



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 07:09 AM UTC

PDB ID : 1MQ1 / pdb_00001mq1
Title : Ca²⁺-S100B-TRTK-12 complex
Authors : McClintock, K.A.; Shaw, G.S.
Deposited on : 2002-09-13

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
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

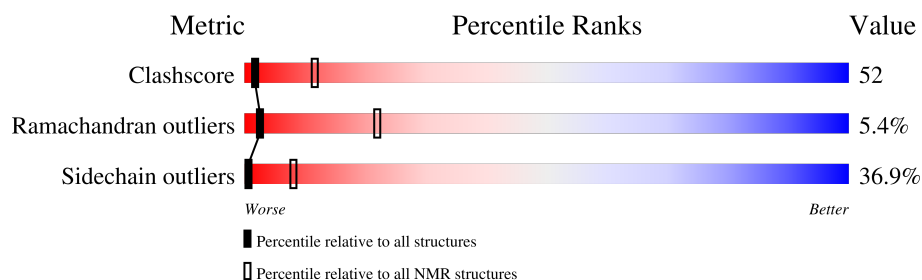
1 Overall quality at a glance

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	91	
1	B	91	
2	C	12	
2	D	12	

2 Ensemble composition and analysis

This entry contains 17 models. Model 16 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:19, A:24-A:40, A:48-A:88, B:1-B:19, B:24-B:40, B:48-B:88, C:2-C:12, D:1-D:12 (177)	1.05	16

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, 5, 7, 12, 13, 14, 15, 16, 17
2	3, 6, 10, 11
3	4, 8, 9

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3322 atoms, of which 1632 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called S-100 protein, beta chain.

Mol	Chain	Residues	Atoms						Trace
1	A	91	Total	C	H	N	O	S	0
			1445	465	704	118	152	6	
1	B	91	Total	C	H	N	O	S	0
			1445	465	704	118	152	6	

- Molecule 2 is a protein called F-actin capping protein alpha-1 subunit.

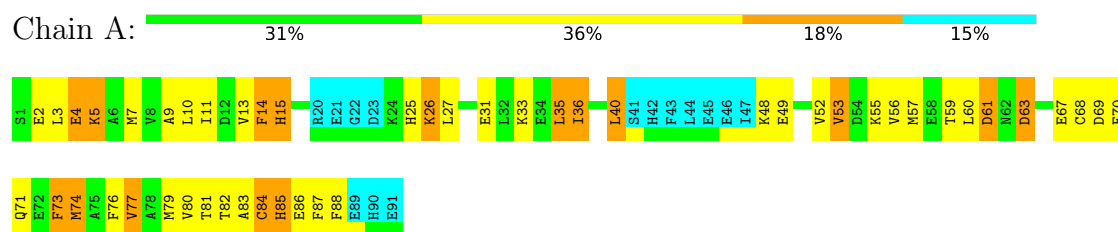
Mol	Chain	Residues	Atoms					Trace
2	C	12	Total	C	H	N	O	0
			216	66	112	19	19	
2	D	12	Total	C	H	N	O	0
			216	66	112	19	19	

4.2 Scores per residue for each member of the ensemble

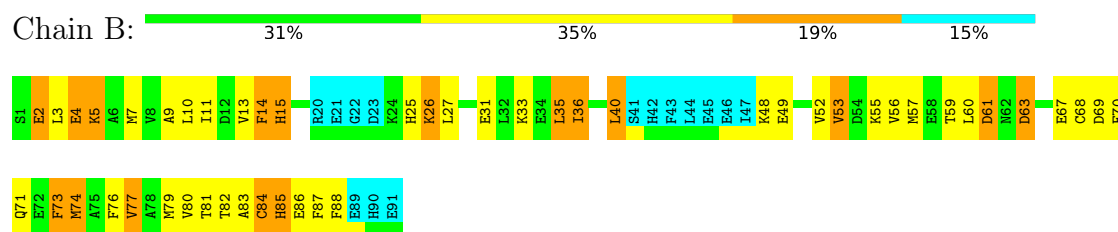
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

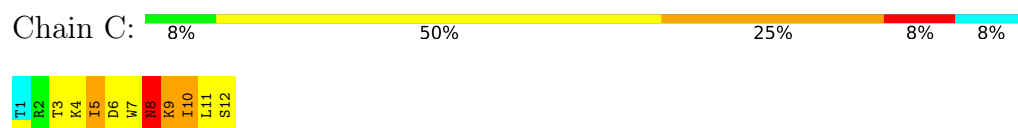
- Molecule 1: S-100 protein, beta chain



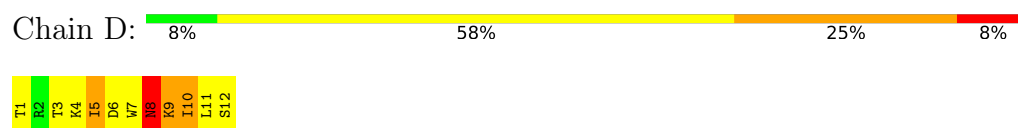
- Molecule 1: S-100 protein, beta chain



- Molecule 2: F-actin capping protein alpha-1 subunit

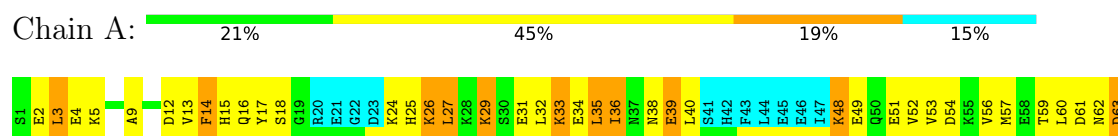


- Molecule 2: F-actin capping protein alpha-1 subunit



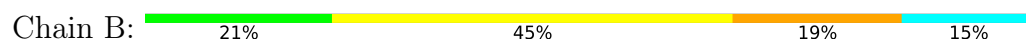
4.2.2 Score per residue for model 2

- Molecule 1: S-100 protein, beta chain

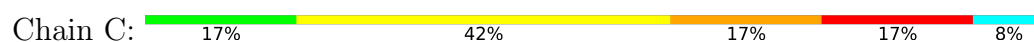




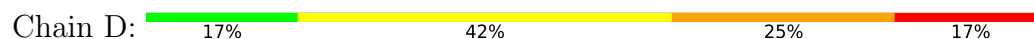
- Molecule 1: S-100 protein, beta chain



- Molecule 2: F-actin capping protein alpha-1 subunit

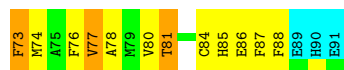
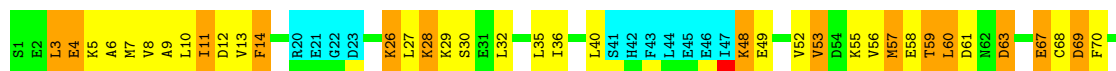


