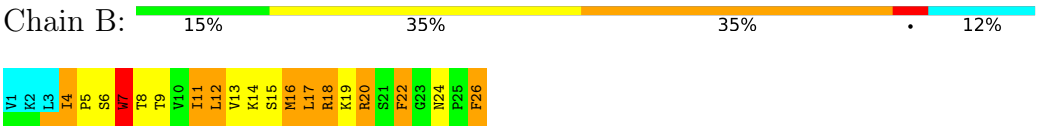
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

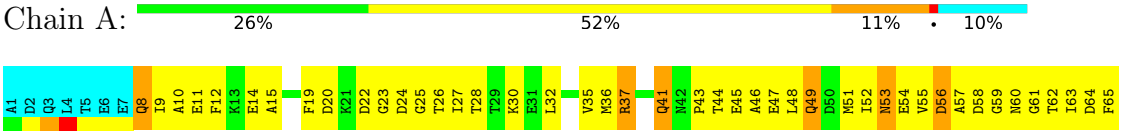
Chain B:

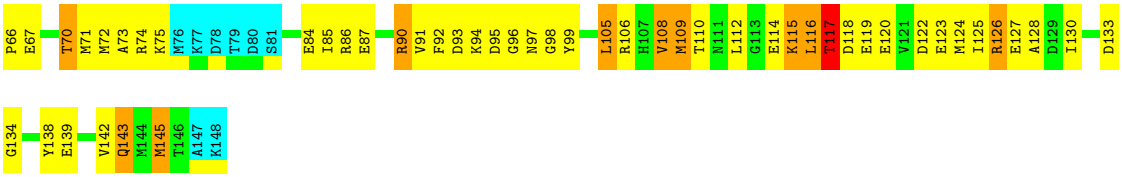


4.2.24 Score per residue for model 24

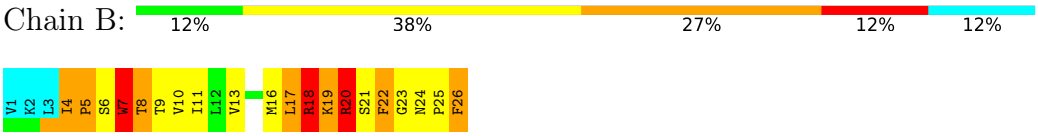
• Molecule 1: Calmodulin-1

Chain A:



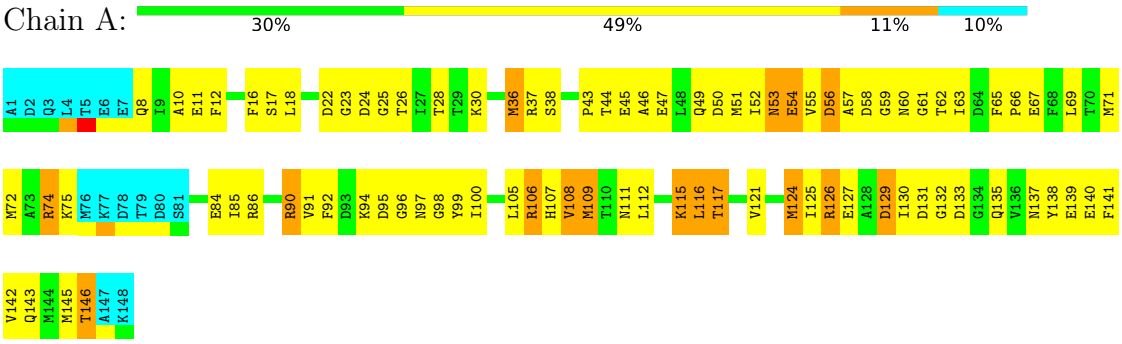


• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

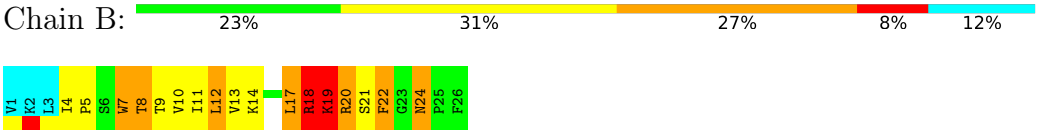


4.2.25 Score per residue for model 25

• Molecule 1: Calmodulin-1

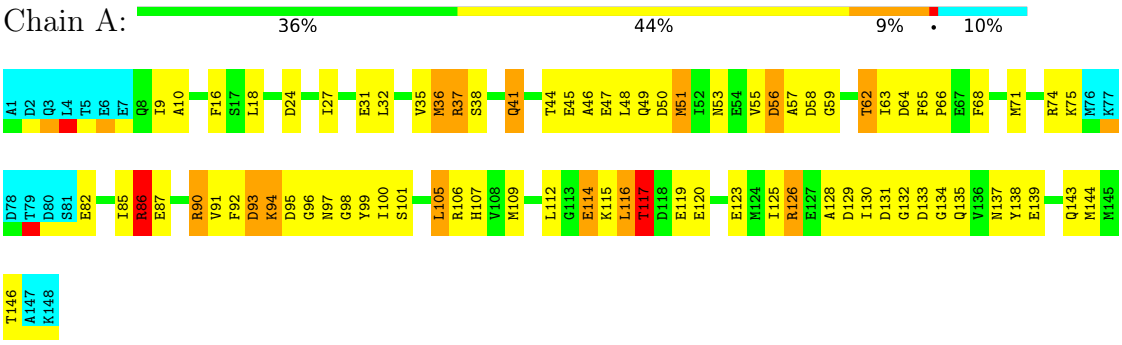


• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1



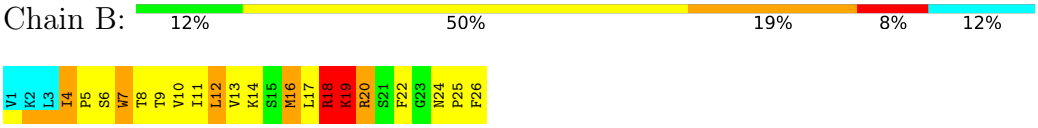
4.2.26 Score per residue for model 26

• Molecule 1: Calmodulin-1



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

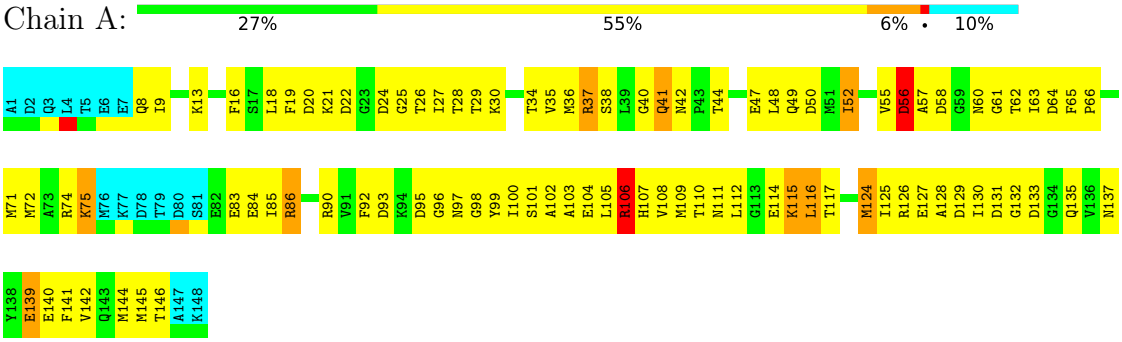
Chain B:



4.2.27 Score per residue for model 27

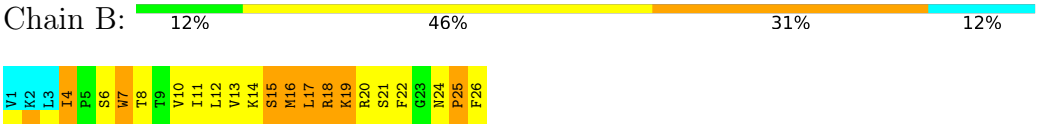
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

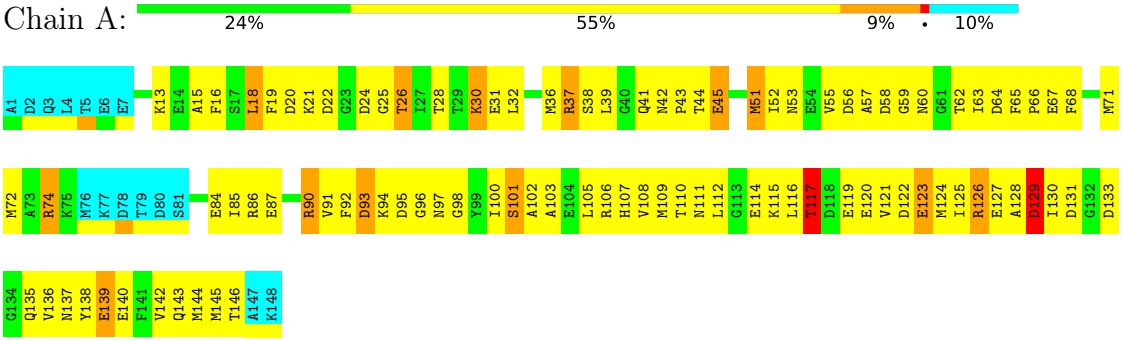
Chain B:



4.2.28 Score per residue for model 28

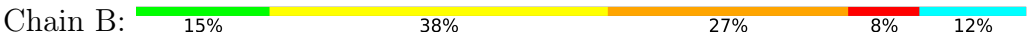
• Molecule 1: Calmodulin-1

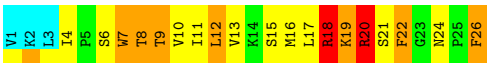
Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

Chain B:

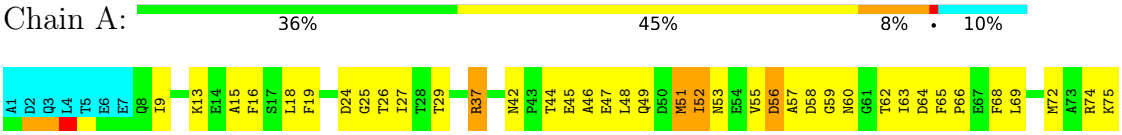




4.2.29 Score per residue for model 29

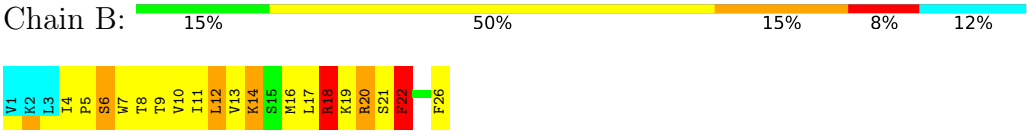
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

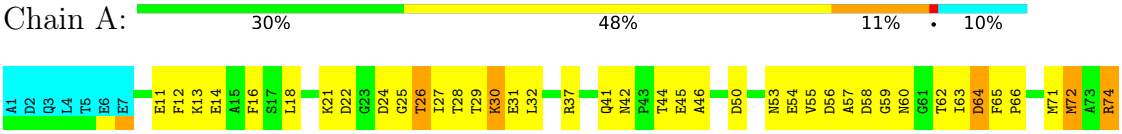
Chain B:



4.2.30 Score per residue for model 30

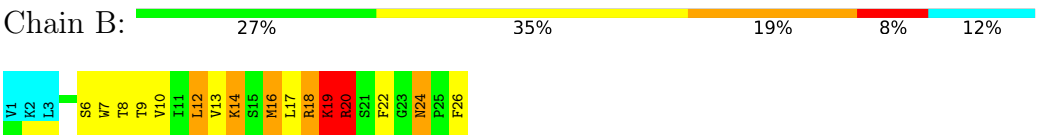
• Molecule 1: Calmodulin-1

Chain A:



• Molecule 2: Calcium/calmodulin-dependent protein kinase kinase 1

Chain B:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 30 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
X-PLOR	refinement	3.8.5.1
X-PLOR	structure solution	3.8.5.1

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: CA

There are no covalent bond-length or bond-angle outliers.

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	5.8±0.5
2	B	0.0±0.0	1.9±0.2
All	All	0	232

There are no bond-length outliers.

There are no bond-angle outliers.

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)
1	A	90	ARG	Sidechain	30
1	A	126	ARG	Sidechain	30
1	A	37	ARG	Sidechain	29
1	A	86	ARG	Sidechain	29
1	A	106	ARG	Sidechain	29
2	B	18	ARG	Sidechain	29
2	B	20	ARG	Sidechain	29
1	A	74	ARG	Sidechain	27

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	1050	987	987	84±11
2	B	189	203	203	34±7
All	All	37290	35700	35700	2924

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 40.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:LEU:HD12	1:A:125:ILE:HD11	1.10	1.22	26	18
1:A:145:MET:HE3	2:B:12:LEU:HD21	1.02	1.05	28	1
1:A:145:MET:CE	2:B:12:LEU:HD21	1.00	1.86	28	2
1:A:105:LEU:CD1	1:A:125:ILE:HD11	0.95	1.92	9	25
1:A:116:LEU:HD11	2:B:17:LEU:O	0.92	1.64	18	5
1:A:112:LEU:HD11	2:B:13:VAL:HG12	0.91	1.42	19	19
2:B:6:SER:O	2:B:10:VAL:HG23	0.91	1.66	16	3
1:A:109:MET:HA	2:B:17:LEU:HD21	0.90	1.43	6	20
2:B:7:TRP:O	2:B:10:VAL:HG22	0.90	1.66	5	10
1:A:105:LEU:HD12	1:A:125:ILE:CD1	0.90	1.96	14	8
2:B:17:LEU:HD22	2:B:17:LEU:O	0.90	1.67	11	1
1:A:87:GLU:HB3	2:B:9:THR:HG21	0.87	1.44	8	13
1:A:109:MET:SD	1:A:116:LEU:HD13	0.87	2.10	25	3
1:A:145:MET:HE2	2:B:24:ASN:HB2	0.86	1.48	11	1
1:A:109:MET:HE2	1:A:116:LEU:HD13	0.86	1.47	17	1
1:A:88:ALA:HB2	2:B:12:LEU:CD1	0.86	2.01	20	2
1:A:128:ALA:O	1:A:130:ILE:HD12	0.85	1.71	17	4
1:A:18:LEU:HD11	1:A:112:LEU:O	0.83	1.73	14	25
1:A:92:PHE:CZ	2:B:13:VAL:HG13	0.83	2.07	24	7
1:A:142:VAL:HG13	1:A:146:THR:HG21	0.83	1.49	5	1
2:B:4:ILE:HG22	2:B:5:PRO:CD	0.83	2.04	9	1
1:A:65:PHE:O	1:A:69:LEU:HD12	0.81	1.75	5	6
1:A:112:LEU:CD1	2:B:13:VAL:HG12	0.81	2.05	4	24
1:A:91:VAL:HG12	1:A:108:VAL:HG21	0.80	1.53	11	19
1:A:75:LYS:HG3	2:B:8:THR:HG21	0.80	1.53	17	4
1:A:18:LEU:HD12	1:A:112:LEU:O	0.79	1.78	28	2
2:B:4:ILE:HD13	2:B:5:PRO:HD2	0.79	1.54	4	1
1:A:18:LEU:HD13	2:B:14:LYS:HG3	0.78	1.55	16	6
1:A:72:MET:CE	2:B:11:ILE:HG21	0.78	2.09	24	1
1:A:16:PHE:CE1	1:A:27:ILE:HD11	0.78	2.14	12	2
2:B:17:LEU:O	2:B:17:LEU:HD13	0.77	1.79	11	1
1:A:18:LEU:HD13	2:B:14:LYS:CD	0.77	2.08	30	1
1:A:72:MET:SD	2:B:11:ILE:HG21	0.77	2.20	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:VAL:O	1:A:146:THR:HG22	0.76	1.81	30	4
2:B:13:VAL:O	2:B:17:LEU:HD13	0.76	1.80	8	6
1:A:27:ILE:O	1:A:62:THR:HG22	0.76	1.81	2	2
2:B:8:THR:O	2:B:12:LEU:HD13	0.76	1.81	5	1
1:A:25:GLY:O	1:A:26:THR:HG23	0.76	1.81	7	14
1:A:91:VAL:HG11	2:B:13:VAL:HG11	0.75	1.56	19	4
1:A:105:LEU:HD11	1:A:125:ILE:HD11	0.75	1.58	10	1
1:A:102:ALA:HB1	1:A:121:VAL:HG12	0.75	1.57	10	3
1:A:32:LEU:HD23	1:A:48:LEU:CD2	0.75	2.11	9	2
1:A:91:VAL:HG12	1:A:108:VAL:CG2	0.75	2.12	11	6
1:A:105:LEU:HD13	1:A:125:ILE:HD11	0.74	1.59	11	9
1:A:18:LEU:HD13	2:B:14:LYS:HD3	0.74	1.58	30	1
1:A:55:VAL:HG22	1:A:71:MET:SD	0.74	2.21	9	5
1:A:124:MET:HE2	2:B:22:PHE:CD1	0.74	2.16	27	2
1:A:112:LEU:HD11	2:B:13:VAL:HG13	0.74	1.59	20	1
1:A:65:PHE:CE2	1:A:69:LEU:HD11	0.74	2.17	29	1
1:A:142:VAL:HG13	1:A:146:THR:CG2	0.73	2.12	5	1
1:A:72:MET:HE1	2:B:11:ILE:HG21	0.73	1.59	24	1
1:A:112:LEU:HD12	2:B:17:LEU:CD2	0.73	2.13	28	2
1:A:116:LEU:HD21	2:B:19:LYS:O	0.73	1.84	17	5
1:A:55:VAL:HG21	2:B:7:TRP:CD1	0.73	2.19	3	9
1:A:85:ILE:HG21	1:A:142:VAL:HG22	0.72	1.59	19	7
2:B:24:ASN:N	2:B:25:PRO:CD	0.72	2.52	13	7
1:A:28:THR:HG22	1:A:62:THR:HG22	0.72	1.58	12	3
2:B:4:ILE:HG23	2:B:5:PRO:HD2	0.72	1.61	13	14
1:A:72:MET:HE1	2:B:11:ILE:CG2	0.72	2.14	24	1
1:A:112:LEU:HD12	2:B:17:LEU:HD22	0.71	1.61	21	4
1:A:55:VAL:HG13	1:A:71:MET:HG3	0.71	1.62	23	1
1:A:85:ILE:CD1	1:A:146:THR:HG21	0.71	2.16	16	3
1:A:116:LEU:HD23	1:A:120:GLU:HG2	0.71	1.62	6	1
1:A:52:ILE:HG12	1:A:63:ILE:HD11	0.71	1.62	4	2
1:A:116:LEU:HD21	2:B:19:LYS:CA	0.71	2.16	15	5
1:A:85:ILE:HG23	1:A:141:PHE:CD1	0.70	2.21	19	4
1:A:27:ILE:HD12	1:A:63:ILE:HG21	0.70	1.64	4	5
1:A:112:LEU:HD11	2:B:13:VAL:CG1	0.70	2.17	19	10
2:B:8:THR:HA	2:B:11:ILE:HD12	0.70	1.64	24	1
1:A:31:GLU:O	1:A:35:VAL:HG23	0.69	1.88	15	5
1:A:72:MET:HE1	2:B:26:PHE:CZ	0.69	2.23	11	7
1:A:146:THR:HG23	1:A:146:THR:O	0.69	1.86	13	11
1:A:12:PHE:CD2	1:A:68:PHE:CZ	0.69	2.81	8	1
1:A:39:LEU:CD2	1:A:112:LEU:HD21	0.69	2.18	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:MET:CB	2:B:17:LEU:HD21	0.69	2.17	11	1
2:B:4:ILE:HG22	2:B:5:PRO:HD2	0.69	1.64	9	1
1:A:29:THR:HG21	1:A:49:GLN:NE2	0.68	2.03	17	2
2:B:5:PRO:HB3	2:B:9:THR:HG21	0.68	1.64	25	2
1:A:29:THR:HG21	1:A:49:GLN:OE1	0.68	1.89	11	1
1:A:116:LEU:HD21	2:B:19:LYS:HA	0.68	1.64	9	5
1:A:92:PHE:CE2	1:A:105:LEU:HD21	0.68	2.24	26	4
1:A:61:GLY:O	1:A:62:THR:HG23	0.68	1.88	24	4
1:A:55:VAL:CG1	1:A:63:ILE:HD12	0.67	2.19	4	5
1:A:55:VAL:CG2	2:B:7:TRP:CD1	0.67	2.77	21	16
1:A:72:MET:CE	2:B:26:PHE:CZ	0.67	2.78	18	8
1:A:55:VAL:HG12	1:A:63:ILE:HD12	0.67	1.64	4	1
2:B:12:LEU:HD12	2:B:13:VAL:N	0.67	2.05	16	1
1:A:91:VAL:HG21	2:B:13:VAL:HG21	0.67	1.66	19	1
1:A:88:ALA:HB2	2:B:12:LEU:HD11	0.67	1.65	16	2
1:A:88:ALA:HB2	2:B:12:LEU:HD22	0.66	1.66	13	4
2:B:10:VAL:HG23	2:B:11:ILE:HD12	0.66	1.67	25	1
1:A:87:GLU:HG3	2:B:9:THR:HG23	0.66	1.67	24	1
1:A:91:VAL:CG1	2:B:13:VAL:HG21	0.66	2.21	9	3
1:A:65:PHE:CE1	1:A:69:LEU:HD11	0.66	2.26	14	2
1:A:124:MET:CE	2:B:22:PHE:CD1	0.66	2.79	10	2
1:A:109:MET:HB3	2:B:17:LEU:HD21	0.66	1.66	11	1
1:A:112:LEU:HD13	2:B:17:LEU:HD22	0.66	1.67	20	2
1:A:145:MET:HE2	2:B:24:ASN:H	0.66	1.50	23	1
1:A:39:LEU:O	1:A:39:LEU:HD13	0.66	1.91	11	1
2:B:17:LEU:O	2:B:17:LEU:CD2	0.66	2.43	11	1
1:A:91:VAL:HG11	2:B:13:VAL:HG21	0.65	1.67	9	9
1:A:68:PHE:CZ	2:B:11:ILE:HD13	0.65	2.27	2	2
1:A:124:MET:HE2	2:B:22:PHE:CD2	0.65	2.26	5	2
1:A:114:GLU:HG2	1:A:116:LEU:HD12	0.65	1.69	19	4
1:A:55:VAL:HG23	2:B:7:TRP:CD1	0.65	2.27	16	10
1:A:55:VAL:HG21	2:B:7:TRP:NE1	0.65	2.05	4	4
1:A:32:LEU:HD13	2:B:7:TRP:CH2	0.65	2.27	7	4
1:A:32:LEU:HD22	1:A:52:ILE:CD1	0.65	2.22	8	1
1:A:92:PHE:CE1	2:B:13:VAL:HG13	0.65	2.27	21	4
1:A:124:MET:HE3	2:B:22:PHE:CD1	0.64	2.27	10	1
1:A:43:PRO:HA	2:B:4:ILE:HD11	0.64	1.69	23	4
2:B:4:ILE:HG22	2:B:5:PRO:HD3	0.64	1.69	9	1
1:A:125:ILE:HG23	1:A:136:VAL:HG23	0.64	1.68	19	2
1:A:18:LEU:HD23	1:A:18:LEU:O	0.64	1.93	13	2
1:A:124:MET:CE	2:B:22:PHE:CD2	0.64	2.81	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:ALA:HB2	2:B:22:PHE:HD2	0.64	1.51	15	2
1:A:85:ILE:HG23	1:A:141:PHE:CE1	0.64	2.28	13	5
1:A:84:GLU:CG	2:B:12:LEU:HD11	0.64	2.23	7	1
1:A:92:PHE:CE1	1:A:105:LEU:HD23	0.64	2.28	13	1
1:A:16:PHE:CZ	1:A:65:PHE:N	0.64	2.66	27	17
1:A:51:MET:CE	2:B:7:TRP:CD1	0.64	2.80	4	3
1:A:138:TYR:CE1	1:A:142:VAL:HG21	0.64	2.28	15	1
2:B:17:LEU:H	2:B:17:LEU:HD13	0.63	1.53	17	3
1:A:116:LEU:HD11	2:B:17:LEU:C	0.63	2.12	12	1
1:A:105:LEU:HD11	2:B:22:PHE:HZ	0.63	1.51	16	1
1:A:92:PHE:CE1	1:A:108:VAL:HG11	0.63	2.27	6	9
1:A:92:PHE:HB3	1:A:100:ILE:HD13	0.63	1.70	28	16
1:A:55:VAL:HG22	1:A:71:MET:HG3	0.63	1.70	30	4
1:A:117:THR:O	1:A:121:VAL:HG23	0.63	1.93	30	10
2:B:5:PRO:HB2	2:B:10:VAL:HG13	0.63	1.71	17	1
1:A:87:GLU:CB	2:B:9:THR:HG21	0.63	2.23	19	4
1:A:65:PHE:CZ	1:A:69:LEU:HD11	0.63	2.28	14	1
1:A:39:LEU:HD23	1:A:112:LEU:HD21	0.62	1.69	11	1
1:A:36:MET:HE1	1:A:51:MET:SD	0.62	2.33	16	2
1:A:55:VAL:CG1	1:A:63:ILE:HG23	0.62	2.25	20	2
1:A:82:GLU:HA	1:A:85:ILE:HD12	0.62	1.69	2	3
1:A:65:PHE:N	1:A:66:PRO:HD2	0.62	2.10	19	30
1:A:91:VAL:HG11	2:B:13:VAL:CG1	0.62	2.25	19	1
1:A:72:MET:CE	2:B:26:PHE:CE1	0.62	2.82	18	4
1:A:28:THR:HG22	1:A:62:THR:CG2	0.62	2.25	11	2
1:A:145:MET:HE3	2:B:24:ASN:HB2	0.61	1.70	1	4
1:A:19:PHE:CD1	1:A:35:VAL:HG11	0.61	2.30	15	2
2:B:11:ILE:HD13	2:B:11:ILE:N	0.61	2.09	26	6
1:A:75:LYS:CB	2:B:8:THR:HG21	0.61	2.25	25	5
2:B:9:THR:HA	2:B:12:LEU:HD21	0.61	1.72	20	2
1:A:84:GLU:HG2	2:B:12:LEU:HD12	0.61	1.71	17	1
1:A:105:LEU:HD11	2:B:22:PHE:CZ	0.61	2.30	16	5
1:A:112:LEU:CD1	2:B:13:VAL:CG1	0.61	2.79	14	7
2:B:19:LYS:N	2:B:19:LYS:CD	0.60	2.65	14	1
1:A:85:ILE:HG21	1:A:142:VAL:CG2	0.60	2.26	19	2
1:A:19:PHE:CE1	1:A:32:LEU:CD1	0.60	2.85	22	1
1:A:55:VAL:HG21	2:B:7:TRP:CE2	0.60	2.32	4	7
1:A:145:MET:HE3	2:B:12:LEU:CD2	0.60	2.02	28	1
1:A:116:LEU:HD12	1:A:116:LEU:N	0.60	2.12	14	1
2:B:19:LYS:HG2	2:B:20:ARG:N	0.60	2.11	30	2
1:A:85:ILE:HG23	1:A:141:PHE:CE2	0.59	2.31	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:7:TRP:O	2:B:10:VAL:CG2	0.59	2.50	17	10
2:B:17:LEU:O	2:B:19:LYS:N	0.59	2.36	14	5
1:A:142:VAL:CG1	1:A:146:THR:CG2	0.59	2.80	5	1
1:A:27:ILE:HD12	1:A:63:ILE:HB	0.59	1.74	20	13
2:B:11:ILE:CD1	2:B:11:ILE:N	0.59	2.65	23	1
1:A:112:LEU:CD1	2:B:17:LEU:HD22	0.59	2.27	13	6
1:A:98:GLY:O	1:A:99:TYR:CG	0.59	2.55	4	12
2:B:12:LEU:CD1	2:B:26:PHE:CD2	0.59	2.85	4	1
1:A:125:ILE:N	1:A:125:ILE:HD12	0.59	2.12	19	1
1:A:75:LYS:HG2	2:B:8:THR:HG21	0.59	1.75	29	5
1:A:112:LEU:CB	2:B:17:LEU:CD2	0.59	2.80	20	1
1:A:112:LEU:HD13	2:B:14:LYS:HA	0.59	1.73	16	4
1:A:99:TYR:CD1	1:A:99:TYR:N	0.59	2.70	21	2
2:B:12:LEU:HD13	2:B:26:PHE:CD2	0.59	2.33	4	1
1:A:72:MET:HE1	2:B:26:PHE:CE2	0.59	2.32	16	2
1:A:18:LEU:HD13	2:B:14:LYS:CG	0.59	2.27	18	4
1:A:92:PHE:CE1	2:B:13:VAL:HG22	0.59	2.33	21	2
1:A:75:LYS:HB3	2:B:8:THR:HG21	0.59	1.75	30	5
1:A:32:LEU:HD23	1:A:48:LEU:HD22	0.58	1.75	9	1
1:A:68:PHE:CZ	2:B:11:ILE:HD12	0.58	2.33	28	2
1:A:99:TYR:CE2	1:A:137:ASN:OD1	0.58	2.56	26	1
1:A:51:MET:O	2:B:7:TRP:CD1	0.58	2.56	24	5
1:A:16:PHE:CZ	1:A:64:ASP:O	0.58	2.57	11	1
1:A:128:ALA:HB2	2:B:22:PHE:CD2	0.58	2.33	15	1
1:A:27:ILE:HD12	1:A:63:ILE:CB	0.58	2.28	21	7
1:A:142:VAL:HG13	1:A:146:THR:OG1	0.58	1.98	25	2
1:A:102:ALA:HB1	1:A:121:VAL:CG1	0.58	2.29	17	2
2:B:17:LEU:O	2:B:17:LEU:CD1	0.58	2.51	11	1
1:A:99:TYR:CB	1:A:135:GLN:NE2	0.58	2.65	27	1
1:A:98:GLY:O	1:A:99:TYR:CD2	0.58	2.57	13	9
1:A:55:VAL:HB	1:A:63:ILE:HD12	0.58	1.74	20	6
2:B:16:MET:SD	2:B:22:PHE:CD1	0.58	2.97	3	2
1:A:88:ALA:O	1:A:92:PHE:CD2	0.58	2.57	14	5
1:A:27:ILE:HD12	1:A:63:ILE:CG2	0.58	2.29	4	6
1:A:116:LEU:HD23	2:B:19:LYS:O	0.58	1.98	7	1
1:A:98:GLY:O	1:A:99:TYR:CD1	0.58	2.57	24	6
2:B:6:SER:O	2:B:8:THR:N	0.58	2.36	12	11
1:A:92:PHE:CB	1:A:100:ILE:HD13	0.57	2.29	14	2
1:A:65:PHE:N	1:A:66:PRO:CD	0.57	2.67	19	29
1:A:18:LEU:C	1:A:18:LEU:HD23	0.57	2.19	14	11
1:A:92:PHE:CD2	1:A:141:PHE:CE1	0.57	2.92	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:MET:HE1	2:B:7:TRP:CG	0.57	2.34	4	4
2:B:19:LYS:O	2:B:19:LYS:HG2	0.57	1.98	14	1
1:A:72:MET:HE2	2:B:26:PHE:CE1	0.57	2.34	8	3
1:A:99:TYR:CZ	1:A:137:ASN:OD1	0.57	2.57	16	2
1:A:51:MET:SD	2:B:7:TRP:CD1	0.57	2.98	9	8
1:A:88:ALA:CB	2:B:12:LEU:HD22	0.57	2.29	18	5
2:B:4:ILE:CG2	2:B:5:PRO:CD	0.57	2.82	9	1
1:A:68:PHE:CZ	2:B:11:ILE:HG23	0.57	2.33	28	1
1:A:109:MET:CG	2:B:17:LEU:HD21	0.57	2.29	10	1
1:A:112:LEU:HD13	2:B:14:LYS:CA	0.57	2.30	1	1
1:A:72:MET:HE3	2:B:26:PHE:CE1	0.57	2.35	18	2
1:A:55:VAL:O	1:A:57:ALA:N	0.57	2.38	7	29
1:A:75:LYS:CG	2:B:8:THR:HG21	0.57	2.29	17	4
1:A:116:LEU:HD21	2:B:17:LEU:O	0.57	2.00	8	2
1:A:72:MET:SD	2:B:8:THR:HG22	0.56	2.40	20	3
2:B:19:LYS:CD	2:B:19:LYS:O	0.56	2.53	9	1
1:A:11:GLU:OE2	1:A:12:PHE:CE1	0.56	2.57	25	2
1:A:114:GLU:HB3	2:B:17:LEU:HD23	0.56	1.77	19	1
1:A:124:MET:HG2	2:B:22:PHE:CD2	0.56	2.35	2	4
1:A:85:ILE:HG23	1:A:145:MET:SD	0.56	2.39	9	1
1:A:18:LEU:CD1	1:A:112:LEU:O	0.56	2.51	20	17
1:A:116:LEU:N	1:A:116:LEU:CD1	0.56	2.67	14	1
2:B:17:LEU:O	2:B:18:ARG:C	0.56	2.44	29	9
1:A:19:PHE:HA	1:A:35:VAL:HG21	0.56	1.78	7	4