- Molecule 2: F-actin capping protein alpha-1 subunit

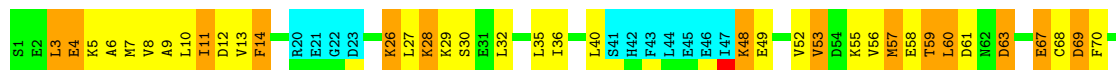


4.2.3 Score per residue for model 3

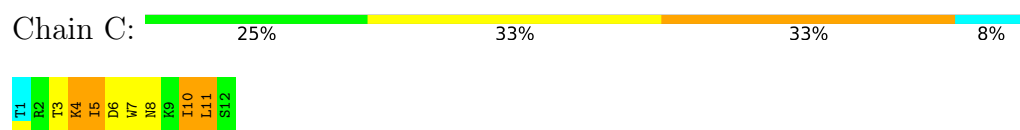
- Molecule 1: S-100 protein, beta chain



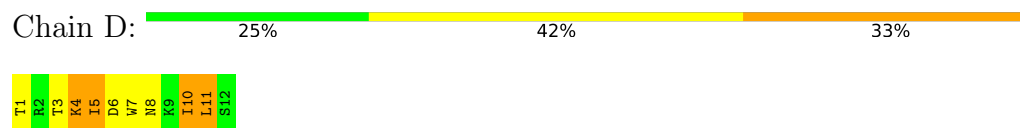
- Molecule 1: S-100 protein, beta chain



- Molecule 2: F-actin capping protein alpha-1 subunit

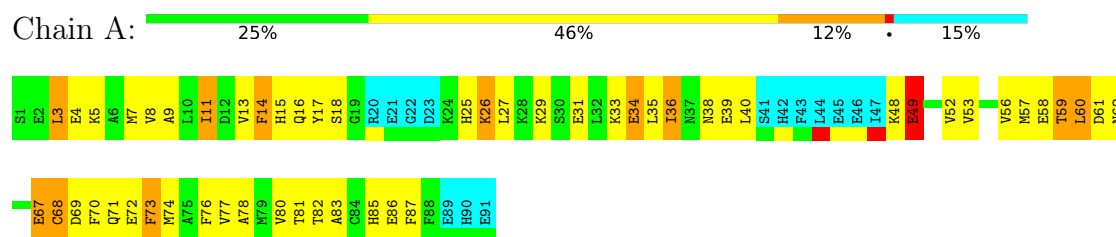


- Molecule 2: F-actin capping protein alpha-1 subunit

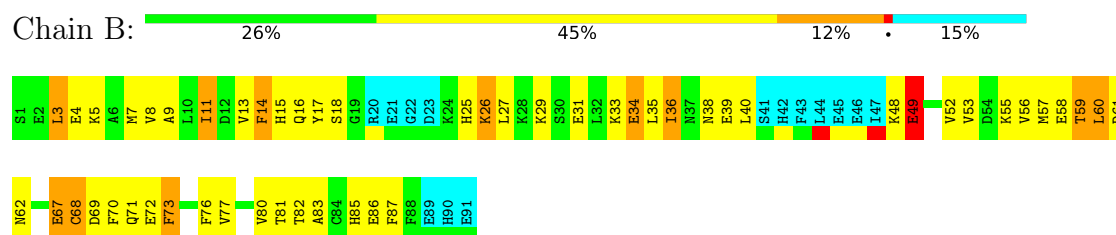


4.2.4 Score per residue for model 4

- Molecule 1: S-100 protein, beta chain



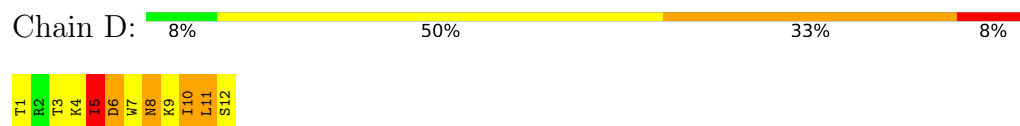
- Molecule 1: S-100 protein, beta chain



- Molecule 2: F-actin capping protein alpha-1 subunit

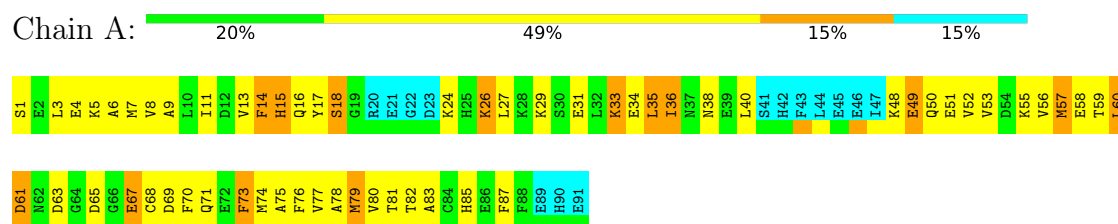


- Molecule 2: F-actin capping protein alpha-1 subunit

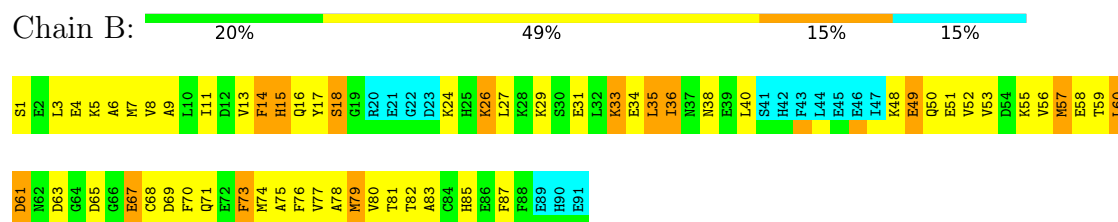


4.2.5 Score per residue for model 5

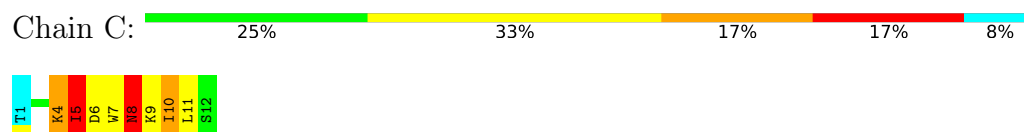
- Molecule 1: S-100 protein, beta chain



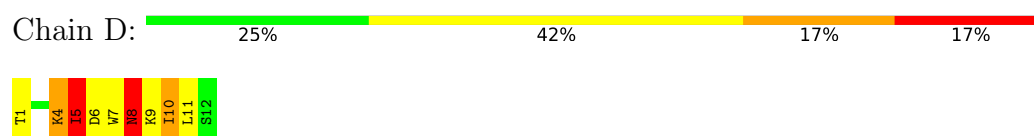
- Molecule 1: S-100 protein, beta chain



- Molecule 2: F-actin capping protein alpha-1 subunit

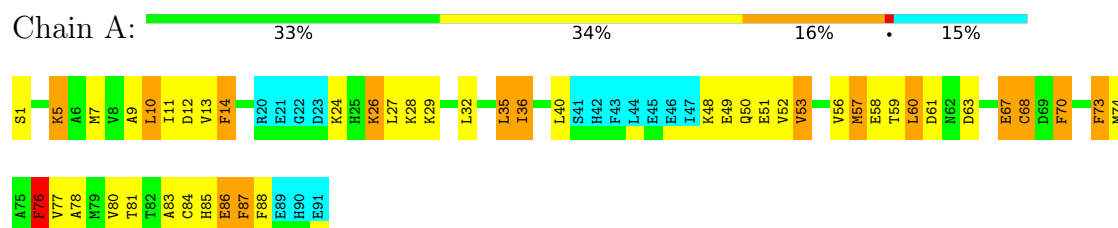


- Molecule 2: F-actin capping protein alpha-1 subunit



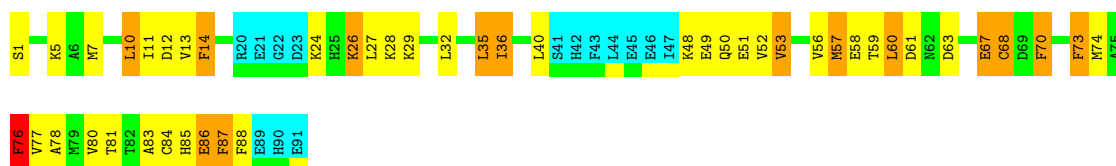
4.2.6 Score per residue for model 6

- Molecule 1: S-100 protein, beta chain



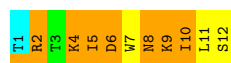
- Molecule 1: S-100 protein, beta chain





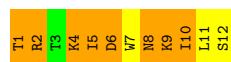
- Molecule 2: F-actin capping protein alpha-1 subunit

Chain C: 8% 25% 58% 8%



- Molecule 2: F-actin capping protein alpha-1 subunit

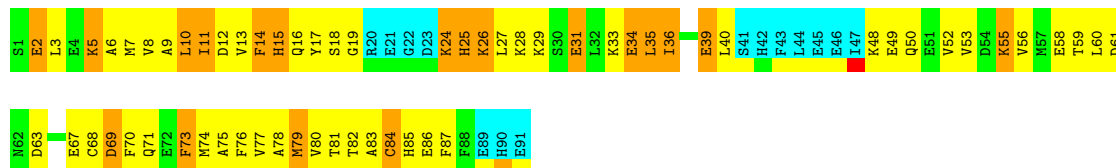
Chain D: 8% 25% 67%



4.2.7 Score per residue for model 7

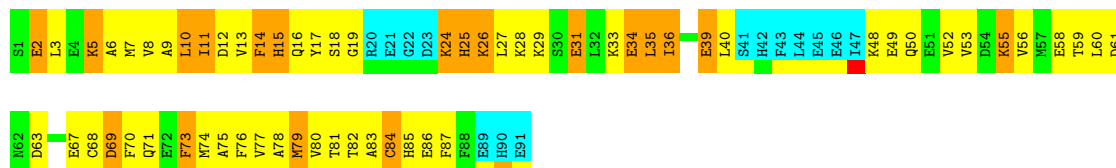
- Molecule 1: S-100 protein, beta chain

Chain A: 16% 47% 21% 15%



- Molecule 1: S-100 protein, beta chain

Chain B: 16% 47% 21% 15%



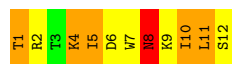
- Molecule 2: F-actin capping protein alpha-1 subunit

Chain C: 8% 42% 33% 8% 8%



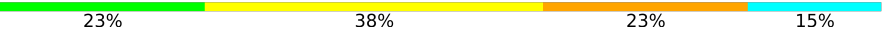
- Molecule 2: F-actin capping protein alpha-1 subunit

Chain D:  8% 42% 42% 8%



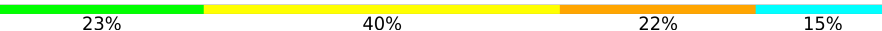
4.2.8 Score per residue for model 8

- Molecule 1: S-100 protein, beta chain

Chain A:  23% 38% 23% 15%



- Molecule 1: S-100 protein, beta chain

Chain B:  23% 40% 22% 15%



- Molecule 2: F-actin capping protein alpha-1 subunit

Chain C:  17% 33% 33% 8% 8%



- Molecule 2: F-actin capping protein alpha-1 subunit

Chain D:  17% 33% 42% 8%

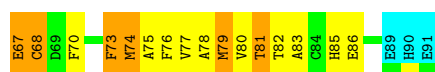


4.2.9 Score per residue for model 9

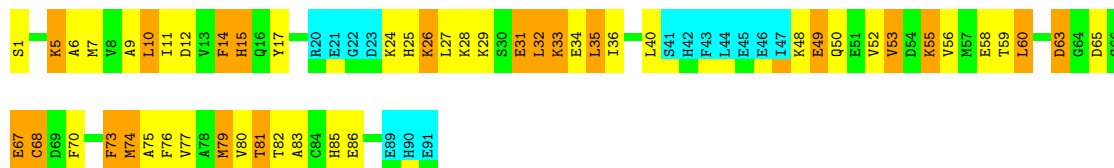
- Molecule 1: S-100 protein, beta chain

Chain A:  27% 34% 23% 15%

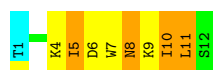
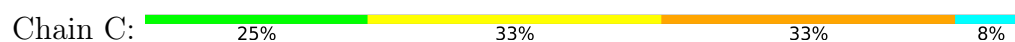