1:A:33:GLY:CA	1:A:48:LEU:HD21	0.56	2.31	16	1
1:A:18:LEU:HD23	1:A:18:LEU:C	0.56	2.21	13	2
1:A:84:GLU:HG2	2:B:12:LEU:HD11	0.56	1.78	7	1
1:A:16:PHE:CE1	1:A:65:PHE:N	0.55	2.74	22	2
2:B:18:ARG:O	2:B:20:ARG:N	0.55	2.39	15	3
1:A:85:ILE:CD1	1:A:146:THR:CG2	0.55	2.83	16	2
1:A:8:GLN:CG	1:A:9:ILE:N	0.55	2.69	16	1
1:A:116:LEU:HD13	2:B:17:LEU:CD2	0.55	2.32	11	1
1:A:55:VAL:HG21	2:B:7:TRP:CG	0.55	2.37	3	4
1:A:145:MET:CE	2:B:24:ASN:CB	0.55	2.84	7	2
1:A:124:MET:O	2:B:22:PHE:CD2	0.55	2.60	13	2
1:A:89:PHE:CE1	1:A:93:ASP:OD2	0.55	2.58	22	1
1:A:120:GLU:CG	1:A:121:VAL:N	0.55	2.69	21	2
2:B:24:ASN:N	2:B:25:PRO:HD3	0.55	2.16	10	4
1:A:16:PHE:CZ	1:A:64:ASP:C	0.55	2.80	29	15
1:A:60:ASN:OD1	1:A:61:GLY:N	0.55	2.40	4	14
2:B:17:LEU:HD13	2:B:17:LEU:N	0.55	2.16	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:THR:O	1:A:48:LEU:HD22	0.55	2.01	16	2
1:A:116:LEU:CD2	2:B:19:LYS:O	0.55	2.54	7	6
2:B:19:LYS:CD	2:B:19:LYS:C	0.55	2.75	24	12
1:A:42:ASN:N	1:A:43:PRO:CD	0.55	2.70	19	2
1:A:92:PHE:HE1	2:B:13:VAL:HG22	0.55	1.60	10	2
1:A:91:VAL:CG1	1:A:108:VAL:CG2	0.55	2.83	11	2
2:B:20:ARG:O	2:B:20:ARG:HG2	0.55	2.00	10	2
1:A:67:GLU:O	1:A:71:MET:CG	0.55	2.54	19	2
1:A:128:ALA:O	1:A:130:ILE:N	0.55	2.40	3	15
2:B:6:SER:CB	2:B:9:THR:OG1	0.55	2.54	5	2
1:A:51:MET:HE1	2:B:7:TRP:CA	0.55	2.32	5	1
1:A:122:ASP:OD1	1:A:123:GLU:N	0.55	2.40	9	1
2:B:12:LEU:HG	2:B:26:PHE:CE2	0.55	2.37	11	2
1:A:18:LEU:HD21	1:A:112:LEU:O	0.54	2.01	11	3
1:A:141:PHE:CE1	2:B:16:MET:CE	0.54	2.91	17	1
1:A:92:PHE:CE2	1:A:105:LEU:CD2	0.54	2.90	19	2
1:A:16:PHE:CE1	1:A:64:ASP:C	0.54	2.81	7	10
1:A:72:MET:HE2	2:B:26:PHE:CZ	0.54	2.37	2	4
1:A:116:LEU:CD1	2:B:17:LEU:O	0.54	2.55	26	2
1:A:105:LEU:CD1	1:A:125:ILE:CD1	0.54	2.80	26	9
1:A:28:THR:CG2	1:A:62:THR:HG22	0.54	2.32	11	2
1:A:125:ILE:HG22	1:A:129:ASP:OD2	0.54	2.03	18	2
1:A:88:ALA:HB2	2:B:12:LEU:HD13	0.54	1.77	6	1
1:A:98:GLY:C	1:A:99:TYR:CG	0.54	2.81	27	6
1:A:139:GLU:O	1:A:143:GLN:N	0.54	2.40	10	6
1:A:145:MET:O	2:B:24:ASN:ND2	0.54	2.40	12	2
1:A:39:LEU:CD2	1:A:112:LEU:CD2	0.54	2.86	11	1
2:B:19:LYS:O	2:B:20:ARG:CB	0.54	2.54	14	2
1:A:95:ASP:OD1	1:A:96:GLY:N	0.54	2.41	2	15
1:A:68:PHE:HZ	2:B:11:ILE:HG23	0.54	1.63	28	3
1:A:85:ILE:HD11	1:A:146:THR:HG21	0.54	1.80	16	1
1:A:44:THR:CG2	1:A:47:GLU:CG	0.54	2.86	20	1
1:A:36:MET:CE	1:A:51:MET:CE	0.53	2.86	22	3
1:A:56:ASP:OD2	1:A:60:ASN:N	0.53	2.42	29	1
1:A:20:ASP:OD2	1:A:25:GLY:N	0.53	2.41	4	1
2:B:24:ASN:N	2:B:25:PRO:HD2	0.53	2.17	13	2
2:B:17:LEU:CD2	2:B:17:LEU:C	0.53	2.77	27	2
1:A:52:ILE:CG2	1:A:53:ASN:N	0.53	2.71	25	4
1:A:133:ASP:OD1	1:A:133:ASP:N	0.53	2.40	22	8
1:A:28:THR:CG2	1:A:62:THR:CG2	0.53	2.85	11	1
1:A:116:LEU:CD2	2:B:19:LYS:HA	0.53	2.33	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ASP:N	1:A:22:ASP:OD1	0.53	2.41	10	6
2:B:5:PRO:CB	2:B:9:THR:HG21	0.53	2.34	25	2
1:A:61:GLY:C	1:A:62:THR:HG23	0.53	2.24	25	2
2:B:19:LYS:CD	2:B:20:ARG:N	0.53	2.72	16	3
2:B:20:ARG:O	2:B:20:ARG:CG	0.53	2.57	10	3
1:A:60:ASN:ND2	1:A:62:THR:OG1	0.53	2.42	27	6
2:B:9:THR:O	2:B:12:LEU:N	0.53	2.41	19	3
2:B:5:PRO:O	2:B:7:TRP:N	0.53	2.42	17	1
1:A:44:THR:HG23	1:A:45:GLU:N	0.53	2.18	25	2
2:B:19:LYS:CG	2:B:19:LYS:O	0.53	2.55	10	1
1:A:25:GLY:O	1:A:26:THR:CG2	0.53	2.57	3	14
2:B:7:TRP:O	2:B:9:THR:N	0.53	2.42	25	9
1:A:8:GLN:O	1:A:11:GLU:CG	0.53	2.57	2	1
1:A:123:GLU:O	1:A:127:GLU:CG	0.53	2.57	4	2
1:A:89:PHE:C	1:A:89:PHE:CD1	0.53	2.82	3	6
1:A:109:MET:CE	1:A:121:VAL:HG22	0.53	2.33	4	1
1:A:95:ASP:OD1	1:A:95:ASP:N	0.53	2.42	22	6
1:A:61:GLY:O	1:A:62:THR:CG2	0.53	2.56	27	4
1:A:25:GLY:C	1:A:26:THR:HG23	0.53	2.24	12	12
1:A:97:ASN:OD1	1:A:98:GLY:N	0.53	2.42	12	14
1:A:105:LEU:HD11	2:B:22:PHE:CE2	0.53	2.39	5	2
1:A:40:GLY:O	1:A:41:GLN:CG	0.53	2.57	18	2
1:A:55:VAL:O	1:A:56:ASP:C	0.53	2.47	16	2
1:A:68:PHE:HZ	2:B:11:ILE:HD12	0.53	1.64	16	2
2:B:4:ILE:CG2	2:B:5:PRO:HD2	0.52	2.32	9	13
1:A:12:PHE:CB	1:A:69:LEU:CD2	0.52	2.88	22	1
1:A:133:ASP:OD1	1:A:134:GLY:N	0.52	2.43	24	8
1:A:105:LEU:O	1:A:109:MET:CG	0.52	2.57	7	2
1:A:131:ASP:OD1	1:A:132:GLY:N	0.52	2.42	10	13
1:A:24:ASP:OD1	1:A:25:GLY:N	0.52	2.42	10	11
1:A:16:PHE:CD1	1:A:16:PHE:O	0.52	2.62	15	1
2:B:16:MET:CG	2:B:22:PHE:O	0.52	2.57	26	1
1:A:8:GLN:O	1:A:12:PHE:CD2	0.52	2.63	2	2
1:A:58:ASP:OD1	1:A:59:GLY:N	0.52	2.43	23	13
2:B:19:LYS:O	2:B:19:LYS:HD3	0.52	2.05	9	2
1:A:60:ASN:N	1:A:60:ASN:OD1	0.52	2.42	25	4
1:A:93:ASP:O	1:A:96:GLY:N	0.52	2.43	11	9
2:B:8:THR:O	2:B:12:LEU:N	0.52	2.42	10	1
2:B:5:PRO:CB	2:B:9:THR:CG2	0.52	2.88	12	2
2:B:12:LEU:HB3	2:B:26:PHE:CE2	0.52	2.40	16	2
1:A:109:MET:SD	1:A:116:LEU:N	0.52	2.83	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ASN:OD1	1:A:62:THR:N	0.52	2.43	4	1
1:A:85:ILE:HD13	1:A:146:THR:HG21	0.52	1.81	4	1
1:A:22:ASP:OD1	1:A:23:GLY:N	0.52	2.42	5	6
2:B:17:LEU:HD22	2:B:17:LEU:C	0.52	2.24	11	1
1:A:72:MET:HE1	2:B:11:ILE:HB	0.52	1.81	20	1
1:A:24:ASP:OD1	1:A:24:ASP:N	0.52	2.43	15	19
2:B:19:LYS:O	2:B:21:SER:N	0.52	2.42	4	2
1:A:117:THR:O	1:A:121:VAL:CG2	0.52	2.57	5	7
1:A:21:LYS:N	1:A:31:GLU:OE2	0.52	2.43	7	1
1:A:109:MET:SD	2:B:17:LEU:CD2	0.52	2.98	9	1
1:A:133:ASP:OD1	1:A:135:GLN:N	0.52	2.43	3	5
1:A:51:MET:O	2:B:7:TRP:NE1	0.52	2.43	15	6
2:B:12:LEU:HD13	2:B:26:PHE:CE2	0.52	2.40	4	1
1:A:65:PHE:O	1:A:69:LEU:CD1	0.52	2.57	21	2
1:A:95:ASP:N	1:A:95:ASP:OD1	0.52	2.42	25	5
1:A:47:GLU:N	1:A:47:GLU:OE1	0.52	2.43	7	1
1:A:57:ALA:N	1:A:67:GLU:OE2	0.52	2.43	21	2
1:A:36:MET:SD	2:B:4:ILE:CG2	0.52	2.98	16	1
1:A:141:PHE:CE1	2:B:16:MET:HE2	0.52	2.40	17	1
1:A:44:THR:HG22	1:A:47:GLU:CG	0.52	2.35	20	1
1:A:133:ASP:N	1:A:133:ASP:OD1	0.52	2.43	7	3
1:A:12:PHE:CD2	1:A:68:PHE:CE2	0.52	2.98	8	1
1:A:87:GLU:N	1:A:87:GLU:OE1	0.52	2.42	23	1
1:A:11:GLU:OE2	1:A:12:PHE:CD1	0.52	2.63	25	1
1:A:53:ASN:O	1:A:56:ASP:N	0.52	2.43	3	1
1:A:144:MET:O	2:B:24:ASN:ND2	0.52	2.43	16	4
1:A:134:GLY:O	1:A:135:GLN:CG	0.52	2.58	21	3
2:B:5:PRO:HB3	2:B:9:THR:CG2	0.52	2.35	25	3
1:A:98:GLY:C	1:A:99:TYR:CD2	0.51	2.84	8	3
2:B:16:MET:O	2:B:19:LYS:CG	0.51	2.58	8	1
1:A:133:ASP:OD2	1:A:135:GLN:NE2	0.51	2.42	9	1
1:A:109:MET:HB3	2:B:17:LEU:CD2	0.51	2.33	11	1
1:A:93:ASP:OD1	1:A:96:GLY:N	0.51	2.42	19	1
1:A:112:LEU:CD1	2:B:13:VAL:HG13	0.51	2.35	20	1
2:B:6:SER:OG	2:B:7:TRP:N	0.51	2.44	5	1
1:A:36:MET:CE	1:A:51:MET:SD	0.51	2.98	16	3
1:A:124:MET:CG	2:B:22:PHE:CD2	0.51	2.94	6	2
2:B:19:LYS:CD	2:B:21:SER:O	0.51	2.58	8	1
1:A:109:MET:HE1	1:A:116:LEU:HB2	0.51	1.81	13	2
1:A:100:ILE:HG22	1:A:100:ILE:O	0.51	2.04	21	1
1:A:127:GLU:OE2	2:B:20:ARG:CZ	0.51	2.59	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:O	1:A:21:LYS:N	0.51	2.43	28	5
2:B:20:ARG:CD	2:B:20:ARG:O	0.51	2.58	7	2
1:A:41:GLN:OE1	1:A:42:ASN:N	0.51	2.44	2	1
1:A:72:MET:HE1	2:B:26:PHE:CE1	0.51	2.39	4	2
1:A:11:GLU:OE2	2:B:18:ARG:CD	0.51	2.59	10	1
1:A:19:PHE:CD1	1:A:32:LEU:CD1	0.51	2.94	23	1
1:A:99:TYR:HB3	1:A:135:GLN:NE2	0.51	2.20	27	1
1:A:131:ASP:N	1:A:131:ASP:OD1	0.51	2.44	8	5
1:A:58:ASP:OD1	1:A:58:ASP:N	0.51	2.42	23	4
1:A:71:MET:O	1:A:73:ALA:N	0.51	2.44	6	2
1:A:97:ASN:N	1:A:97:ASN:OD1	0.51	2.43	7	3
1:A:84:GLU:OE2	2:B:12:LEU:HD23	0.51	2.05	12	1
1:A:32:LEU:HD22	2:B:7:TRP:CZ2	0.51	2.40	22	3
1:A:51:MET:SD	2:B:4:ILE:HG21	0.51	2.45	10	1
2:B:18:ARG:CG	2:B:19:LYS:CD	0.51	2.88	26	1
1:A:38:SER:O	1:A:111:ASN:ND2	0.51	2.44	2	4
1:A:109:MET:HE1	1:A:121:VAL:HG22	0.51	1.83	4	1
1:A:72:MET:SD	2:B:11:ILE:CG2	0.51	2.98	14	3
2:B:24:ASN:OD1	2:B:24:ASN:N	0.51	2.44	9	1
1:A:58:ASP:N	1:A:58:ASP:OD1	0.51	2.43	12	2
1:A:87:GLU:HB3	2:B:9:THR:CG2	0.50	2.34	5	11
1:A:117:THR:HG22	1:A:118:ASP:H	0.50	1.66	2	3
1:A:39:LEU:HD23	1:A:112:LEU:CD2	0.50	2.36	11	1
1:A:124:MET:HG2	2:B:22:PHE:CD1	0.50	2.41	11	1
1:A:51:MET:HE3	2:B:6:SER:O	0.50	2.06	23	1
1:A:32:LEU:HD22	2:B:7:TRP:CH2	0.50	2.41	28	1
1:A:89:PHE:HB2	1:A:141:PHE:CE2	0.50	2.41	5	3
1:A:92:PHE:HB3	1:A:100:ILE:CD1	0.50	2.36	5	9
1:A:109:MET:CG	1:A:110:THR:N	0.50	2.74	28	4
1:A:129:ASP:OD2	1:A:134:GLY:N	0.50	2.44	7	1
2:B:18:ARG:C	2:B:19:LYS:CD	0.50	2.79	2	2
1:A:8:GLN:HG3	1:A:9:ILE:N	0.50	2.20	16	1
1:A:40:GLY:O	1:A:41:GLN:NE2	0.50	2.44	19	1
1:A:109:MET:O	1:A:112:LEU:N	0.50	2.44	20	1
2:B:13:VAL:CG1	2:B:14:LYS:N	0.50	2.73	20	1
2:B:18:ARG:HG3	2:B:19:LYS:CD	0.50	2.36	23	1
1:A:44:THR:HG23	1:A:46:ALA:H	0.50	1.67	25	1
1:A:45:GLU:OE1	1:A:46:ALA:N	0.50	2.44	30	1
1:A:116:LEU:CG	1:A:120:GLU:OE2	0.50	2.59	3	1
1:A:39:LEU:HD23	1:A:108:VAL:HG23	0.50	1.82	4	1
1:A:55:VAL:CG2	2:B:7:TRP:NE1	0.50	2.75	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:MET:HE3	2:B:7:TRP:CD1	0.50	2.41	2	3
1:A:116:LEU:HD12	1:A:116:LEU:H	0.50	1.67	3	4
2:B:16:MET:SD	2:B:22:PHE:CE1	0.50	3.04	3	1
2:B:10:VAL:HG23	2:B:11:ILE:CD1	0.50	2.36	25	2
1:A:42:ASN:N	1:A:43:PRO:HD3	0.50	2.22	19	3
2:B:16:MET:O	2:B:21:SER:O	0.50	2.30	9	2
1:A:58:ASP:OD1	1:A:60:ASN:N	0.50	2.45	27	1
1:A:89:PHE:CE2	1:A:138:TYR:HA	0.50	2.42	17	4
1:A:108:VAL:HG11	2:B:13:VAL:CG1	0.50	2.37	18	1
1:A:12:PHE:CD2	1:A:69:LEU:HD23	0.50	2.41	22	1
1:A:51:MET:CE	2:B:6:SER:O	0.50	2.60	23	2
1:A:19:PHE:CE2	2:B:11:ILE:CD1	0.50	2.95	16	4
1:A:99:TYR:CE1	1:A:137:ASN:OD1	0.50	2.64	16	3
1:A:109:MET:CA	2:B:17:LEU:HD21	0.50	2.36	8	2
2:B:13:VAL:HG12	2:B:14:LYS:N	0.50	2.22	20	1
2:B:19:LYS:CD	2:B:20:ARG:HB2	0.50	2.37	25	1
1:A:71:MET:HG3	1:A:72:MET:N	0.50	2.20	1	1
1:A:60:ASN:OD1	1:A:60:ASN:N	0.50	2.45	17	11
1:A:101:SER:O	1:A:104:GLU:N	0.50	2.45	16	3
2:B:16:MET:O	2:B:18:ARG:N	0.50	2.43	16	6
2:B:24:ASN:CB	2:B:25:PRO:CD	0.50	2.89	16	1
2:B:12:LEU:HA	2:B:26:PHE:CZ	0.50	2.42	18	1
1:A:71:MET:CG	1:A:72:MET:N	0.49	2.74	1	1
1:A:22:ASP:OD1	1:A:22:ASP:N	0.49	2.43	17	6
1:A:41:GLN:OE1	1:A:41:GLN:CA	0.49	2.58	2	1
1:A:64:ASP:N	1:A:67:GLU:OE1	0.49	2.45	4	1
1:A:40:GLY:O	1:A:41:GLN:CB	0.49	2.60	27	1
2:B:11:ILE:N	2:B:11:ILE:HD12	0.49	2.22	27	1
2:B:19:LYS:HD2	2:B:20:ARG:N	0.49	2.22	1	3
1:A:124:MET:HG2	2:B:22:PHE:CE2	0.49	2.41	6	2
1:A:115:LYS:O	1:A:116:LEU:O	0.49	2.29	10	15
1:A:142:VAL:O	1:A:144:MET:N	0.49	2.45	4	2
1:A:11:GLU:OE1	1:A:11:GLU:CA	0.49	2.60	11	1
1:A:39:LEU:O	1:A:39:LEU:CD1	0.49	2.60	11	1
1:A:120:GLU:OE2	2:B:20:ARG:NH2	0.49	2.43	26	1
1:A:142:VAL:O	1:A:146:THR:OG1	0.49	2.30	4	1
1:A:64:ASP:N	1:A:64:ASP:OD1	0.49	2.43	18	1
1:A:98:GLY:C	1:A:99:TYR:CD1	0.49	2.86	26	2
1:A:99:TYR:CD2	1:A:137:ASN:OD1	0.49	2.64	26	1
1:A:27:ILE:O	1:A:62:THR:CG2	0.49	2.59	2	1
1:A:72:MET:CE	2:B:26:PHE:CE2	0.49	2.95	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:ASP:OD1	1:A:97:ASN:N	0.49	2.45	12	2
1:A:12:PHE:CE2	1:A:72:MET:HG3	0.49	2.43	16	1
1:A:145:MET:CE	2:B:24:ASN:HB2	0.49	2.36	20	3
1:A:120:GLU:OE2	2:B:20:ARG:NE	0.49	2.45	26	1
1:A:99:TYR:CE1	1:A:137:ASN:HB2	0.49	2.42	7	4
1:A:109:MET:HG3	1:A:110:THR:N	0.49	2.22	11	7
1:A:44:THR:O	1:A:46:ALA:N	0.49	2.43	6	1
1:A:122:ASP:OD1	1:A:122:ASP:C	0.49	2.51	9	1
1:A:97:ASN:OD1	1:A:99:TYR:N	0.49	2.44	20	3
1:A:56:ASP:OD1	1:A:59:GLY:N	0.49	2.45	25	1
2:B:19:LYS:O	2:B:20:ARG:HG2	0.49	2.08	4	1
1:A:109:MET:CE	1:A:116:LEU:HB2	0.49	2.38	7	3
1:A:124:MET:CG	2:B:21:SER:HA	0.49	2.37	16	1
1:A:131:ASP:OD1	1:A:131:ASP:N	0.49	2.43	25	7
1:A:146:THR:O	1:A:146:THR:CG2	0.49	2.61	6	5
1:A:12:PHE:CG	1:A:69:LEU:HD23	0.49	2.43	22	1
1:A:56:ASP:OD2	1:A:59:GLY:CA	0.49	2.60	29	1
1:A:87:GLU:OE1	2:B:9:THR:OG1	0.49	2.31	6	2
2:B:4:ILE:CG1	2:B:5:PRO:HD2	0.49	2.37	8	1
1:A:92:PHE:CZ	1:A:105:LEU:HD21	0.49	2.43	19	1
1:A:112:LEU:HB3	2:B:17:LEU:CD2	0.49	2.37	20	1
2:B:5:PRO:HB2	2:B:9:THR:CB	0.49	2.38	24	1
1:A:44:THR:HG22	1:A:45:GLU:N	0.49	2.22	28	1
1:A:19:PHE:CD1	1:A:32:LEU:HD12	0.49	2.43	1	3
1:A:109:MET:O	1:A:114:GLU:O	0.49	2.31	11	8
2:B:7:TRP:O	2:B:10:VAL:N	0.49	2.45	26	3
1:A:64:ASP:OD1	1:A:67:GLU:N	0.49	2.42	16	1
1:A:136:VAL:HG13	1:A:140:GLU:HB3	0.49	1.83	17	1
1:A:8:GLN:O	1:A:12:PHE:CG	0.49	2.65	19	1
1:A:43:PRO:HB3	2:B:4:ILE:HG21	0.49	1.83	24	1
1:A:142:VAL:O	1:A:145:MET:N	0.48	2.45	15	5
1:A:71:MET:CE	2:B:7:TRP:HB3	0.48	2.38	5	1
1:A:144:MET:SD	2:B:24:ASN:OD1	0.48	2.72	26	1
1:A:133:ASP:OD1	1:A:135:GLN:CG	0.48	2.60	3	1
2:B:17:LEU:N	2:B:17:LEU:HD22	0.48	2.23	3	2
1:A:110:THR:HG23	1:A:115:LYS:HB3	0.48	1.83	4	1
1:A:84:GLU:OE2	2:B:12:LEU:CD2	0.48	2.62	12	1
1:A:92:PHE:CE1	1:A:105:LEU:CD2	0.48	2.96	12	3
1:A:55:VAL:HG13	1:A:71:MET:CB	0.48	2.38	19	2
1:A:116:LEU:O	1:A:117:THR:O	0.48	2.30	3	18
2:B:22:PHE:O	2:B:23:GLY:O	0.48	2.32	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:GLY:C	1:A:26:THR:CG2	0.48	2.81	29	6
1:A:105:LEU:O	1:A:109:MET:N	0.48	2.43	4	1
2:B:6:SER:C	2:B:9:THR:HG1	0.48	2.12	5	1
2:B:5:PRO:O	2:B:6:SER:C	0.48	2.52	10	2
1:A:28:THR:OG1	1:A:31:GLU:CG	0.48	2.61	15	2
2:B:12:LEU:O	2:B:15:SER:OG	0.48	2.32	21	1
1:A:16:PHE:CE1	1:A:65:PHE:HA	0.48	2.43	22	1
1:A:18:LEU:HD13	2:B:14:LYS:HD2	0.48	1.83	30	1
1:A:67:GLU:O	1:A:70:THR:OG1	0.48	2.31	24	3
1:A:57:ALA:N	1:A:67:GLU:OE1	0.48	2.45	6	2
1:A:16:PHE:CD1	1:A:27:ILE:HD11	0.48	2.43	12	1
1:A:12:PHE:CE1	1:A:72:MET:HG3	0.48	2.44	13	1
2:B:21:SER:OG	2:B:22:PHE:N	0.48	2.47	13	1
1:A:29:THR:CG2	1:A:49:GLN:NE2	0.48	2.76	17	1
1:A:84:GLU:OE2	2:B:8:THR:CB	0.48	2.61	19	1
1:A:87:GLU:CB	2:B:9:THR:CG2	0.48	2.91	28	2
1:A:38:SER:OG	1:A:39:LEU:N	0.48	2.46	21	1
1:A:92:PHE:HE1	2:B:13:VAL:HG13	0.48	1.68	21	1
1:A:41:GLN:NE2	2:B:5:PRO:CG	0.48	2.76	26	1
1:A:114:GLU:CG	1:A:115:LYS:N	0.48	2.76	17	4
1:A:109:MET:SD	2:B:17:LEU:HD21	0.48	2.48	9	1
1:A:109:MET:CG	2:B:17:LEU:CD2	0.48	2.92	10	1
1:A:116:LEU:HD21	2:B:20:ARG:H	0.48	1.67	10	1
1:A:97:ASN:OD1	1:A:97:ASN:N	0.48	2.46	17	3
1:A:119:GLU:CG	1:A:120:GLU:N	0.48	2.76	24	2
1:A:65:PHE:CE2	1:A:69:LEU:CD1	0.48	2.93	29	1
1:A:39:LEU:HD23	1:A:108:VAL:CG2	0.48	2.39	4	1
1:A:55:VAL:HG13	1:A:71:MET:SD	0.48	2.49	6	1
1:A:36:MET:HE1	1:A:51:MET:CE	0.48	2.39	7	2
2:B:9:THR:HA	2:B:12:LEU:CD2	0.48	2.38	16	2
1:A:16:PHE:CE2	1:A:65:PHE:HA	0.48	2.43	26	1
1:A:38:SER:O	1:A:111:ASN:OD1	0.48	2.32	27	1
1:A:120:GLU:HG3	1:A:121:VAL:N	0.48	2.23	21	2
1:A:71:MET:HE1	2:B:8:THR:HG23	0.48	1.84	6	1
1:A:71:MET:CE	2:B:8:THR:HG23	0.48	2.39	25	2
1:A:134:GLY:C	1:A:135:GLN:CG	0.48	2.82	29	4
1:A:98:GLY:O	1:A:137:ASN:ND2	0.48	2.46	11	2
1:A:89:PHE:CE2	1:A:138:TYR:CG	0.48	3.02	13	1
1:A:44:THR:HG22	1:A:45:GLU:H	0.48	1.67	30	1
1:A:20:ASP:OD2	1:A:24:ASP:OD1	0.48	2.32	23	4
1:A:109:MET:CG	1:A:115:LYS:HA	0.48	2.38	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:GLY:O	1:A:137:ASN:OD1	0.48	2.31	27	7
1:A:137:ASN:OD1	1:A:137:ASN:N	0.48	2.46	20	4
1:A:55:VAL:HG13	1:A:71:MET:HB2	0.48	1.85	19	2
1:A:115:LYS:O	1:A:116:LEU:C	0.48	2.53	4	24
1:A:44:THR:HG22	1:A:47:GLU:HG3	0.48	1.85	3	2
1:A:75:LYS:HG3	2:B:8:THR:CG2	0.48	2.39	5	3
1:A:39:LEU:HD11	1:A:91:VAL:HG13	0.48	1.86	11	1
2:B:20:ARG:O	2:B:21:SER:C	0.48	2.51	13	1
1:A:91:VAL:CG1	1:A:108:VAL:HG21	0.47	2.37	24	3
2:B:24:ASN:CB	2:B:25:PRO:HD3	0.47	2.38	17	1
2:B:25:PRO:O	2:B:26:PHE:O	0.47	2.32	27	1
2:B:7:TRP:O	2:B:8:THR:C	0.47	2.52	25	17
1:A:92:PHE:CE2	2:B:13:VAL:HG22	0.47	2.44	9	2
1:A:86:ARG:CD	1:A:138:TYR:OH	0.47	2.62	8	1
1:A:105:LEU:HD13	1:A:124:MET:SD	0.47	2.49	14	1
1:A:144:MET:O	2:B:24:ASN:OD1	0.47	2.32	17	4
2:B:6:SER:O	2:B:7:TRP:CB	0.47	2.62	23	2
1:A:16:PHE:CD1	1:A:65:PHE:HA	0.47	2.44	22	1
1:A:55:VAL:HG13	1:A:71:MET:CG	0.47	2.36	23	1
2:B:22:PHE:O	2:B:24:ASN:OD1	0.47	2.33	23	1
1:A:116:LEU:HB3	1:A:121:VAL:HG23	0.47	1.84	3	3
2:B:19:LYS:HD2	2:B:20:ARG:CG	0.47	2.39	7	2
1:A:57:ALA:CB	1:A:67:GLU:HG2	0.47	2.39	5	1
1:A:89:PHE:HB2	1:A:141:PHE:CD2	0.47	2.44	23	3
1:A:11:GLU:CG	1:A:12:PHE:N	0.47	2.77	8	1
1:A:16:PHE:CZ	1:A:63:ILE:HG22	0.47	2.44	11	1
1:A:16:PHE:CE1	1:A:27:ILE:CD1	0.47	2.96	12	1
1:A:33:GLY:HA2	1:A:48:LEU:HD21	0.47	1.86	16	1
1:A:124:MET:CE	2:B:21:SER:O	0.47	2.63	19	2
1:A:114:GLU:HG2	1:A:116:LEU:CD1	0.47	2.40	26	2
1:A:15:ALA:HB1	1:A:68:PHE:CZ	0.47	2.44	22	3
2:B:20:ARG:O	2:B:22:PHE:N	0.47	2.47	24	1
1:A:55:VAL:O	1:A:67:GLU:OE1	0.47	2.33	5	2
1:A:29:THR:O	1:A:48:LEU:HD13	0.47	2.10	9	2
1:A:93:ASP:OD2	1:A:97:ASN:N	0.47	2.47	24	1
2:B:23:GLY:C	2:B:25:PRO:CD	0.47	2.83	24	1
1:A:65:PHE:C	1:A:65:PHE:CD1	0.47	2.88	27	2
1:A:56:ASP:OD2	1:A:61:GLY:N	0.47	2.47	15	2
2:B:5:PRO:CB	2:B:10:VAL:HG13	0.47	2.37	17	1
1:A:71:MET:CE	1:A:72:MET:N	0.47	2.77	18	1
1:A:55:VAL:HG11	1:A:63:ILE:HG23	0.47	1.86	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ASP:O	1:A:23:GLY:N	0.47	2.43	23	1
1:A:44:THR:OG1	1:A:45:GLU:N	0.47	2.47	24	2
1:A:20:ASP:OD1	1:A:23:GLY:N	0.47	2.45	4	1
2:B:19:LYS:O	2:B:20:ARG:HB3	0.47	2.09	6	3
2:B:20:ARG:CZ	2:B:20:ARG:CB	0.47	2.93	16	1
1:A:84:GLU:OE1	2:B:26:PHE:O	0.47	2.32	18	1
1:A:137:ASN:OD1	1:A:140:GLU:CB	0.47	2.63	20	1
1:A:16:PHE:CZ	1:A:65:PHE:CA	0.47	2.97	25	1
1:A:22:ASP:OD2	1:A:24:ASP:OD1	0.47	2.32	21	2
1:A:44:THR:CG2	1:A:47:GLU:HG3	0.47	2.40	3	2
1:A:119:GLU:HG3	1:A:120:GLU:N	0.47	2.24	26	3
1:A:85:ILE:HD11	1:A:146:THR:CG2	0.47	2.40	4	2
1:A:93:ASP:O	1:A:95:ASP:N	0.47	2.48	16	4
2:B:6:SER:O	2:B:9:THR:HB	0.47	2.10	29	2
2:B:19:LYS:HD3	2:B:21:SER:O	0.47	2.10	8	1
1:A:94:LYS:HA	1:A:94:LYS:CE	0.47	2.39	9	2
1:A:92:PHE:CZ	2:B:16:MET:SD	0.47	3.07	16	1
1:A:55:VAL:HG11	1:A:63:ILE:CG2	0.47	2.40	20	1
1:A:116:LEU:HB3	1:A:121:VAL:CG2	0.47	2.39	21	1
1:A:15:ALA:CB	1:A:68:PHE:CZ	0.47	2.97	22	3
1:A:44:THR:HG22	1:A:47:GLU:OE2	0.47	2.09	27	1
2:B:18:ARG:O	2:B:19:LYS:HB2	0.47	2.10	4	4
1:A:136:VAL:HG12	1:A:137:ASN:N	0.47	2.25	8	4
1:A:44:THR:O	1:A:45:GLU:CB	0.47	2.63	6	1
2:B:12:LEU:C	2:B:12:LEU:HD23	0.47	2.30	15	1
2:B:18:ARG:HG2	2:B:19:LYS:N	0.47	2.24	17	1
1:A:92:PHE:CE2	2:B:16:MET:SD	0.47	3.07	20	1
1:A:142:VAL:O	1:A:146:THR:HG23	0.47	2.09	3	1
2:B:24:ASN:O	2:B:24:ASN:ND2	0.47	2.47	10	1
1:A:139:GLU:O	1:A:143:GLN:CB	0.47	2.63	14	2
1:A:36:MET:HA	1:A:39:LEU:HD12	0.47	1.87	22	2
2:B:19:LYS:CD	2:B:19:LYS:N	0.47	2.78	2	3
1:A:144:MET:O	2:B:23:GLY:O	0.47	2.33	6	1
1:A:124:MET:HE2	2:B:21:SER:O	0.47	2.10	8	1
1:A:93:ASP:O	1:A:94:LYS:C	0.46	2.54	28	23
1:A:24:ASP:OD2	1:A:26:THR:OG1	0.46	2.33	14	11
2:B:6:SER:O	2:B:7:TRP:C	0.46	2.53	7	3
2:B:19:LYS:O	2:B:19:LYS:HG3	0.46	2.10	10	1
1:A:58:ASP:OD2	1:A:67:GLU:OE2	0.46	2.34	11	2
1:A:99:TYR:CE1	1:A:135:GLN:HG3	0.46	2.45	16	1
1:A:137:ASN:OD1	1:A:140:GLU:OE2	0.46	2.33	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:ASP:OD1	1:A:67:GLU:OE2	0.46	2.32	28	1
1:A:92:PHE:HE2	1:A:105:LEU:HD21	0.46	1.63	28	1
1:A:53:ASN:O	1:A:54:GLU:C	0.46	2.54	25	4
2:B:14:LYS:O	2:B:17:LEU:HD22	0.46	2.10	3	2
1:A:145:MET:CG	2:B:24:ASN:O	0.46	2.63	4	1
1:A:109:MET:SD	1:A:115:LYS:CA	0.46	3.03	12	1
1:A:109:MET:SD	1:A:115:LYS:HA	0.46	2.50	12	2
1:A:44:THR:CG2	1:A:47:GLU:HG2	0.46	2.40	20	1
1:A:89:PHE:CE1	1:A:138:TYR:HA	0.46	2.44	21	1
1:A:101:SER:O	1:A:102:ALA:C	0.46	2.53	28	20
1:A:22:ASP:OD2	1:A:31:GLU:OE2	0.46	2.33	7	1
1:A:107:HIS:O	1:A:111:ASN:OD1	0.46	2.33	21	7
2:B:18:ARG:O	2:B:18:ARG:CG	0.46	2.62	8	1
1:A:15:ALA:O	1:A:18:LEU:N	0.46	2.48	13	1
1:A:14:GLU:O	1:A:17:SER:OG	0.46	2.34	20	1
1:A:135:GLN:CD	1:A:135:GLN:N	0.46	2.69	26	1
1:A:16:PHE:CE1	1:A:64:ASP:O	0.46	2.68	7	5
1:A:144:MET:O	2:B:24:ASN:N	0.46	2.47	2	1
2:B:16:MET:O	2:B:19:LYS:HG3	0.46	2.10	8	1
1:A:71:MET:HE2	1:A:72:MET:N	0.46	2.26	18	1
1:A:125:ILE:O	1:A:129:ASP:N	0.46	2.44	28	1
1:A:84:GLU:HG3	1:A:85:ILE:N	0.46	2.26	3	1
1:A:131:ASP:OD2	1:A:133:ASP:OD2	0.46	2.33	28	3
1:A:92:PHE:O	1:A:104:GLU:OE1	0.46	2.34	5	3
1:A:55:VAL:HB	1:A:63:ILE:CD1	0.46	2.41	24	2
1:A:36:MET:CB	1:A:43:PRO:HG3	0.46	2.41	25	2
1:A:16:PHE:CZ	1:A:65:PHE:HA	0.46	2.45	10	2
2:B:24:ASN:OD1	2:B:26:PHE:OXT	0.46	2.34	14	1
1:A:89:PHE:CZ	1:A:138:TYR:HB2	0.46	2.46	21	1
1:A:28:THR:OG1	1:A:31:GLU:OE1	0.46	2.34	9	1
1:A:65:PHE:CD1	1:A:65:PHE:O	0.46	2.69	19	2
2:B:14:LYS:CD	2:B:14:LYS:O	0.46	2.64	17	1
2:B:6:SER:O	2:B:9:THR:CB	0.46	2.64	29	1
1:A:51:MET:SD	2:B:7:TRP:N	0.46	2.89	3	1
1:A:133:ASP:OD1	1:A:135:GLN:HG2	0.46	2.11	3	1
1:A:145:MET:HE1	2:B:24:ASN:HB3	0.46	1.86	7	1
1:A:139:GLU:CG	1:A:140:GLU:N	0.46	2.79	8	1
1:A:119:GLU:O	1:A:122:ASP:OD1	0.46	2.34	9	1
1:A:12:PHE:CZ	1:A:72:MET:HG3	0.46	2.46	16	1
2:B:12:LEU:HB3	2:B:26:PHE:CZ	0.46	2.45	16	1
1:A:20:ASP:OD1	1:A:24:ASP:OD1	0.46	2.34	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:PHE:CE1	1:A:105:LEU:HD21	0.46	2.46	24	1
1:A:129:ASP:O	1:A:132:GLY:N	0.46	2.48	25	1
1:A:93:ASP:OD1	1:A:95:ASP:OD1	0.46	2.34	30	1
1:A:27:ILE:CD1	1:A:63:ILE:HB	0.46	2.41	1	7
1:A:83:GLU:O	1:A:87:GLU:OE1	0.46	2.34	1	2
1:A:123:GLU:O	1:A:127:GLU:CB	0.46	2.64	16	2
1:A:83:GLU:OE1	1:A:87:GLU:OE1	0.46	2.34	19	1
1:A:36:MET:O	1:A:41:GLN:O	0.46	2.34	24	1
1:A:56:ASP:OD1	1:A:60:ASN:N	0.46	2.49	25	1
1:A:82:GLU:HG3	1:A:83:GLU:N	0.46	2.25	30	1
1:A:145:MET:HG3	2:B:24:ASN:O	0.46	2.11	4	1
1:A:129:ASP:OD2	1:A:135:GLN:N	0.46	2.49	13	1
1:A:37:ARG:NE	1:A:41:GLN:O	0.46	2.49	15	1
1:A:27:ILE:HB	1:A:63:ILE:CG1	0.46	2.41	24	2
2:B:23:GLY:C	2:B:25:PRO:HD3	0.46	2.31	24	1
1:A:142:VAL:O	1:A:146:THR:CG2	0.46	2.60	30	1
1:A:32:LEU:HD23	1:A:48:LEU:HD21	0.46	1.86	5	1
1:A:72:MET:HG2	2:B:11:ILE:HD12	0.46	1.87	6	1
1:A:42:ASN:O	1:A:42:ASN:OD1	0.46	2.33	28	2
1:A:75:LYS:HB2	2:B:8:THR:HG21	0.46	1.87	8	2
1:A:109:MET:HG2	2:B:17:LEU:CD2	0.46	2.41	10	1
1:A:27:ILE:CG1	1:A:63:ILE:HB	0.45	2.41	18	12
2:B:8:THR:O	2:B:11:ILE:N	0.45	2.49	14	2
1:A:55:VAL:O	1:A:67:GLU:HG2	0.45	2.11	25	2
1:A:11:GLU:HG2	1:A:12:PHE:N	0.45	2.26	19	1
2:B:21:SER:O	2:B:22:PHE:CB	0.45	2.64	22	1
2:B:21:SER:O	2:B:22:PHE:CG	0.45	2.69	22	1
1:A:105:LEU:N	1:A:105:LEU:CD2	0.45	2.79	30	1
1:A:83:GLU:O	1:A:87:GLU:OE2	0.45	2.34	23	2
1:A:32:LEU:HD22	1:A:52:ILE:HD11	0.45	1.89	8	1
1:A:50:ASP:O	1:A:54:GLU:OE1	0.45	2.34	17	1
1:A:14:GLU:HA	1:A:17:SER:OG	0.45	2.11	20	1
1:A:12:PHE:CE1	1:A:72:MET:HG2	0.45	2.45	21	1
1:A:41:GLN:NE2	2:B:5:PRO:HG3	0.45	2.27	26	1
1:A:24:ASP:OD1	1:A:26:THR:N	0.45	2.50	1	2