- Molecule 1: S-100 protein, beta chain



- Molecule 2: F-actin capping protein alpha-1 subunit

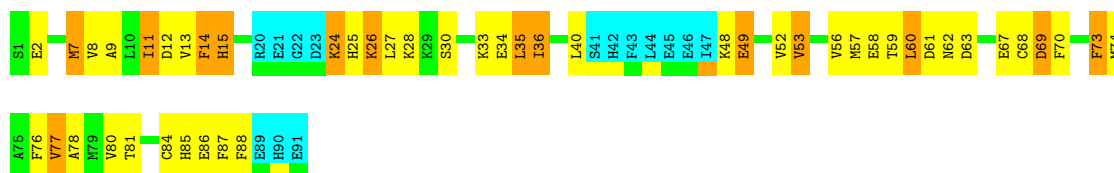


- Molecule 2: F-actin capping protein alpha-1 subunit

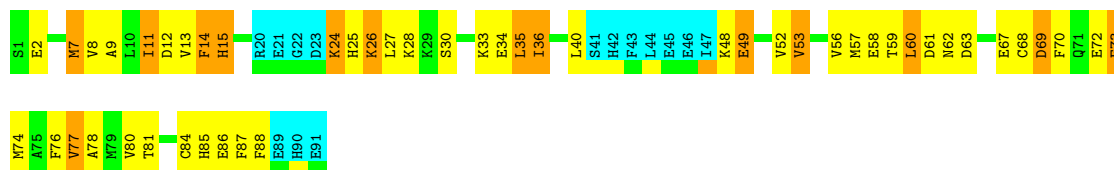


4.2.10 Score per residue for model 10

- Molecule 1: S-100 protein, beta chain

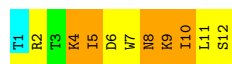


- Molecule 1: S-100 protein, beta chain



- Molecule 2: F-actin capping protein alpha-1 subunit

Chain C: 



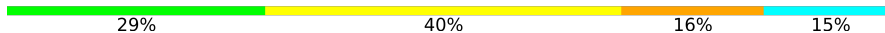
- Molecule 2: F-actin capping protein alpha-1 subunit

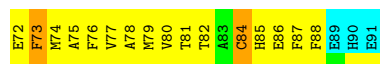
Chain D: 



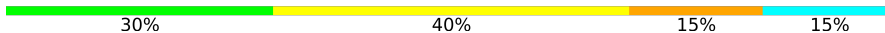
4.2.11 Score per residue for model 11

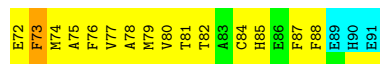
- Molecule 1: S-100 protein, beta chain

Chain A: 



- Molecule 1: S-100 protein, beta chain

Chain B: 



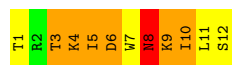
- Molecule 2: F-actin capping protein alpha-1 subunit

Chain C: 



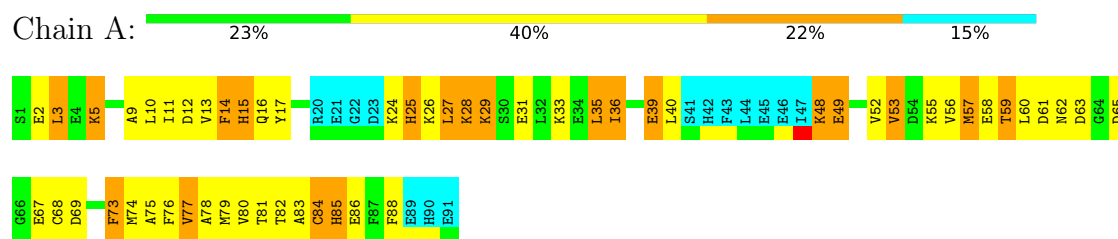
- Molecule 2: F-actin capping protein alpha-1 subunit

Chain D: 