1:A:11:GLU:HG3	1:A:12:PHE:N	0.45	2.26	2	2
1:A:28:THR:HA	1:A:62:THR:HG22	0.45	1.87	2	1
1:A:137:ASN:N	1:A:140:GLU:OE1	0.45	2.49	6	1
1:A:109:MET:HA	2:B:17:LEU:CD2	0.45	2.42	12	6
1:A:109:MET:HG2	1:A:114:GLU:O	0.45	2.12	19	2
1:A:11:GLU:OE1	1:A:12:PHE:CD1	0.45	2.69	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:5:PRO:HB2	2:B:10:VAL:HG23	0.45	1.89	20	1
1:A:19:PHE:N	1:A:19:PHE:CD1	0.45	2.84	2	1
1:A:101:SER:O	1:A:103:ALA:N	0.45	2.49	27	8
2:B:17:LEU:H	2:B:17:LEU:HD22	0.45	1.71	3	1
1:A:51:MET:CE	2:B:7:TRP:CG	0.45	2.99	4	1
1:A:134:GLY:O	1:A:135:GLN:HG2	0.45	2.12	30	2
1:A:93:ASP:OD1	1:A:99:TYR:O	0.45	2.33	12	1
1:A:109:MET:SD	1:A:115:LYS:O	0.45	2.74	12	3
1:A:69:LEU:N	1:A:69:LEU:CD2	0.45	2.80	13	2
1:A:30:LYS:HG3	1:A:31:GLU:N	0.45	2.27	22	2
1:A:137:ASN:OD1	1:A:140:GLU:HB2	0.45	2.11	20	1
1:A:12:PHE:CB	1:A:69:LEU:HD23	0.45	2.41	22	1
1:A:84:GLU:HG2	1:A:85:ILE:N	0.45	2.27	27	1
2:B:11:ILE:HD12	2:B:11:ILE:H	0.45	1.70	27	1
1:A:129:ASP:OD1	1:A:133:ASP:N	0.45	2.46	30	1
2:B:6:SER:O	2:B:9:THR:N	0.45	2.46	7	1
2:B:20:ARG:O	2:B:21:SER:OG	0.45	2.34	16	1
1:A:109:MET:CG	2:B:17:LEU:HG	0.45	2.40	17	1
1:A:65:PHE:O	1:A:69:LEU:HD13	0.45	2.12	21	1
1:A:68:PHE:CZ	2:B:11:ILE:CD1	0.45	2.99	2	1
1:A:115:LYS:O	1:A:115:LYS:CG	0.45	2.64	20	3
1:A:128:ALA:HB3	1:A:136:VAL:HG22	0.45	1.88	13	1
1:A:92:PHE:CZ	2:B:13:VAL:HG22	0.45	2.47	14	2
2:B:23:GLY:O	2:B:24:ASN:OD1	0.45	2.34	15	1
1:A:88:ALA:HB2	2:B:12:LEU:HD12	0.45	1.85	20	1
1:A:141:PHE:O	1:A:145:MET:SD	0.45	2.74	21	1
1:A:126:ARG:O	1:A:127:GLU:C	0.45	2.55	13	5
1:A:60:ASN:CG	1:A:61:GLY:N	0.45	2.70	10	3
1:A:95:ASP:OD2	1:A:97:ASN:OD1	0.45	2.34	19	1
1:A:16:PHE:CE1	1:A:65:PHE:CA	0.45	3.00	22	1
1:A:36:MET:HB3	1:A:43:PRO:CD	0.45	2.42	25	1
1:A:129:ASP:OD2	1:A:133:ASP:N	0.45	2.43	29	3
2:B:19:LYS:O	2:B:20:ARG:CG	0.45	2.65	4	1
1:A:119:GLU:HA	1:A:122:ASP:OD2	0.45	2.12	9	1
1:A:105:LEU:HD13	1:A:125:ILE:CD1	0.45	2.41	24	1
2:B:16:MET:HG3	2:B:22:PHE:O	0.45	2.11	26	1
2:B:14:LYS:O	2:B:14:LYS:HE3	0.45	2.12	30	1
1:A:143:GLN:HG3	1:A:144:MET:N	0.45	2.27	4	1
1:A:100:ILE:N	1:A:136:VAL:O	0.45	2.44	7	2
1:A:124:MET:SD	2:B:21:SER:O	0.45	2.75	11	1
1:A:41:GLN:NE2	2:B:4:ILE:HA	0.45	2.27	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:ILE:O	1:A:86:ARG:C	0.45	2.56	26	1
2:B:15:SER:O	2:B:24:ASN:ND2	0.45	2.45	27	1
1:A:72:MET:HE2	2:B:26:PHE:HZ	0.45	1.72	29	1
2:B:24:ASN:O	2:B:24:ASN:OD1	0.45	2.34	2	1
1:A:56:ASP:O	1:A:57:ALA:C	0.45	2.54	27	6
1:A:95:ASP:OD1	1:A:95:ASP:C	0.45	2.56	3	1
1:A:115:LYS:O	1:A:115:LYS:HG3	0.45	2.12	4	2
1:A:92:PHE:O	1:A:94:LYS:N	0.45	2.46	5	1
1:A:138:TYR:O	1:A:139:GLU:C	0.45	2.55	19	14
1:A:71:MET:O	1:A:72:MET:C	0.45	2.54	6	3
1:A:145:MET:HE1	2:B:24:ASN:CB	0.45	2.42	7	1
2:B:18:ARG:O	2:B:19:LYS:HB3	0.45	2.11	24	2
1:A:108:VAL:HG13	1:A:112:LEU:HD12	0.45	1.87	14	1
1:A:36:MET:SD	1:A:41:GLN:OE1	0.45	2.75	15	1
1:A:94:LYS:HG3	1:A:95:ASP:N	0.45	2.26	19	3
2:B:15:SER:O	2:B:18:ARG:CG	0.45	2.64	16	1
1:A:116:LEU:HD13	2:B:17:LEU:HB2	0.45	1.89	17	1
1:A:136:VAL:CG1	1:A:140:GLU:HB3	0.45	2.43	17	1
2:B:13:VAL:O	2:B:16:MET:HB2	0.45	2.12	27	2
1:A:82:GLU:CG	1:A:83:GLU:N	0.45	2.80	30	1
1:A:8:GLN:O	1:A:11:GLU:HG2	0.44	2.11	2	1
1:A:58:ASP:CG	1:A:59:GLY:N	0.44	2.70	22	2
1:A:56:ASP:OD1	1:A:59:GLY:CA	0.44	2.65	25	1
2:B:12:LEU:CD2	2:B:26:PHE:CE2	0.44	3.00	27	1
1:A:39:LEU:O	1:A:94:LYS:NZ	0.44	2.43	1	1
1:A:142:VAL:O	1:A:143:GLN:C	0.44	2.56	22	5
1:A:84:GLU:CG	1:A:85:ILE:N	0.44	2.81	3	1
1:A:140:GLU:O	1:A:142:VAL:N	0.44	2.50	23	5
1:A:94:LYS:HE3	1:A:107:HIS:CD2	0.44	2.47	23	1
1:A:114:GLU:OE2	2:B:18:ARG:O	0.44	2.35	28	1
1:A:85:ILE:CG2	1:A:141:PHE:CE1	0.44	2.99	30	1
1:A:114:GLU:HG3	1:A:115:LYS:N	0.44	2.27	19	6
1:A:40:GLY:O	1:A:41:GLN:HG2	0.44	2.11	23	2
1:A:33:GLY:HA2	1:A:43:PRO:CG	0.44	2.42	10	1
1:A:144:MET:SD	2:B:23:GLY:CA	0.44	3.05	21	1
1:A:116:LEU:HD23	1:A:120:GLU:HB3	0.44	1.89	30	1
1:A:28:THR:OG1	1:A:31:GLU:OE2	0.44	2.35	1	2
2:B:19:LYS:C	2:B:19:LYS:HD3	0.44	2.33	11	5
1:A:100:ILE:O	1:A:135:GLN:HB2	0.44	2.12	3	2
2:B:13:VAL:O	2:B:16:MET:HB3	0.44	2.13	3	2
1:A:24:ASP:CG	1:A:26:THR:OG1	0.44	2.56	10	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:LEU:CD2	1:A:69:LEU:N	0.44	2.80	15	1
1:A:116:LEU:HD21	2:B:19:LYS:N	0.44	2.28	15	1
1:A:124:MET:HG3	2:B:21:SER:HA	0.44	1.90	16	1
1:A:93:ASP:HA	1:A:104:GLU:OE2	0.44	2.13	17	1
2:B:12:LEU:HG	2:B:26:PHE:CD2	0.44	2.48	18	1
1:A:117:THR:N	1:A:120:GLU:OE2	0.44	2.44	21	1
2:B:12:LEU:O	2:B:16:MET:SD	0.44	2.76	26	1
1:A:89:PHE:O	1:A:90:ARG:C	0.44	2.56	17	4
1:A:41:GLN:OE1	1:A:41:GLN:HA	0.44	2.12	2	1
1:A:58:ASP:OD2	1:A:60:ASN:CG	0.44	2.56	15	6
1:A:26:THR:HA	1:A:63:ILE:O	0.44	2.12	12	15
1:A:84:GLU:HG2	2:B:12:LEU:CD2	0.44	2.43	5	1
1:A:105:LEU:O	1:A:109:MET:HG3	0.44	2.13	30	3
1:A:109:MET:HG3	2:B:17:LEU:HD21	0.44	1.89	24	2
1:A:16:PHE:CE1	1:A:68:PHE:HB2	0.44	2.48	11	1
1:A:124:MET:HE1	2:B:17:LEU:HA	0.44	1.89	11	1
1:A:85:ILE:CG2	1:A:141:PHE:CD1	0.44	3.00	30	2
1:A:11:GLU:HG2	1:A:12:PHE:CD1	0.44	2.47	19	2
1:A:15:ALA:O	1:A:19:PHE:CD2	0.44	2.70	24	2
1:A:44:THR:HG22	1:A:47:GLU:HG2	0.44	1.87	25	1
1:A:61:GLY:C	1:A:62:THR:CG2	0.44	2.86	25	1
1:A:92:PHE:HA	1:A:108:VAL:HG21	0.44	1.88	28	1
2:B:24:ASN:O	2:B:24:ASN:CG	0.44	2.56	28	2
1:A:60:ASN:OD1	1:A:60:ASN:C	0.44	2.56	4	1
1:A:75:LYS:HB3	2:B:8:THR:CG2	0.44	2.41	9	2
1:A:137:ASN:OD1	1:A:140:GLU:CG	0.44	2.66	18	3
1:A:71:MET:SD	1:A:72:MET:N	0.44	2.90	16	1
2:B:24:ASN:HB3	2:B:25:PRO:HD3	0.44	1.90	17	1
1:A:100:ILE:HB	1:A:136:VAL:O	0.44	2.12	28	1
1:A:116:LEU:HD23	1:A:120:GLU:OE2	0.44	2.12	3	1
1:A:15:ALA:HB2	2:B:14:LYS:CD	0.44	2.43	11	1
1:A:112:LEU:HD12	2:B:13:VAL:HG12	0.44	1.89	12	2
2:B:14:LYS:CD	2:B:14:LYS:C	0.44	2.86	17	1
1:A:108:VAL:O	1:A:112:LEU:N	0.44	2.51	20	1
1:A:107:HIS:CD2	1:A:107:HIS:N	0.44	2.86	25	1
1:A:93:ASP:HA	1:A:104:GLU:OE1	0.44	2.12	6	2
1:A:95:ASP:OD2	1:A:97:ASN:CG	0.44	2.56	24	4
1:A:145:MET:HA	2:B:24:ASN:ND2	0.44	2.28	9	1
1:A:140:GLU:O	1:A:141:PHE:C	0.44	2.56	19	8
1:A:84:GLU:OE2	2:B:8:THR:HB	0.44	2.13	19	1
1:A:112:LEU:HD13	2:B:17:LEU:CD2	0.44	2.41	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:18:ARG:HD3	2:B:19:LYS:CD	0.44	2.43	2	1
1:A:57:ALA:HA	1:A:74:ARG:NH2	0.44	2.28	3	1
1:A:68:PHE:O	1:A:71:MET:HG3	0.44	2.13	3	1
1:A:55:VAL:HG22	1:A:71:MET:HE2	0.44	1.89	4	1
1:A:92:PHE:CD1	1:A:108:VAL:HG11	0.44	2.48	12	3
1:A:124:MET:HE3	2:B:21:SER:O	0.44	2.12	7	1
2:B:4:ILE:CB	2:B:5:PRO:CD	0.44	2.96	9	1
1:A:45:GLU:O	1:A:46:ALA:C	0.44	2.56	19	6
1:A:58:ASP:CG	1:A:60:ASN:OD1	0.44	2.55	13	3
1:A:118:ASP:O	1:A:122:ASP:OD2	0.44	2.36	11	1
1:A:144:MET:O	2:B:23:GLY:HA3	0.44	2.12	18	1
1:A:125:ILE:N	1:A:125:ILE:CD1	0.44	2.80	19	1
1:A:52:ILE:CG2	1:A:61:GLY:O	0.44	2.65	21	1
1:A:8:GLN:NE2	2:B:26:PHE:OXT	0.44	2.51	24	1
1:A:16:PHE:CE2	1:A:65:PHE:HB2	0.43	2.48	14	1
1:A:55:VAL:CG1	1:A:71:MET:CB	0.43	2.96	19	1
1:A:114:GLU:CG	1:A:116:LEU:HD12	0.43	2.40	19	1
1:A:128:ALA:O	1:A:140:GLU:CD	0.43	2.57	20	1
2:B:8:THR:O	2:B:9:THR:C	0.43	2.57	14	5
2:B:13:VAL:O	2:B:16:MET:HG3	0.43	2.13	5	1
1:A:70:THR:O	1:A:71:MET:C	0.43	2.56	15	2
1:A:14:GLU:C	1:A:17:SER:OG	0.43	2.56	20	1
1:A:36:MET:CE	1:A:51:MET:HE2	0.43	2.42	22	1
1:A:72:MET:HE1	2:B:12:LEU:CD2	0.43	2.43	27	1
1:A:20:ASP:O	1:A:21:LYS:C	0.43	2.57	1	3
1:A:43:PRO:HA	2:B:4:ILE:CD1	0.43	2.42	1	3
1:A:142:VAL:CG1	1:A:146:THR:HG21	0.43	2.30	5	1
1:A:52:ILE:HG13	1:A:63:ILE:HD11	0.43	1.89	12	3
1:A:64:ASP:CB	1:A:66:PRO:HD2	0.43	2.44	18	3
1:A:19:PHE:HD1	1:A:35:VAL:HG21	0.43	1.71	27	1
1:A:22:ASP:OD2	1:A:24:ASP:CG	0.43	2.57	4	7
1:A:87:GLU:HB3	2:B:9:THR:OG1	0.43	2.13	3	1
2:B:24:ASN:OD1	2:B:26:PHE:CD1	0.43	2.71	3	1
1:A:85:ILE:CD1	1:A:146:THR:HB	0.43	2.42	5	1
1:A:139:GLU:O	1:A:142:VAL:N	0.43	2.51	6	3
2:B:12:LEU:O	2:B:16:MET:HB2	0.43	2.14	8	1
1:A:55:VAL:CG2	1:A:71:MET:SD	0.43	3.02	9	2
1:A:65:PHE:CE1	1:A:69:LEU:CD1	0.43	3.01	16	1
1:A:89:PHE:O	1:A:92:PHE:N	0.43	2.51	29	2
1:A:92:PHE:O	1:A:104:GLU:CD	0.43	2.57	18	1
2:B:5:PRO:HB2	2:B:9:THR:HB	0.43	1.89	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:ASP:OD1	1:A:133:ASP:OD1	0.43	2.37	25	1
1:A:143:GLN:O	1:A:143:GLN:CD	0.43	2.57	25	1
1:A:129:ASP:OD2	1:A:133:ASP:CG	0.43	2.57	3	1
1:A:71:MET:HE1	2:B:7:TRP:HB3	0.43	1.91	5	1
1:A:51:MET:HG3	1:A:52:ILE:N	0.43	2.27	11	1
1:A:55:VAL:HG22	1:A:71:MET:CE	0.43	2.43	11	1
1:A:109:MET:HB2	2:B:17:LEU:HD21	0.43	1.90	11	1
1:A:133:ASP:OD2	1:A:135:GLN:O	0.43	2.35	17	1
1:A:9:ILE:O	1:A:10:ALA:C	0.43	2.56	20	4
1:A:43:PRO:O	1:A:44:THR:O	0.43	2.36	19	1
1:A:139:GLU:O	1:A:143:GLN:HB2	0.43	2.13	19	1
1:A:145:MET:HE3	2:B:24:ASN:CB	0.43	2.43	25	2
1:A:38:SER:O	1:A:39:LEU:C	0.43	2.57	23	5
1:A:44:THR:O	1:A:45:GLU:C	0.43	2.57	23	5
2:B:26:PHE:CD1	2:B:26:PHE:N	0.43	2.87	10	1
1:A:38:SER:O	1:A:111:ASN:CG	0.43	2.57	22	2
1:A:41:GLN:NE2	2:B:5:PRO:CD	0.43	2.81	26	1
1:A:92:PHE:CE2	2:B:22:PHE:CE2	0.43	3.06	26	1
2:B:16:MET:SD	2:B:22:PHE:O	0.43	2.77	27	1
1:A:58:ASP:OD2	1:A:67:GLU:CD	0.43	2.57	28	1
1:A:124:MET:HE1	2:B:16:MET:O	0.43	2.13	30	1
1:A:51:MET:SD	2:B:6:SER:C	0.43	2.97	3	1
1:A:123:GLU:O	1:A:127:GLU:HB2	0.43	2.14	16	3
1:A:22:ASP:CG	1:A:23:GLY:N	0.43	2.72	25	2
1:A:72:MET:HG2	2:B:11:ILE:CD1	0.43	2.44	6	1
1:A:51:MET:HG3	2:B:4:ILE:HD12	0.43	1.91	7	1
2:B:16:MET:O	2:B:17:LEU:C	0.43	2.57	10	1
2:B:19:LYS:CG	2:B:20:ARG:N	0.43	2.81	20	2
1:A:127:GLU:OE2	2:B:20:ARG:NE	0.43	2.52	24	1
1:A:134:GLY:O	1:A:135:GLN:HG3	0.43	2.14	1	1
1:A:112:LEU:CD1	2:B:17:LEU:CD2	0.43	2.95	12	1
1:A:28:THR:OG1	1:A:31:GLU:HG3	0.43	2.13	15	1
1:A:29:THR:HG21	1:A:49:GLN:CD	0.43	2.34	17	1
1:A:12:PHE:CZ	1:A:72:MET:HG2	0.43	2.49	21	1
1:A:58:ASP:CG	1:A:67:GLU:OE2	0.43	2.55	23	1
1:A:131:ASP:CG	1:A:133:ASP:OD1	0.43	2.57	25	1
2:B:6:SER:O	2:B:10:VAL:CG2	0.43	2.61	27	1
1:A:120:GLU:OE2	2:B:19:LYS:NZ	0.43	2.51	7	1
1:A:24:ASP:OD1	1:A:26:THR:OG1	0.43	2.37	9	1
2:B:17:LEU:HD13	2:B:17:LEU:C	0.43	2.35	11	1
1:A:87:GLU:OE2	2:B:6:SER:OG	0.43	2.37	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:MET:CE	1:A:51:MET:HE3	0.43	2.44	22	1
1:A:51:MET:SD	2:B:5:PRO:O	0.43	2.77	23	1
1:A:116:LEU:O	1:A:121:VAL:HG23	0.43	2.14	28	1
1:A:58:ASP:OD1	1:A:58:ASP:C	0.43	2.57	30	1
2:B:14:LYS:O	2:B:14:LYS:CE	0.43	2.67	30	1
1:A:30:LYS:O	1:A:31:GLU:C	0.43	2.56	28	5
1:A:95:ASP:OD2	1:A:97:ASN:HB3	0.43	2.13	3	3
2:B:19:LYS:O	2:B:20:ARG:C	0.43	2.57	4	1
2:B:16:MET:HG3	2:B:17:LEU:N	0.43	2.29	5	1
1:A:65:PHE:O	1:A:69:LEU:HD23	0.43	2.14	8	1
2:B:13:VAL:O	2:B:17:LEU:HD12	0.43	2.14	11	1
1:A:110:THR:OG1	1:A:115:LYS:HG2	0.43	2.14	16	1
1:A:52:ILE:O	1:A:56:ASP:HB2	0.43	2.14	29	3
1:A:108:VAL:O	1:A:112:LEU:HB2	0.43	2.14	24	1
1:A:133:ASP:OD2	1:A:135:GLN:CG	0.43	2.67	25	1
1:A:85:ILE:HG23	1:A:141:PHE:HE1	0.43	1.70	30	1
1:A:126:ARG:HD2	1:A:127:GLU:N	0.42	2.29	6	1
1:A:86:ARG:HD2	1:A:138:TYR:OH	0.42	2.13	8	1
1:A:134:GLY:C	1:A:135:GLN:HG3	0.42	2.34	29	4
1:A:112:LEU:HD13	2:B:13:VAL:HG12	0.42	1.91	14	1
2:B:20:ARG:C	2:B:21:SER:OG	0.42	2.57	16	1
1:A:41:GLN:HB3	2:B:4:ILE:CD1	0.42	2.43	21	1
1:A:20:ASP:OD2	1:A:26:THR:N	0.42	2.50	27	1
1:A:125:ILE:O	1:A:129:ASP:OD2	0.42	2.37	28	1
1:A:39:LEU:HA	1:A:111:ASN:OD1	0.42	2.14	1	1
1:A:83:GLU:HG3	1:A:84:GLU:N	0.42	2.29	1	1
1:A:64:ASP:OD1	1:A:65:PHE:N	0.42	2.48	7	1
2:B:5:PRO:O	2:B:9:THR:HB	0.42	2.13	10	1
1:A:126:ARG:O	1:A:129:ASP:N	0.42	2.52	13	1
1:A:144:MET:O	2:B:24:ASN:CG	0.42	2.57	17	2
1:A:40:GLY:O	1:A:41:GLN:CD	0.42	2.57	19	1
2:B:18:ARG:HG3	2:B:19:LYS:HD2	0.42	1.90	26	2
1:A:84:GLU:HA	1:A:87:GLU:OE2	0.42	2.13	24	1
1:A:58:ASP:OD1	1:A:60:ASN:CB	0.42	2.67	27	1
1:A:99:TYR:HB2	1:A:135:GLN:NE2	0.42	2.29	27	1
1:A:130:ILE:CD1	1:A:144:MET:HE1	0.42	2.44	5	1
1:A:105:LEU:C	1:A:109:MET:HG3	0.42	2.35	7	1
1:A:106:ARG:HA	1:A:109:MET:HG2	0.42	1.92	8	2
1:A:138:TYR:O	1:A:140:GLU:N	0.42	2.52	19	2
1:A:16:PHE:CE1	1:A:63:ILE:HG22	0.42	2.50	11	1
2:B:6:SER:O	2:B:7:TRP:HB2	0.42	2.13	23	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:GLU:OE2	2:B:8:THR:OG1	0.42	2.30	19	1
1:A:22:ASP:O	1:A:23:GLY:C	0.42	2.57	22	1
1:A:129:ASP:CG	1:A:133:ASP:OD1	0.42	2.57	25	1
1:A:18:LEU:CD1	2:B:14:LYS:HD3	0.42	2.37	30	1
1:A:137:ASN:OD1	1:A:137:ASN:C	0.42	2.56	4	1
1:A:89:PHE:CD2	1:A:141:PHE:CD2	0.42	3.07	6	1
1:A:120:GLU:O	1:A:121:VAL:C	0.42	2.57	7	2
2:B:20:ARG:C	2:B:20:ARG:HD3	0.42	2.35	10	1
1:A:58:ASP:OD1	1:A:60:ASN:CG	0.42	2.57	13	1
1:A:129:ASP:OD2	1:A:133:ASP:OD1	0.42	2.36	15	1
1:A:145:MET:HE3	2:B:16:MET:HE1	0.42	1.92	9	1
2:B:17:LEU:N	2:B:17:LEU:CD1	0.42	2.83	12	1
2:B:21:SER:O	2:B:22:PHE:HB2	0.42	2.14	13	1
1:A:47:GLU:O	1:A:48:LEU:C	0.42	2.58	16	3
1:A:66:PRO:O	1:A:70:THR:OG1	0.42	2.33	16	1
1:A:120:GLU:O	1:A:124:MET:HB2	0.42	2.15	16	1
1:A:58:ASP:OD2	1:A:60:ASN:N	0.42	2.52	22	1
2:B:17:LEU:O	2:B:18:ARG:HB3	0.42	2.14	25	1
1:A:71:MET:O	1:A:75:LYS:HE3	0.42	2.15	1	1
1:A:118:ASP:O	1:A:119:GLU:C	0.42	2.57	20	4
1:A:100:ILE:O	1:A:135:GLN:CB	0.42	2.68	14	2
1:A:128:ALA:O	1:A:129:ASP:C	0.42	2.58	12	1
1:A:22:ASP:OD1	1:A:24:ASP:CG	0.42	2.57	15	1
1:A:36:MET:SD	2:B:5:PRO:HG2	0.42	2.55	17	1
1:A:63:ILE:HA	1:A:67:GLU:OE1	0.42	2.14	18	1
1:A:12:PHE:HB3	1:A:69:LEU:CD2	0.42	2.44	22	1
1:A:68:PHE:CD1	1:A:68:PHE:C	0.42	2.92	22	1
2:B:11:ILE:O	2:B:12:LEU:C	0.42	2.57	23	3
1:A:139:GLU:O	1:A:140:GLU:C	0.42	2.57	20	4
2:B:19:LYS:C	2:B:19:LYS:CD	0.42	2.88	6	1
1:A:58:ASP:OD2	1:A:60:ASN:OD1	0.42	2.37	10	1
1:A:64:ASP:OD1	1:A:66:PRO:HD2	0.42	2.15	10	2
1:A:92:PHE:O	1:A:104:GLU:HB3	0.42	2.15	18	3
2:B:5:PRO:CG	2:B:10:VAL:HG22	0.42	2.45	20	1
1:A:99:TYR:HA	1:A:136:VAL:O	0.42	2.15	29	1
2:B:7:TRP:C	2:B:9:THR:N	0.42	2.73	25	5
1:A:11:GLU:O	1:A:14:GLU:HB3	0.42	2.14	11	1
1:A:88:ALA:HA	2:B:13:VAL:CG2	0.42	2.45	19	1
1:A:89:PHE:HA	1:A:141:PHE:CE2	0.42	2.49	19	1
1:A:52:ILE:HG23	1:A:61:GLY:O	0.42	2.14	21	1
2:B:19:LYS:CD	2:B:20:ARG:HB3	0.42	2.45	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:GLN:NE2	2:B:26:PHE:O	0.42	2.52	24	1
1:A:108:VAL:CG1	2:B:13:VAL:CG1	0.42	2.98	27	1
1:A:124:MET:HE3	2:B:16:MET:O	0.42	2.15	27	1
1:A:24:ASP:OD1	1:A:24:ASP:C	0.42	2.57	1	1
2:B:5:PRO:HB2	2:B:9:THR:HG21	0.42	1.91	4	1
1:A:16:PHE:CE2	1:A:65:PHE:CA	0.42	3.03	13	1
1:A:133:ASP:OD1	1:A:135:GLN:O	0.42	2.38	28	2
1:A:99:TYR:CD1	1:A:135:GLN:CD	0.42	2.93	14	1
1:A:126:ARG:O	1:A:128:ALA:N	0.42	2.53	16	2
1:A:63:ILE:C	1:A:64:ASP:OD1	0.42	2.57	18	1
1:A:64:ASP:OD2	1:A:67:GLU:OE1	0.42	2.38	19	1
1:A:37:ARG:HA	1:A:41:GLN:O	0.42	2.15	24	1
1:A:22:ASP:OD2	1:A:24:ASP:CB	0.42	2.68	25	1
1:A:42:ASN:O	1:A:42:ASN:CG	0.42	2.59	29	1
1:A:95:ASP:OD2	1:A:97:ASN:ND2	0.42	2.53	29	1
1:A:68:PHE:CE2	2:B:11:ILE:CD1	0.42	3.03	2	1
2:B:18:ARG:C	2:B:19:LYS:HD2	0.42	2.35	2	2
1:A:27:ILE:HA	1:A:31:GLU:OE1	0.42	2.15	5	1
1:A:28:THR:OG1	1:A:31:GLU:CD	0.42	2.58	5	2
1:A:51:MET:SD	2:B:4:ILE:CG2	0.42	3.08	10	1
1:A:58:ASP:OD2	1:A:60:ASN:HB3	0.42	2.15	10	1
1:A:129:ASP:OD1	1:A:132:GLY:N	0.42	2.53	12	1
1:A:72:MET:SD	1:A:72:MET:O	0.42	2.78	13	1
1:A:123:GLU:O	1:A:124:MET:C	0.42	2.57	24	1
1:A:129:ASP:O	1:A:130:ILE:C	0.42	2.57	25	1
1:A:142:VAL:HG13	1:A:146:THR:CB	0.42	2.45	25	1
1:A:99:TYR:HB3	1:A:135:GLN:OE1	0.41	2.16	8	2
1:A:67:GLU:O	1:A:71:MET:HB2	0.41	2.15	6	2
1:A:31:GLU:O	1:A:32:LEU:C	0.41	2.58	11	1
1:A:71:MET:SD	1:A:71:MET:C	0.41	2.98	16	1
1:A:65:PHE:HB3	1:A:66:PRO:HD3	0.41	1.92	21	4
1:A:44:THR:O	1:A:48:LEU:HD12	0.41	2.15	24	1
1:A:45:GLU:O	1:A:48:LEU:HB2	0.41	2.15	24	1
2:B:24:ASN:H	2:B:25:PRO:CD	0.41	2.27	26	1
1:A:34:THR:O	1:A:37:ARG:N	0.41	2.53	27	1
1:A:41:GLN:NE2	1:A:41:GLN:HA	0.41	2.29	6	1
1:A:57:ALA:HB3	1:A:67:GLU:OE1	0.41	2.16	6	1
1:A:36:MET:HE1	1:A:51:MET:HE2	0.41	1.93	7	1
1:A:8:GLN:O	1:A:12:PHE:CD1	0.41	2.73	8	1
2:B:12:LEU:CD1	2:B:13:VAL:HG23	0.41	2.45	16	1
1:A:24:ASP:CG	1:A:25:GLY:N	0.41	2.73	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:LEU:O	1:A:108:VAL:N	0.41	2.53	30	1
2:B:17:LEU:C	2:B:17:LEU:CD2	0.41	2.88	3	1
1:A:64:ASP:O	1:A:65:PHE:C	0.41	2.58	5	1
1:A:109:MET:SD	2:B:17:LEU:HG	0.41	2.55	9	1
1:A:109:MET:SD	1:A:116:LEU:CD1	0.41	3.01	10	1
1:A:131:ASP:OD2	1:A:140:GLU:CD	0.41	2.58	10	1
1:A:107:HIS:O	1:A:111:ASN:CG	0.41	2.58	13	2
1:A:106:ARG:NH2	1:A:106:ARG:HG2	0.41	2.30	15	1
1:A:72:MET:HE1	2:B:26:PHE:HZ	0.41	1.76	18	1
2:B:12:LEU:CD1	2:B:26:PHE:CD1	0.41	3.03	18	1
1:A:106:ARG:O	1:A:110:THR:OG1	0.41	2.38	19	1
1:A:16:PHE:CE2	1:A:64:ASP:C	0.41	2.93	26	1
1:A:24:ASP:C	1:A:24:ASP:OD1	0.41	2.58	26	1
1:A:19:PHE:CE1	1:A:32:LEU:HD13	0.41	2.51	28	1
1:A:128:ALA:O	1:A:130:ILE:CD1	0.41	2.67	30	1
1:A:105:LEU:O	1:A:109:MET:CB	0.41	2.69	4	1
2:B:16:MET:CG	2:B:22:PHE:CE1	0.41	3.03	4	1
2:B:10:VAL:HG23	2:B:11:ILE:HD13	0.41	1.92	5	1
1:A:38:SER:O	1:A:40:GLY:N	0.41	2.53	11	1
1:A:131:ASP:CG	1:A:133:ASP:OD2	0.41	2.58	14	1
2:B:18:ARG:HB3	2:B:19:LYS:HD3	0.41	1.91	14	1
1:A:48:LEU:O	1:A:51:MET:N	0.41	2.54	24	1
1:A:133:ASP:OD1	1:A:135:GLN:HB2	0.41	2.15	28	1
1:A:143:GLN:NE2	1:A:143:GLN:HA	0.41	2.30	28	1
1:A:45:GLU:CG	1:A:46:ALA:N	0.41	2.84	29	1
2:B:23:GLY:O	2:B:24:ASN:C	0.41	2.57	2	1
2:B:19:LYS:C	2:B:19:LYS:HD2	0.41	2.34	10	1
1:A:22:ASP:OD2	1:A:24:ASP:OD2	0.41	2.39	12	1
1:A:92:PHE:HE1	1:A:105:LEU:HD23	0.41	1.74	13	1
1:A:15:ALA:O	1:A:18:LEU:HB3	0.41	2.16	14	1
2:B:20:ARG:CZ	2:B:20:ARG:HB2	0.41	2.45	16	1
1:A:14:GLU:CA	1:A:17:SER:OG	0.41	2.69	20	1
1:A:84:GLU:HA	1:A:87:GLU:OE1	0.41	2.15	5	1
1:A:44:THR:CG2	1:A:45:GLU:N	0.41	2.83	9	1
1:A:11:GLU:OE2	2:B:18:ARG:HD3	0.41	2.15	10	1
1:A:51:MET:CG	1:A:52:ILE:N	0.41	2.83	11	1
2:B:18:ARG:CG	2:B:19:LYS:N	0.41	2.84	11	1
1:A:75:LYS:HG2	2:B:8:THR:CG2	0.41	2.45	18	1
1:A:139:GLU:HG3	1:A:140:GLU:N	0.41	2.30	19	1
1:A:32:LEU:HD21	1:A:51:MET:CE	0.41	2.45	24	1
1:A:46:ALA:O	1:A:47:GLU:C	0.41	2.57	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:11:ILE:N	2:B:11:ILE:HD13	0.41	2.30	28	1
1:A:27:ILE:HB	1:A:63:ILE:HB	0.41	1.92	4	2
2:B:20:ARG:CD	2:B:20:ARG:C	0.41	2.89	7	1
1:A:54:GLU:HG3	1:A:55:VAL:HG23	0.41	1.92	8	1
1:A:120:GLU:CG	2:B:20:ARG:HB3	0.41	2.46	8	1
1:A:20:ASP:HA	1:A:31:GLU:OE2	0.41	2.16	23	2
1:A:145:MET:O	2:B:24:ASN:HB2	0.41	2.16	10	1
2:B:18:ARG:HG3	2:B:19:LYS:N	0.41	2.30	11	1
1:A:131:ASP:OD1	1:A:133:ASP:CG	0.41	2.58	14	1
1:A:16:PHE:CD1	1:A:16:PHE:C	0.41	2.92	15	1
1:A:18:LEU:HD11	1:A:112:LEU:C	0.41	2.35	26	1
1:A:28:THR:O	1:A:29:THR:C	0.41	2.58	27	1
1:A:34:THR:O	1:A:35:VAL:C	0.41	2.59	27	1
1:A:51:MET:HE1	2:B:7:TRP:N	0.41	2.31	5	1
1:A:133:ASP:OD2	1:A:135:GLN:HG2	0.41	2.16	22	2
2:B:18:ARG:C	2:B:19:LYS:HG3	0.41	2.36	9	1
1:A:106:ARG:HA	1:A:109:MET:HB3	0.41	1.93	13	1
1:A:137:ASN:OD1	1:A:140:GLU:HG3	0.41	2.15	18	1
1:A:91:VAL:CG2	2:B:13:VAL:HG21	0.41	2.43	19	1
1:A:41:GLN:OE1	2:B:4:ILE:HA	0.41	2.16	5	1
1:A:130:ILE:CD1	1:A:144:MET:CE	0.41	2.98	5	1
1:A:51:MET:O	1:A:54:GLU:HG2	0.41	2.15	8	1
1:A:94:LYS:CG	1:A:95:ASP:N	0.41	2.84	12	1
1:A:74:ARG:O	1:A:75:LYS:C	0.41	2.57	13	1
1:A:92:PHE:CE2	1:A:141:PHE:CE1	0.41	3.08	15	1
1:A:140:GLU:C	1:A:142:VAL:N	0.41	2.74	23	1
1:A:17:SER:O	1:A:18:LEU:C	0.41	2.60	25	1
2:B:10:VAL:O	2:B:14:LYS:HB2	0.41	2.16	29	1
2:B:25:PRO:O	2:B:26:PHE:C	0.41	2.57	1	1
1:A:27:ILE:O	1:A:62:THR:HA	0.41	2.16	2	1
1:A:122:ASP:O	1:A:123:GLU:C	0.41	2.57	8	2
1:A:106:ARG:O	1:A:109:MET:HB2	0.41	2.16	6	1
1:A:109:MET:HG2	2:B:17:LEU:HD21	0.41	1.93	10	1
1:A:15:ALA:O	1:A:16:PHE:C	0.41	2.57	13	1
1:A:11:GLU:CG	1:A:12:PHE:CD1	0.41	3.04	19	1
1:A:112:LEU:HB2	2:B:17:LEU:CD2	0.41	2.45	20	1
2:B:11:ILE:O	2:B:15:SER:N	0.41	2.54	28	1
1:A:42:ASN:CG	1:A:42:ASN:O	0.41	2.59	30	1
1:A:24:ASP:CG	1:A:26:THR:HG1	0.40	2.20	1	1
1:A:134:GLY:C	1:A:135:GLN:OE1	0.40	2.60	5	1
1:A:85:ILE:CG2	1:A:141:PHE:CE2	0.40	3.02	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:9:THR:O	2:B:10:VAL:C	0.40	2.59	19	1
1:A:120:GLU:OE2	2:B:19:LYS:HE3	0.40	2.16	24	1
2:B:16:MET:O	2:B:17:LEU:O	0.40	2.39	24	1
1:A:22:ASP:OD2	1:A:24:ASP:HB3	0.40	2.16	25	1
2:B:19:LYS:N	2:B:19:LYS:HD2	0.40	2.30	2	1
1:A:40:GLY:O	1:A:41:GLN:OE1	0.40	2.39	4	1
1:A:144:MET:SD	1:A:144:MET:C	0.40	3.00	9	1
1:A:15:ALA:CA	2:B:14:LYS:HD2	0.40	2.46	11	1
1:A:70:THR:HG22	1:A:74:ARG:HG3	0.40	1.93	13	1
1:A:101:SER:C	1:A:103:ALA:N	0.40	2.75	13	1
2:B:23:GLY:O	2:B:24:ASN:CB	0.40	2.69	17	1
1:A:95:ASP:OD2	1:A:104:GLU:HG3	0.40	2.16	21	1
1:A:87:GLU:N	1:A:87:GLU:CD	0.40	2.73	23	1
1:A:36:MET:CE	2:B:5:PRO:HG2	0.40	2.46	24	1
1:A:109:MET:HB3	1:A:114:GLU:O	0.40	2.16	26	1
2:B:18:ARG:CG	2:B:19:LYS:HD2	0.40	2.46	26	1
1:A:115:LYS:O	1:A:115:LYS:HG2	0.40	2.15	2	1
1:A:84:GLU:CG	2:B:12:LEU:CD1	0.40	2.99	7	1
1:A:88:ALA:CB	2:B:12:LEU:CD1	0.40	2.99	16	1
1:A:108:VAL:O	1:A:109:MET:C	0.40	2.59	17	1
1:A:48:LEU:O	1:A:49:GLN:C	0.40	2.60	24	1
1:A:52:ILE:O	1:A:54:GLU:N	0.40	2.54	24	1
1:A:93:ASP:OD2	1:A:96:GLY:HA2	0.40	2.16	24	1
2:B:18:ARG:NE	2:B:18:ARG:HA	0.40	2.31	26	1
1:A:108:VAL:CG1	1:A:109:MET:N	0.40	2.85	3	1
2:B:12:LEU:C	2:B:12:LEU:CD2	0.40	2.90	6	1
1:A:89:PHE:CD1	1:A:89:PHE:C	0.40	2.94	9	1
1:A:72:MET:HE3	2:B:11:ILE:HG22	0.40	1.91	10	1
1:A:109:MET:C	1:A:114:GLU:O	0.40	2.60	11	1
2:B:17:LEU:O	2:B:17:LEU:CG	0.40	2.69	11	1
1:A:125:ILE:HD12	1:A:125:ILE:H	0.40	1.74	19	1
2:B:9:THR:HA	2:B:12:LEU:CG	0.40	2.47	20	1
2:B:8:THR:O	2:B:11:ILE:HB	0.40	2.16	23	1
1:A:95:ASP:OD2	1:A:97:ASN:CB	0.40	2.69	24	1
1:A:75:LYS:O	1:A:75:LYS:HG3	0.40	2.16	2	1
1:A:109:MET:HE3	1:A:116:LEU:HB2	0.40	1.93	7	1
1:A:36:MET:HB2	1:A:43:PRO:HG3	0.40	1.94	8	1
1:A:13:LYS:O	1:A:17:SER:OG	0.40	2.39	20	1
2:B:5:PRO:HB2	2:B:10:VAL:CG2	0.40	2.46	20	1
2:B:24:ASN:O	2:B:26:PHE:N	0.40	2.54	23	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	133/148 (90%)	112±3 (84±2%)	17±3 (13±2%)	4±1 (3±1%)	8 42
2	B	22/26 (85%)	14±2 (62±8%)	5±2 (24±9%)	3±1 (13±6%)	1 5
All	All	4650/5220 (89%)	3773 (81%)	677 (15%)	200 (4%)	5 29