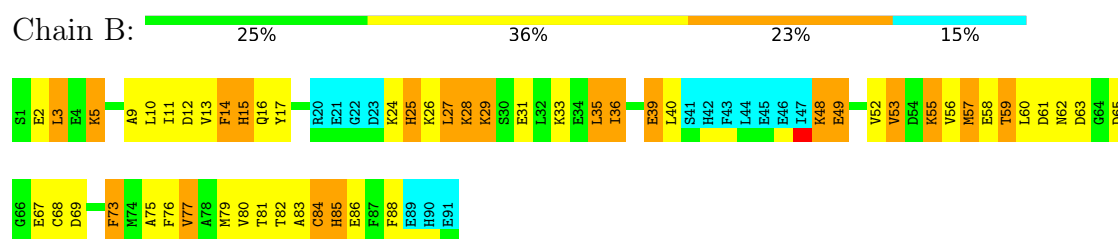


4.2.12 Score per residue for model 12

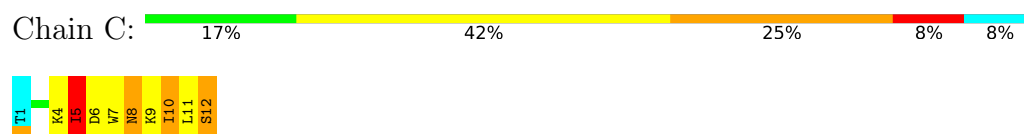
- Molecule 1: S-100 protein, beta chain



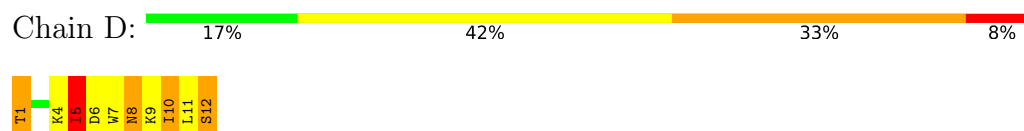
- Molecule 1: S-100 protein, beta chain



- Molecule 2: F-actin capping protein alpha-1 subunit

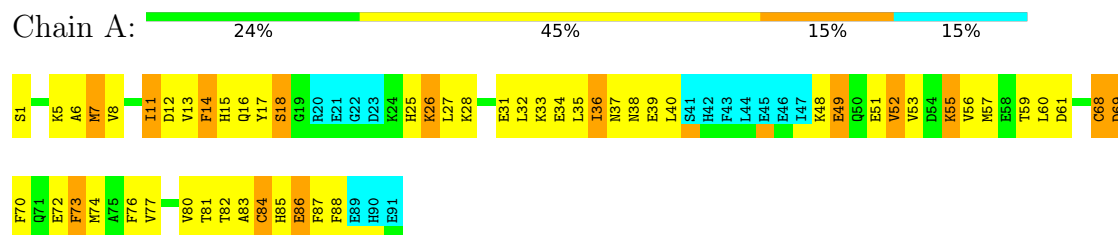


- Molecule 2: F-actin capping protein alpha-1 subunit

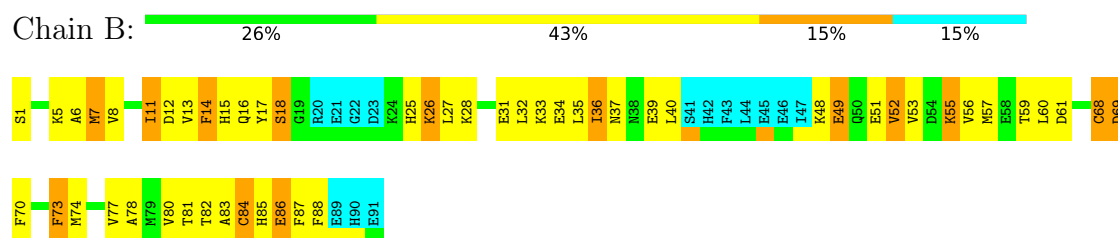


4.2.13 Score per residue for model 13

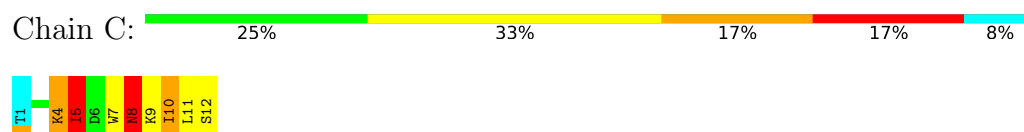
- Molecule 1: S-100 protein, beta chain



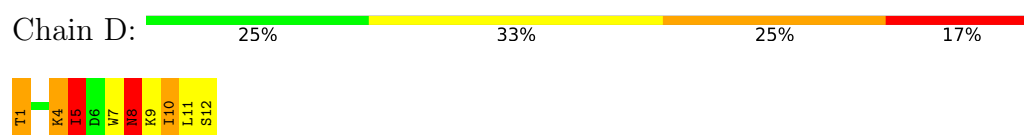
- Molecule 1: S-100 protein, beta chain



- Molecule 2: F-actin capping protein alpha-1 subunit

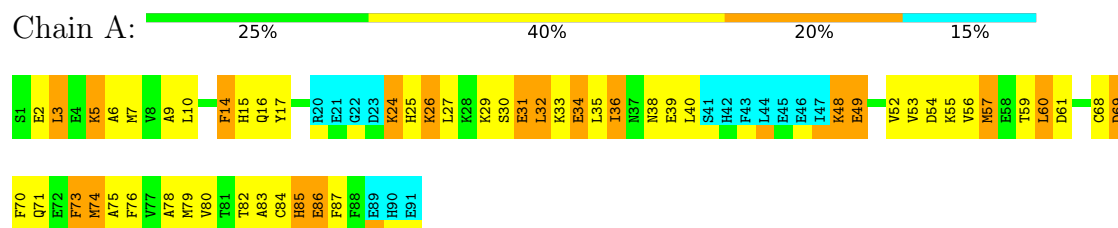


- Molecule 2: F-actin capping protein alpha-1 subunit

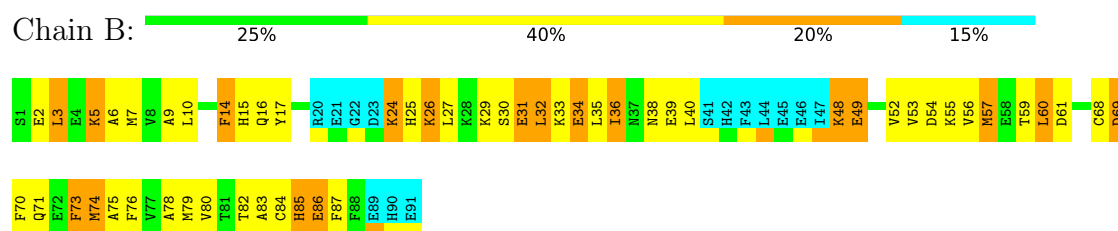


4.2.14 Score per residue for model 14

- Molecule 1: S-100 protein, beta chain



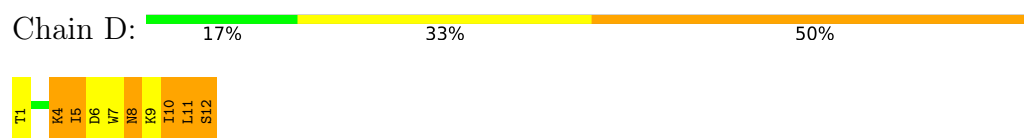
- Molecule 1: S-100 protein, beta chain



- Molecule 2: F-actin capping protein alpha-1 subunit

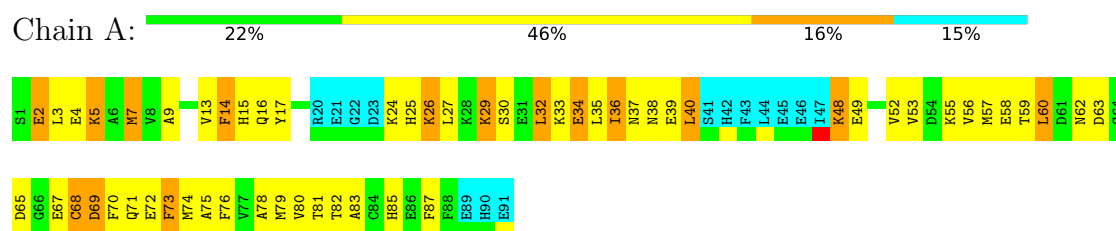


- Molecule 2: F-actin capping protein alpha-1 subunit

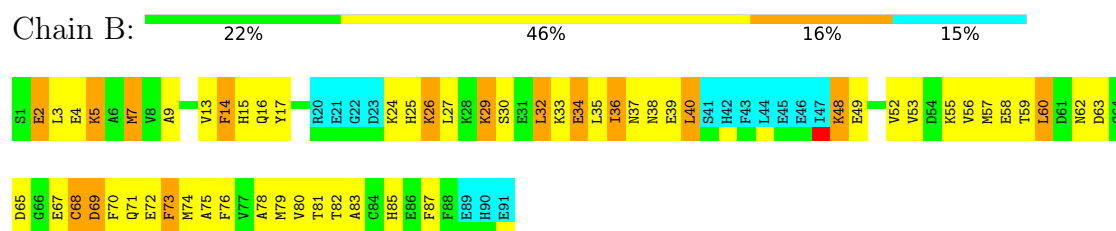


4.2.15 Score per residue for model 15

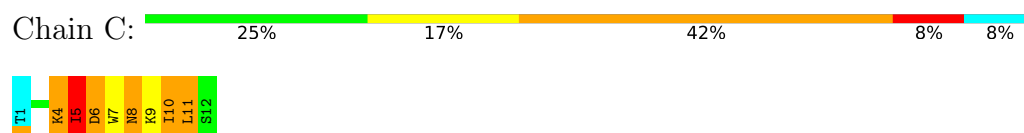
- Molecule 1: S-100 protein, beta chain



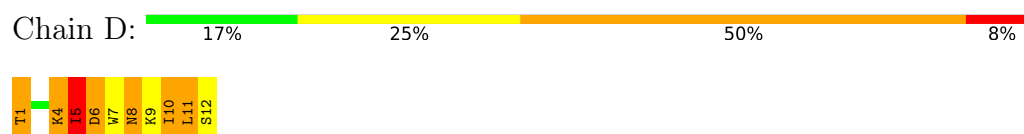
- Molecule 1: S-100 protein, beta chain



- Molecule 2: F-actin capping protein alpha-1 subunit



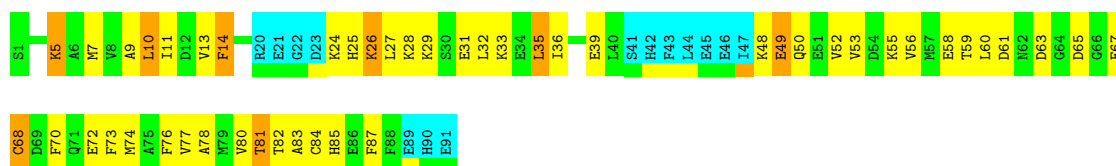
- Molecule 2: F-actin capping protein alpha-1 subunit



4.2.16 Score per residue for model 16 (medoid)

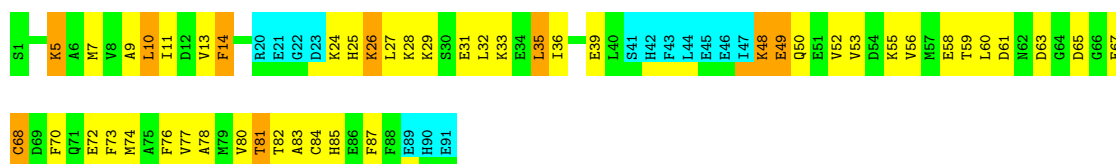
- Molecule 1: S-100 protein, beta chain





- Molecule 1: S-100 protein, beta chain

Chain B: 32% 43% 10% 15%



- Molecule 2: F-actin capping protein alpha-1 subunit

Chain C: 8% 58% 17% 8% 8%



- Molecule 2: F-actin capping protein alpha-1 subunit

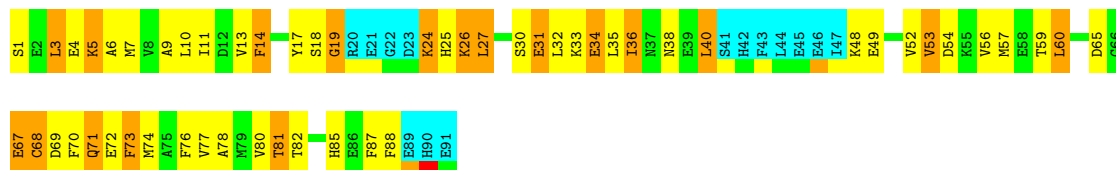
Chain D: 8% 67% 17% 8%



4.2.17 Score per residue for model 17

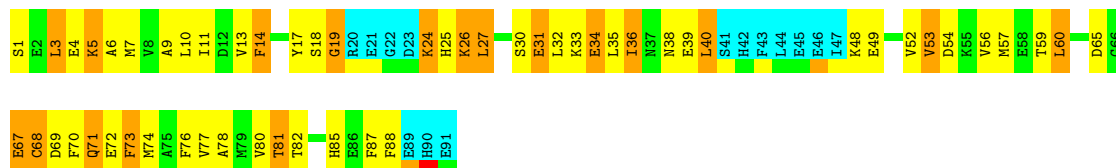
- Molecule 1: S-100 protein, beta chain

Chain A: 25% 40% 20% 15%



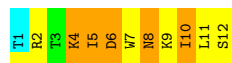
- Molecule 1: S-100 protein, beta chain

Chain B: 24% 41% 20% 15%



- Molecule 2: F-actin capping protein alpha-1 subunit

Chain C:  8% 42% 42% 8%



- Molecule 2: F-actin capping protein alpha-1 subunit

Chain D:  8% 50% 42%



5 Refinement protocol and experimental data overview

Of the 80 calculated structures, 17 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
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	619	603	600	61±11
1	B	619	603	600	61±10
2	C	97	103	104	24±4
2	D	104	112	113	25±4
All	All	24463	24157	24089	2538