All 29 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	56	ASP	27
1	A	117	THR	21
1	A	116	LEU	21
1	A	129	ASP	19
2	B	7	TRP	17
2	B	18	ARG	11
2	B	19	LYS	9
2	B	8	THR	7
2	B	5	PRO	7
2	B	4	ILE	6
2	B	17	LEU	6
2	B	23	GLY	6
1	A	20	ASP	5
1	A	40	GLY	5
2	B	22	PHE	5
2	B	21	SER	4
2	B	20	ARG	4
2	B	6	SER	4
1	A	44	THR	3
1	A	41	GLN	3
2	B	24	ASN	2
1	A	143	GLN	1
1	A	24	ASP	1
1	A	72	MET	1
1	A	60	ASN	1
1	A	61	GLY	1

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Mol	Chain	Res	Type	Models (Total)
1	A	94	LYS	1
2	B	25	PRO	1
1	A	21	LYS	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	113/126 (90%)	90±4 (80±4%)	23±4 (20±4%)	3 33
2	B	22/25 (88%)	15±2 (68±9%)	7±2 (32±9%)	1 14
All	All	4050/4530 (89%)	3160 (78%)	890 (22%)	3 30

All 103 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	53	ASN	27
1	A	117	THR	25
2	B	22	PHE	25
2	B	20	ARG	21
2	B	19	LYS	20
1	A	108	VAL	18
1	A	94	LYS	17
2	B	7	TRP	17
2	B	12	LEU	17
1	A	115	LYS	16
2	B	14	LYS	16
1	A	49	GLN	16
1	A	90	ARG	15
2	B	16	MET	15
1	A	124	MET	15
1	A	129	ASP	15
1	A	41	GLN	14
2	B	18	ARG	14
1	A	37	ARG	14
1	A	72	MET	14
1	A	30	LYS	13