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 52.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ILE:HG23	1:A:40:LEU:HD12	1.08	1.12	17	6
2:C:4:LYS:O	2:C:5:ILE:HG23	1.03	1.53	13	2
2:D:4:LYS:O	2:D:5:ILE:HG23	1.03	1.53	13	2
1:B:36:ILE:HG23	1:B:40:LEU:HD12	1.03	1.12	17	6
2:C:10:ILE:HG23	2:C:11:LEU:HD22	1.02	1.27	3	2
2:D:10:ILE:HG23	2:D:11:LEU:HD22	1.02	1.27	3	2
2:C:4:LYS:C	2:C:5:ILE:HD13	0.98	1.83	17	11
2:D:4:LYS:C	2:D:5:ILE:HD13	0.97	1.83	17	11
1:A:40:LEU:HD21	1:B:3:LEU:HD13	0.94	1.40	11	2
1:A:3:LEU:HD13	1:B:40:LEU:HD21	0.91	1.39	11	2
1:A:60:LEU:HD11	1:A:76:PHE:CD1	0.91	2.01	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:LEU:HD23	1:A:7:MET:HE3	0.91	1.43	8	1
1:B:60:LEU:HD11	1:B:76:PHE:CD1	0.90	2.01	2	5
1:B:52:VAL:O	1:B:56:VAL:HG23	0.89	1.67	8	13
1:A:52:VAL:O	1:A:56:VAL:HG23	0.88	1.67	8	13
1:B:36:ILE:HA	1:B:40:LEU:HD12	0.87	1.46	11	8
2:D:4:LYS:O	2:D:5:ILE:HD12	0.87	1.68	13	5
2:C:7:TRP:CD2	2:C:11:LEU:HD13	0.87	2.05	15	2
1:B:3:LEU:HD23	1:B:7:MET:HE3	0.87	1.44	8	1
1:A:59:THR:HG21	2:C:10:ILE:HG22	0.86	1.47	13	7
2:C:4:LYS:O	2:C:5:ILE:HD12	0.86	1.68	13	5
2:D:7:TRP:CD2	2:D:11:LEU:HD13	0.86	2.05	15	2
1:A:36:ILE:HA	1:A:40:LEU:HD12	0.85	1.46	11	8
2:C:5:ILE:HD13	2:C:7:TRP:CD1	0.85	2.06	9	4
1:A:59:THR:HG23	2:C:8:ASN:HB3	0.85	1.47	9	4
1:B:11:ILE:HG23	1:B:70:PHE:CD1	0.85	2.07	3	3
2:D:5:ILE:HD13	2:D:7:TRP:CD1	0.85	2.06	9	4
1:A:26:LYS:O	1:A:27:LEU:HD13	0.85	1.72	12	7
1:A:36:ILE:CG2	1:A:40:LEU:HD12	0.84	2.01	17	3
1:B:59:THR:HG21	2:D:10:ILE:HG22	0.84	1.48	13	7
1:B:36:ILE:CG2	1:B:40:LEU:HD12	0.84	2.01	17	3
1:B:26:LYS:O	1:B:27:LEU:HD13	0.83	1.72	12	7
1:B:59:THR:HG23	2:D:8:ASN:CB	0.83	2.02	9	4
1:A:11:ILE:HG23	1:A:70:PHE:CD1	0.83	2.07	3	3
1:B:36:ILE:HG23	1:B:40:LEU:HD13	0.83	1.50	13	2
1:A:59:THR:HG23	2:C:8:ASN:CB	0.83	2.02	9	4
1:B:59:THR:HG23	2:D:8:ASN:HB3	0.83	1.47	9	4
2:D:10:ILE:HD12	2:D:11:LEU:HD12	0.83	1.50	15	2
2:C:5:ILE:HD11	2:C:11:LEU:HD12	0.82	1.51	5	4
1:A:33:LYS:HG2	1:A:53:VAL:HG11	0.82	1.51	12	4
2:C:10:ILE:HD12	2:C:11:LEU:HD12	0.82	1.50	15	2
1:A:36:ILE:HG23	1:A:40:LEU:HD13	0.82	1.50	13	2
1:B:70:PHE:CZ	1:B:74:MET:HE2	0.81	2.10	5	2
1:B:33:LYS:HG2	1:B:53:VAL:HG11	0.81	1.51	12	4
2:C:10:ILE:CG2	2:C:11:LEU:HD22	0.81	2.05	3	1
1:A:70:PHE:CZ	1:A:74:MET:HE2	0.80	2.10	5	2
2:D:5:ILE:HD11	2:D:11:LEU:HD12	0.80	1.51	5	5
2:D:10:ILE:CG2	2:D:11:LEU:HD22	0.80	2.05	3	1
1:B:83:ALA:HB2	2:D:6:ASP:HB2	0.79	1.54	15	3
1:A:83:ALA:HB2	2:C:6:ASP:HB2	0.79	1.54	15	3
1:A:11:ILE:HD11	1:B:85:HIS:CE1	0.79	2.13	1	2
1:A:81:THR:OG1	1:B:74:MET:HE3	0.78	1.79	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:MET:HE3	1:B:81:THR:OG1	0.77	1.79	7	1
1:A:85:HIS:CE1	1:B:11:ILE:HD11	0.77	2.13	1	2
1:A:77:VAL:HG13	1:B:7:MET:HE3	0.77	1.54	5	1
1:B:53:VAL:HA	1:B:56:VAL:HG12	0.77	1.56	11	4
1:A:7:MET:HE3	1:B:77:VAL:HG13	0.77	1.54	5	1
1:B:17:TYR:CD1	1:B:35:LEU:HD11	0.77	2.15	4	11
1:B:11:ILE:HG23	1:B:70:PHE:CE1	0.76	2.15	3	1
1:A:17:TYR:CD1	1:A:35:LEU:HD11	0.76	2.14	4	11
1:B:73:PHE:O	1:B:77:VAL:HG22	0.76	1.79	3	6
1:B:10:LEU:HD13	1:B:74:MET:HE1	0.76	1.57	1	1
1:B:56:VAL:HB	2:D:10:ILE:HD12	0.76	1.56	13	1
1:A:13:VAL:HG12	1:A:35:LEU:HD11	0.76	1.58	6	4
1:A:73:PHE:O	1:A:77:VAL:HG22	0.76	1.79	3	6
1:A:60:LEU:HD13	1:A:76:PHE:HB2	0.76	1.58	17	3
1:A:53:VAL:HA	1:A:56:VAL:HG12	0.76	1.56	11	4
1:A:11:ILE:HG23	1:A:70:PHE:CE1	0.75	2.15	3	1
2:C:7:TRP:CD2	2:C:11:LEU:HD23	0.75	2.16	3	2
2:D:7:TRP:CD2	2:D:11:LEU:HD23	0.75	2.16	3	2
1:A:56:VAL:HB	2:C:10:ILE:HD12	0.75	1.56	13	1
1:A:10:LEU:HD13	1:A:74:MET:HE1	0.75	1.57	1	1
1:B:13:VAL:HG12	1:B:35:LEU:HD11	0.75	1.58	6	4
1:B:80:VAL:HG13	2:D:7:TRP:NE1	0.75	1.97	8	10
1:A:80:VAL:HG13	2:C:7:TRP:NE1	0.75	1.97	8	10
1:B:88:PHE:CZ	2:D:3:THR:HG23	0.74	2.17	11	1
1:A:14:PHE:CD2	1:A:27:LEU:HD13	0.74	2.17	11	1
1:B:77:VAL:O	1:B:81:THR:HG23	0.74	1.82	12	3
1:A:77:VAL:O	1:A:81:THR:HG23	0.74	1.82	12	3
1:B:60:LEU:HD13	1:B:76:PHE:HB2	0.74	1.58	17	3
1:B:9:ALA:O	1:B:13:VAL:HG23	0.73	1.83	1	6
1:B:13:VAL:HG21	1:B:39:GLU:OE1	0.73	1.83	12	1
1:A:88:PHE:CZ	2:C:3:THR:HG23	0.73	2.17	11	1
2:D:1:THR:HG22	2:D:6:ASP:HB2	0.73	1.60	2	2
1:A:33:LYS:CE	1:A:53:VAL:HG12	0.73	2.13	5	3
1:B:14:PHE:CD2	1:B:27:LEU:HD13	0.73	2.17	11	1
1:B:80:VAL:HG22	2:D:7:TRP:CE2	0.73	2.19	3	4
1:A:31:GLU:O	1:A:35:LEU:HD22	0.73	1.83	9	9
1:B:33:LYS:CE	1:B:53:VAL:HG12	0.73	2.13	5	3
1:A:13:VAL:HG21	1:A:39:GLU:OE1	0.73	1.83	12	1
1:A:7:MET:HE2	1:B:77:VAL:HG13	0.73	1.59	7	2
1:B:33:LYS:HG3	1:B:53:VAL:HG11	0.73	1.61	17	5
1:B:31:GLU:O	1:B:35:LEU:HD22	0.73	1.83	9	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LEU:HD11	1:A:74:MET:HE2	0.72	1.60	16	1
1:A:49:GLU:O	1:A:52:VAL:HG22	0.72	1.85	14	13
2:C:4:LYS:O	2:C:5:ILE:CG2	0.72	2.36	13	2
1:A:33:LYS:HG3	1:A:53:VAL:HG11	0.72	1.61	10	5
1:B:60:LEU:HD11	1:B:76:PHE:CG	0.72	2.20	7	1
1:A:80:VAL:HG22	2:C:7:TRP:CE2	0.72	2.19	3	4
1:B:10:LEU:HD11	1:B:74:MET:HE2	0.72	1.60	16	1
1:A:9:ALA:O	1:A:13:VAL:HG23	0.72	1.84	1	6
2:D:4:LYS:O	2:D:5:ILE:CG2	0.72	2.36	13	2
1:A:49:GLU:O	1:A:53:VAL:HG23	0.72	1.85	5	13
1:B:49:GLU:O	1:B:53:VAL:HG23	0.72	1.85	5	13
1:A:60:LEU:HD11	1:A:76:PHE:CG	0.72	2.20	7	1
1:B:59:THR:HG22	2:D:8:ASN:HB2	0.72	1.60	8	4
1:A:77:VAL:HG13	1:B:7:MET:HE2	0.72	1.59	7	2
2:C:7:TRP:HE3	2:C:10:ILE:HG21	0.71	1.46	14	5
2:C:7:TRP:CE3	2:C:10:ILE:HG21	0.71	2.20	14	11
1:B:17:TYR:CG	1:B:35:LEU:HD11	0.71	2.21	8	3
1:A:17:TYR:CG	1:A:35:LEU:HD11	0.71	2.21	8	3
2:D:7:TRP:HE3	2:D:10:ILE:HG21	0.71	1.46	14	5
1:B:53:VAL:HA	1:B:56:VAL:CG1	0.71	2.16	14	4
1:A:59:THR:HG22	2:C:8:ASN:HB2	0.71	1.60	8	4
1:A:76:PHE:CE1	1:A:80:VAL:HG21	0.71	2.21	2	9
2:D:7:TRP:CE3	2:D:10:ILE:HG21	0.71	2.20	14	11
1:B:17:TYR:CD1	1:B:35:LEU:HD21	0.71	2.21	14	2
2:C:10:ILE:CD1	2:C:11:LEU:HD12	0.71	2.16	15	1
1:B:76:PHE:CE1	1:B:80:VAL:HG21	0.70	2.21	2	9
2:D:5:ILE:N	2:D:5:ILE:HD13	0.70	2.01	5	1
2:D:10:ILE:HG23	2:D:11:LEU:HD12	0.70	1.62	9	4
1:A:60:LEU:HD21	1:A:76:PHE:CD1	0.70	2.21	12	3
2:D:10:ILE:CD1	2:D:11:LEU:HD12	0.70	2.16	15	1
2:C:10:ILE:HG23	2:C:11:LEU:HD12	0.70	1.62	9	4
1:B:60:LEU:HD21	1:B:76:PHE:CD1	0.70	2.21	12	3
1:A:17:TYR:CD1	1:A:35:LEU:HD21	0.70	2.21	14	2
1:B:49:GLU:O	1:B:52:VAL:HG22	0.70	1.85	14	13
2:C:4:LYS:O	2:C:5:ILE:CD1	0.70	2.40	1	5
1:A:53:VAL:HA	1:A:56:VAL:CG1	0.69	2.16	14	4
2:D:1:THR:HG22	2:D:6:ASP:OD2	0.69	1.87	6	1
2:D:4:LYS:O	2:D:5:ILE:CD1	0.69	2.40	1	5
1:B:8:VAL:HA	1:B:11:ILE:HG13	0.69	1.64	3	3
2:C:5:ILE:N	2:C:5:ILE:HD13	0.69	2.01	5	1
1:A:17:TYR:CD2	1:A:35:LEU:HD11	0.69	2.23	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:VAL:HA	1:A:11:ILE:HG13	0.68	1.64	3	3
1:A:33:LYS:CG	1:A:53:VAL:HG11	0.68	2.19	7	4
2:D:5:ILE:CD1	2:D:11:LEU:HD12	0.68	2.18	5	3
2:D:10:ILE:HG23	2:D:11:LEU:HD23	0.68	1.64	2	6
2:C:5:ILE:CD1	2:C:11:LEU:HD12	0.68	2.18	5	3
1:A:60:LEU:HD12	1:A:68:CYS:SG	0.68	2.29	16	2
2:C:10:ILE:HG23	2:C:11:LEU:HD23	0.68	1.64	2	6
1:B:33:LYS:CG	1:B:53:VAL:HG11	0.68	2.18	7	4
1:B:60:LEU:HD12	1:B:68:CYS:SG	0.68	2.29	16	2
1:A:82:THR:HG23	1:B:71:GLN:HA	0.68	1.65	1	2
1:A:7:MET:HE2	1:B:77:VAL:HG12	0.68	1.65	3	1
1:B:48:LYS:HB2	1:B:52:VAL:HG11	0.68	1.65	8	5
1:B:80:VAL:HG22	2:D:7:TRP:CD2	0.68	2.24	3	5
1:B:17:TYR:CD2	1:B:35:LEU:HD11	0.68	2.23	17	1
1:A:11:ILE:HD12	1:A:70:PHE:CE1	0.68	2.24	6	2
1:A:48:LYS:HG2	1:A:52:VAL:HG21	0.68	1.65	15	3
1:B:13:VAL:HG12	1:B:35:LEU:HG	0.67	1.65	13	7
1:A:48:LYS:HB2	1:A:52:VAL:HG11	0.67	1.65	8	5
1:A:80:VAL:HG22	2:C:7:TRP:CD2	0.67	2.24	3	5
1:A:83:ALA:HB1	2:C:5:ILE:HG22	0.67	1.67	13	1
2:D:5:ILE:HG12	2:D:11:LEU:HD22	0.67	1.66	7	2
1:A:13:VAL:HG12	1:A:35:LEU:HG	0.67	1.65	13	7
1:B:11:ILE:HD12	1:B:70:PHE:CE1	0.67	2.24	6	2
1:A:71:GLN:HA	1:B:82:THR:HG23	0.66	1.66	1	2
2:C:5:ILE:HG12	2:C:11:LEU:HD22	0.66	1.66	7	2
2:D:1:THR:HG22	2:D:6:ASP:CG	0.66	2.15	6	4
1:A:32:LEU:HD13	1:A:33:LYS:N	0.66	2.05	15	1
1:B:17:TYR:CG	1:B:35:LEU:HD21	0.66	2.26	15	2
1:A:27:LEU:O	1:A:67:GLU:HB2	0.66	1.90	1	3
1:B:27:LEU:O	1:B:67:GLU:HB2	0.66	1.90	1	3
1:B:48:LYS:HG2	1:B:52:VAL:HG21	0.65	1.66	14	4
1:B:81:THR:HG23	1:B:85:HIS:CG	0.65	2.26	10	1
1:A:81:THR:HG23	1:A:85:HIS:CG	0.65	2.26	10	1
1:A:17:TYR:CG	1:A:35:LEU:HD21	0.65	2.25	15	2
1:B:25:HIS:O	1:B:26:LYS:HG2	0.65	1.92	1	5
1:B:32:LEU:HD13	1:B:33:LYS:N	0.65	2.05	15	1
1:A:25:HIS:O	1:A:26:LYS:HG2	0.65	1.92	1	5
1:A:82:THR:HG23	1:B:71:GLN:HB2	0.65	1.68	15	1
1:A:71:GLN:HB2	1:B:82:THR:HG23	0.65	1.67	15	1
1:A:9:ALA:HB1	1:B:2:GLU:HB2	0.64	1.69	1	5
1:B:83:ALA:HB1	2:D:5:ILE:HG22	0.64	1.67	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:26:LYS:HE2	1:B:69:ASP:HB3	0.64	1.69	14	8
2:D:1:THR:HG22	2:D:6:ASP:CB	0.64	2.23	12	2
1:A:83:ALA:CB	2:C:5:ILE:HA	0.64	2.23	13	1
1:B:83:ALA:CB	2:D:5:ILE:HA	0.64	2.23	13	1
2:C:8:ASN:O	2:C:12:SER:HA	0.64	1.93	16	10
1:B:81:THR:HG23	1:B:85:HIS:HB3	0.64	1.70	13	5
1:B:83:ALA:HB1	2:D:1:THR:O	0.64	1.93	8	3
2:D:8:ASN:O	2:D:12:SER:HA	0.63	1.93	16	10
1:A:26:LYS:HE2	1:A:69:ASP:HB3	0.63	1.70	14	8
1:B:3:LEU:HD23	1:B:7:MET:CE	0.63	2.22	8	1
1:B:76:PHE:HA	1:B:79:MET:HG2	0.63	1.70	5	4
1:A:10:LEU:HD21	1:A:74:MET:CE	0.63	2.23	9	1
1:A:73:PHE:C	1:A:73:PHE:CD1	0.63	2.77	7	7
1:A:2:GLU:HB2	1:B:9:ALA:HB1	0.63	1.70	1	5
1:B:27:LEU:HD23	1:B:68:CYS:O	0.63	1.94	4	3
1:A:56:VAL:HG12	1:A:60:LEU:HD12	0.63	1.70	9	1
1:B:56:VAL:HG12	1:B:60:LEU:HD12	0.63	1.70	9	1
2:D:5:ILE:HD13	2:D:5:ILE:N	0.63	2.09	2	10
1:A:7:MET:O	1:A:11:ILE:HG12	0.62	1.94	8	2
1:B:10:LEU:HD21	1:B:74:MET:CE	0.62	2.23	9	1
2:D:7:TRP:O	2:D:8:ASN:CB	0.62	2.47	14	9
1:A:81:THR:HG23	1:A:85:HIS:HB3	0.62	1.70	13	5
1:A:3:LEU:HD23	1:A:7:MET:CE	0.62	2.22	8	1
1:B:73:PHE:C	1:B:73:PHE:CD1	0.62	2.77	7	7
1:A:27:LEU:HD23	1:A:31:GLU:HB3	0.62	1.70	11	6
1:A:27:LEU:HD23	1:A:68:CYS:O	0.62	1.94	4	4
1:A:36:ILE:HG23	1:A:40:LEU:CD1	0.62	2.07	17	5
1:B:32:LEU:HD12	1:B:53:VAL:CG1	0.62	2.25	8	1
1:B:60:LEU:HD21	1:B:79:MET:HE2	0.62	1.71	2	1
1:A:60:LEU:HD21	1:A:76:PHE:HB2	0.62	1.72	9	2
1:B:27:LEU:HD23	1:B:31:GLU:HB3	0.62	1.70	11	6
2:C:7:TRP:O	2:C:8:ASN:HB2	0.62	1.95	12	9
1:B:78:ALA:O	1:B:82:THR:HG23	0.62	1.94	7	4
2:C:5:ILE:HD13	2:C:5:ILE:N	0.62	2.09	2	9
1:A:80:VAL:HG13	2:C:7:TRP:HE1	0.62	1.55	4	7
1:A:32:LEU:HD12	1:A:53:VAL:CG1	0.61	2.25	8	1
1:A:10:LEU:HD13	1:A:74:MET:SD	0.61	2.35	11	1
1:B:10:LEU:HD13	1:B:74:MET:SD	0.61	2.35	11	1
1:A:59:THR:CG2	2:C:10:ILE:HG22	0.61	2.25	12	2
1:A:76:PHE:HA	1:A:79:MET:HG2	0.61	1.70	11	4
1:B:59:THR:CG2	2:D:10:ILE:HG22	0.61	2.25	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:ALA:O	1:A:82:THR:HG23	0.61	1.94	7	4
1:B:7:MET:O	1:B:11:ILE:HG12	0.61	1.94	8	2
2:C:7:TRP:O	2:C:8:ASN:CB	0.61	2.47	14	9
2:D:7:TRP:CZ3	2:D:10:ILE:HD13	0.61	2.30	13	1
2:C:7:TRP:CZ3	2:C:10:ILE:HD13	0.61	2.30	13	1
1:A:81:THR:HG21	1:B:74:MET:HE3	0.61	1.73	5	1
1:B:60:LEU:HD21	1:B:76:PHE:HB2	0.61	1.72	9	2
1:A:14:PHE:HB3	1:A:73:PHE:CE2	0.61	2.31	4	10
1:A:60:LEU:HD21	1:A:76:PHE:CA	0.61	2.26	6	1
1:A:14:PHE:CD1	1:A:14:PHE:C	0.60	2.79	4	16
1:B:27:LEU:N	1:B:68:CYS:O	0.60	2.34	2	5
1:A:60:LEU:HD21	1:A:79:MET:HE2	0.60	1.71	2	1
2:D:4:LYS:O	2:D:5:ILE:HD13	0.60	1.96	6	4
1:B:10:LEU:HD21	1:B:74:MET:HE1	0.60	1.73	6	3
1:B:60:LEU:HD21	1:B:76:PHE:CA	0.60	2.26	6	1
1:B:14:PHE:HB3	1:B:73:PHE:CE2	0.60	2.31	4	10
1:A:59:THR:HG23	2:C:9:LYS:H	0.60	1.57	6	6
1:B:36:ILE:HG23	1:B:40:LEU:CD1	0.60	2.23	7	5
1:B:11:ILE:HD12	1:B:70:PHE:CG	0.60	2.31	7	1
2:C:4:LYS:O	2:C:5:ILE:HG13	0.60	1.97	12	1
2:D:7:TRP:O	2:D:8:ASN:HB2	0.60	1.95	12	9
2:C:4:LYS:C	2:C:5:ILE:HG23	0.60	2.20	13	1
1:B:14:PHE:C	1:B:14:PHE:CD1	0.60	2.80	10	14
1:A:27:LEU:N	1:A:68:CYS:O	0.60	2.34	2	4
1:B:80:VAL:HG13	2:D:7:TRP:CZ2	0.60	2.32	1	3
1:B:53:VAL:CA	1:B:56:VAL:HG12	0.60	2.27	13	4
1:B:35:LEU:HD23	1:B:35:LEU:O	0.60	1.96	3	2
2:D:10:ILE:C	2:D:10:ILE:HD13	0.60	2.22	15	3
1:B:36:ILE:O	1:B:40:LEU:HB2	0.60	1.97	4	6
1:A:74:MET:HE3	1:B:81:THR:HG21	0.60	1.73	5	1
1:A:53:VAL:CA	1:A:56:VAL:HG12	0.60	2.27	6	4
2:C:10:ILE:C	2:C:10:ILE:HD13	0.60	2.22	15	3
1:B:59:THR:HG23	2:D:9:LYS:H	0.59	1.57	6	6
1:B:48:LYS:HB2	1:B:52:VAL:HG21	0.59	1.74	9	2
1:A:35:LEU:O	1:A:35:LEU:HD23	0.59	1.96	3	2
2:D:5:ILE:CG1	2:D:11:LEU:HG	0.59	2.27	3	5
1:B:59:THR:HG23	2:D:8:ASN:HB2	0.59	1.73	7	1
1:A:74:MET:HA	1:A:74:MET:HE2	0.59	1.74	10	2
1:B:60:LEU:HD21	1:B:76:PHE:N	0.59	2.13	6	1
1:A:11:ILE:HD12	1:A:70:PHE:CG	0.59	2.31	7	1
1:A:27:LEU:HD12	1:A:68:CYS:O	0.59	1.98	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:19:GLY:N	1:B:24:LYS:HB2	0.59	2.13	7	1
1:A:48:LYS:HB2	1:A:52:VAL:HG21	0.59	1.74	9	2
1:B:28:LYS:C	1:B:57:MET:HE1	0.59	2.22	12	1
1:A:80:VAL:HG13	2:C:7:TRP:CZ2	0.59	2.32	1	3
1:B:74:MET:HE2	1:B:74:MET:HA	0.59	1.73	13	2
1:B:52:VAL:O	1:B:56:VAL:HG12	0.59	1.98	14	1
1:B:13:VAL:HG12	1:B:35:LEU:CD1	0.59	2.28	10	3
1:A:10:LEU:HD21	1:A:74:MET:HE1	0.59	1.73	6	3
1:A:52:VAL:O	2:C:10:ILE:HD13	0.59	1.97	12	1
1:A:60:LEU:HD21	1:A:76:PHE:N	0.59	2.12	6	1
1:A:13:VAL:HG12	1:A:35:LEU:CD1	0.59	2.28	10	3
1:A:36:ILE:O	1:A:40:LEU:HB2	0.59	1.97	4	7
2:D:7:TRP:CG	2:D:11:LEU:HD23	0.59	2.33	14	2
1:A:11:ILE:HG22	1:A:15:HIS:CD2	0.59	2.33	8	1
1:A:79:MET:HE3	1:A:80:VAL:HG22	0.59	1.75	9	1
1:B:52:VAL:O	2:D:10:ILE:HD13	0.59	1.97	12	1
2:D:4:LYS:O	2:D:5:ILE:HG13	0.59	1.97	12	1
1:A:2:GLU:HG2	1:B:9:ALA:HB1	0.59	1.75	14	1
2:C:5:ILE:CG1	2:C:11:LEU:HG	0.59	2.27	3	4
1:A:52:VAL:O	1:A:56:VAL:HG12	0.59	1.98	14	1
2:C:7:TRP:CG	2:C:11:LEU:HD23	0.59	2.32	14	2
2:D:5:ILE:HG12	2:D:11:LEU:HG	0.59	1.75	13	2
1:B:60:LEU:HD21	1:B:76:PHE:HA	0.59	1.75	6	1
1:A:28:LYS:C	1:A:57:MET:HE1	0.59	2.22	12	1
2:C:5:ILE:O	2:C:7:TRP:CD1	0.58	2.56	10	6
2:C:4:LYS:O	2:C:5:ILE:HD13	0.58	1.96	6	4
1:A:59:THR:HG23	2:C:8:ASN:HB2	0.58	1.73	7	1
1:B:27:LEU:HD12	1:B:68:CYS:O	0.58	1.98	5	2
1:A:60:LEU:HD21	1:A:76:PHE:HA	0.58	1.74	6	1
2:D:4:LYS:O	2:D:5:ILE:HG12	0.58	1.98	16	6
1:A:40:LEU:HD11	1:B:3:LEU:HD22	0.58	1.76	1	1
2:D:5:ILE:O	2:D:7:TRP:CD1	0.58	2.56	10	6
1:A:79:MET:HE3	1:A:80:VAL:HG23	0.58	1.76	14	1
1:B:79:MET:HE3	1:B:80:VAL:HG23	0.58	1.76	14	1
1:B:80:VAL:HG13	2:D:7:TRP:HE1	0.58	1.57	16	7
2:C:4:LYS:O	2:C:5:ILE:HG12	0.58	1.98	16	6
1:A:10:LEU:HD13	1:A:74:MET:CE	0.58	2.29	1	1
1:B:56:VAL:O	1:B:60:LEU:HD12	0.58	1.99	1	1
2:D:10:ILE:HG23	2:D:11:LEU:N	0.58	2.14	13	15
1:A:19:GLY:N	1:A:24:LYS:HB2	0.58	2.13	7	1
1:B:11:ILE:HG22	1:B:15:HIS:CD2	0.58	2.33	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:VAL:HG12	1:B:7:MET:HE2	0.58	1.74	3	1
1:B:7:MET:HE1	1:B:74:MET:HE1	0.58	1.76	15	1
1:B:32:LEU:HD13	1:B:32:LEU:C	0.57	2.24	17	9
1:A:36:ILE:HA	1:A:40:LEU:CD1	0.57	2.27	11	3
1:A:32:LEU:C	1:A:32:LEU:HD13	0.57	2.25	17	8
2:D:4:LYS:C	2:D:5:ILE:HG23	0.57	2.20	13	1
2:C:5:ILE:HG12	2:C:11:LEU:HG	0.57	1.75	13	2
1:A:78:ALA:HB2	1:B:78:ALA:HB2	0.57	1.75	11	3
1:A:56:VAL:O	1:A:60:LEU:HD12	0.57	1.99	1	1
1:A:26:LYS:CE	1:A:69:ASP:HB3	0.57	2.30	5	1
1:A:32:LEU:HD23	1:A:57:MET:HE2	0.57	1.75	14	1
2:C:10:ILE:HG23	2:C:11:LEU:N	0.57	2.14	13	15
1:A:9:ALA:HB1	1:B:2:GLU:HG2	0.57	1.74	14	1
1:B:27:LEU:HD13	1:B:68:CYS:O	0.57	2.00	15	1
1:A:17:TYR:HD2	1:A:35:LEU:HD11	0.57	1.59	17	1
1:B:32:LEU:CD2	1:B:57:MET:HE2	0.57	2.30	14	1
1:A:32:LEU:CD2	1:A:57:MET:HE2	0.57	2.30	14	1
1:A:27:LEU:HD13	1:A:68:CYS:O	0.57	1.99	15	1
1:B:79:MET:HE3	1:B:80:VAL:HG22	0.57	1.75	9	1
1:B:26:LYS:CE	1:B:69:ASP:HB3	0.57	2.29	5	1
2:D:5:ILE:CG1	2:D:11:LEU:HD12	0.57	2.30	6	4
1:B:60:LEU:HD13	1:B:76:PHE:CE2	0.57	2.35	14	1
2:C:5:ILE:CG1	2:C:11:LEU:HD12	0.56	2.30	6	4
2:D:5:ILE:HD13	2:D:7:TRP:CG	0.56	2.35	9	4
1:A:70:PHE:HZ	1:A:74:MET:HE2	0.56	1.57	5	1
1:A:80:VAL:HG22	2:C:7:TRP:CG	0.56	2.35	11	2
1:B:80:VAL:HG22	2:D:7:TRP:CG	0.56	2.35	11	1
1:A:60:LEU:HD13	1:A:76:PHE:CE2	0.56	2.34	14	1
1:B:32:LEU:HD23	1:B:57:MET:HE2	0.56	1.75	14	1
1:A:36:ILE:CA	1:A:40:LEU:HD12	0.56	2.29	11	2
2:C:5:ILE:HD13	2:C:7:TRP:CG	0.56	2.36	7	4
1:A:4:GLU:O	1:A:8:VAL:HG23	0.56	2.01	5	3
1:B:4:GLU:O	1:B:8:VAL:HG23	0.56	2.01	4	3
1:B:70:PHE:HZ	1:B:74:MET:HE2	0.56	1.57	5	1
1:A:3:LEU:HD22	1:B:40:LEU:HD11	0.56	1.76	1	1
1:B:84:CYS:HB3	2:D:5:ILE:HG22	0.56	1.78	3	2
1:B:10:LEU:HD13	1:B:74:MET:CE	0.56	2.28	1	1
2:D:4:LYS:C	2:D:5:ILE:CD1	0.56	2.79	15	8
1:A:84:CYS:HB3	2:C:5:ILE:HG22	0.56	1.78	3	2
1:A:27:LEU:HD12	1:A:31:GLU:HG2	0.55	1.78	17	1
1:B:14:PHE:CD2	1:B:27:LEU:CD1	0.55	2.89	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:MET:HE1	1:A:74:MET:HE1	0.55	1.76	15	1
2:D:7:TRP:CE3	2:D:11:LEU:HD13	0.55	2.36	15	1
1:A:14:PHE:CD2	1:A:27:LEU:CD1	0.55	2.89	11	1
1:B:39:GLU:O	1:B:40:LEU:HD23	0.55	2.01	11	4
1:A:27:LEU:HB2	1:A:68:CYS:O	0.55	2.02	16	8
1:A:8:VAL:HA	1:A:11:ILE:CG1	0.55	2.32	3	1
1:B:27:LEU:HD12	1:B:31:GLU:HG2	0.55	1.78	17	1
1:A:14:PHE:CD2	1:A:70:PHE:HB2	0.55	2.36	2	6
1:B:14:PHE:CD2	1:B:70:PHE:HB2	0.54	2.36	2	6
2:C:4:LYS:O	2:C:5:ILE:CG1	0.54	2.55	12	5
2:D:4:LYS:O	2:D:5:ILE:CG1	0.54	2.56	12	5
1:B:60:LEU:HD13	1:B:72:GLU:OE1	0.54	2.02	2	1
1:B:36:ILE:HA	1:B:40:LEU:CD1	0.54	2.27	11	3
1:A:74:MET:HE1	1:B:78:ALA:HA	0.54	1.79	15	1
1:A:78:ALA:HA	1:B:74:MET:HE1	0.54	1.79	15	1
2:C:7:TRP:CE3	2:C:11:LEU:HD13	0.54	2.36	15	1
1:B:27:LEU:HB2	1:B:68:CYS:O	0.54	2.02	16	8
2:D:10:ILE:HG23	2:D:11:LEU:H	0.54	1.62	13	6
1:B:8:VAL:HA	1:B:11:ILE:CG1	0.54	2.33	3	1
1:B:29:LYS:HA	1:B:57:MET:HE3	0.54	1.79	2	1
1:A:3:LEU:HD13	1:B:40:LEU:HA	0.54	1.79	2	1
1:A:79:MET:HE3	2:C:6:ASP:O	0.54	2.03	15	1
1:A:29:LYS:HA	1:A:57:MET:HE3	0.54	1.79	2	1
1:B:33:LYS:HE2	1:B:53:VAL:HG12	0.54	1.78	5	1
1:B:59:THR:HG22	2:D:8:ASN:CB	0.54	2.33	15	1
1:A:39:GLU:O	1:A:40:LEU:HD23	0.54	2.01	11	4
2:C:4:LYS:C	2:C:5:ILE:CD1	0.54	2.80	16	6
1:B:36:ILE:CA	1:B:40:LEU:HD12	0.53	2.29	11	1
1:A:83:ALA:HB3	2:C:5:ILE:HA	0.53	1.80	5	1
1:B:79:MET:HE3	2:D:6:ASP:O	0.53	2.03	15	1
2:C:7:TRP:CG	2:C:11:LEU:HD13	0.53	2.38	15	1
1:A:70:PHE:HA	1:A:73:PHE:CD2	0.53	2.38	2	7
2:C:4:LYS:C	2:C:6:ASP:H	0.53	2.11	16	7
2:D:4:LYS:C	2:D:6:ASP:H	0.53	2.11	16	7
1:A:59:THR:HG22	2:C:8:ASN:CB	0.53	2.33	15	1
2:C:10:ILE:HG23	2:C:11:LEU:H	0.53	1.62	13	6
1:A:33:LYS:HE2	1:A:53:VAL:HG12	0.53	1.78	5	1
1:A:30:SER:O	1:A:34:GLU:HB3	0.53	2.03	17	1
1:B:70:PHE:HA	1:B:73:PHE:CD2	0.53	2.38	2	7
1:A:40:LEU:HA	1:B:3:LEU:HD13	0.53	1.79	2	1
1:B:8:VAL:HA	1:B:11:ILE:HG22	0.53	1.81	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:MET:CE	1:B:81:THR:HG21	0.53	2.34	5	1
1:B:83:ALA:HB3	2:D:5:ILE:HA	0.53	1.80	5	1
1:A:60:LEU:HD13	1:A:72:GLU:OE1	0.53	2.02	2	1
1:A:7:MET:HE2	1:B:77:VAL:CG2	0.53	2.34	11	2
1:A:81:THR:HA	1:A:85:HIS:HB2	0.53	1.80	11	1
1:A:26:LYS:C	1:A:27:LEU:HD13	0.53	2.29	12	3
1:A:59:THR:CG2	2:C:8:ASN:HB3	0.53	2.34	12	2
1:B:59:THR:CG2	2:D:8:ASN:HB3	0.53	2.34	12	2
1:A:76:PHE:O	1:A:80:VAL:HG23	0.53	2.04	16	1
2:C:10:ILE:CG2	2:C:11:LEU:N	0.53	2.72	4	11
2:D:10:ILE:CG2	2:D:11:LEU:N	0.53	2.72	4	12
1:B:32:LEU:C	1:B:32:LEU:HD12	0.53	2.29	14	1
1:B:30:SER:O	1:B:34:GLU:HB3	0.53	2.03	17	1
2:C:5:ILE:HB	2:C:7:TRP:CD1	0.53	2.39	5	10
1:B:33:LYS:CD	1:B:53:VAL:HG12	0.53	2.34	5	2
1:A:80:VAL:HA	2:C:5:ILE:O	0.53	2.04	5	1
1:A:77:VAL:CG2	1:B:7:MET:HE2	0.53	2.34	11	2
1:A:8:VAL:HA	1:A:11:ILE:HG22	0.52	1.81	7	2
1:A:19:GLY:CA	1:A:24:LYS:HB2	0.52	2.35	7	1
1:A:32:LEU:HD12	1:A:32:LEU:C	0.52	2.29	14	1
1:A:5:LYS:O	1:A:9:ALA:HB2	0.52	2.04	16	12
1:A:17:TYR:CD1	1:A:35:LEU:CD1	0.52	2.92	9	8
1:A:33:LYS:CD	1:A:53:VAL:HG12	0.52	2.34	5	2
2:D:3:THR:O	2:D:5:ILE:HD13	0.52	2.05	2	2
1:A:76:PHE:CZ	1:A:80:VAL:HG21	0.52	2.40	5	3
2:D:7:TRP:CG	2:D:11:LEU:HD13	0.52	2.38	15	1
2:D:5:ILE:HB	2:D:7:TRP:CD1	0.52	2.39	2	10
1:A:79:MET:HG3	1:A:80:VAL:N	0.52	2.20	2	5
1:B:17:TYR:CD1	1:B:35:LEU:CD1	0.52	2.93	2	