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Mol	Chain	Res	Type	Models (Total)
1	A	54	GLU	13
1	A	74	ARG	13
1	A	126	ARG	13
1	A	56	ASP	12
2	B	21	SER	12
1	A	105	LEU	12
1	A	139	GLU	12
1	A	93	ASP	12
1	A	107	HIS	12
1	A	51	MET	11
1	A	75	LYS	11
1	A	119	GLU	11
1	A	21	LYS	10
1	A	38	SER	10
1	A	143	GLN	10
1	A	101	SER	10
1	A	8	GLN	10
1	A	13	LYS	10
1	A	36	MET	9
1	A	52	ILE	9
1	A	86	ARG	9
1	A	127	GLU	9
1	A	145	MET	9
1	A	45	GLU	9
1	A	106	ARG	9
1	A	71	MET	9
2	B	24	ASN	9
1	A	118	ASP	9
1	A	50	ASP	9
1	A	20	ASP	8
1	A	48	LEU	8
1	A	109	MET	8
1	A	62	THR	8
2	B	6	SER	8
1	A	70	THR	8
1	A	122	ASP	8
2	B	26	PHE	8
1	A	17	SER	7
1	A	28	THR	7
2	B	8	THR	7
1	A	82	GLU	7
1	A	123	GLU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	144	MET	7
1	A	110	THR	6
1	A	69	LEU	6
1	A	11	GLU	6
2	B	15	SER	6
1	A	64	ASP	6
1	A	29	THR	5
1	A	120	GLU	5
2	B	17	LEU	5
2	B	4	ILE	5
1	A	26	THR	5
1	A	39	LEU	4
1	A	99	TYR	4
1	A	135	GLN	4
1	A	138	TYR	4
1	A	14	GLU	4
1	A	67	GLU	3
1	A	68	PHE	3
1	A	83	GLU	3
1	A	42	ASN	3
1	A	87	GLU	3
1	A	22	ASP	3
1	A	47	GLU	2
1	A	130	ILE	2
2	B	9	THR	2
1	A	44	THR	2
1	A	116	LEU	2
1	A	146	THR	2
1	A	111	ASN	1
1	A	140	GLU	1
1	A	84	GLU	1
1	A	16	PHE	1
1	A	60	ASN	1
1	A	91	VAL	1
2	B	13	VAL	1
1	A	104	GLU	1
2	B	11	ILE	1
1	A	114	GLU	1
1	A	18	LEU	1
1	A	12	PHE	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided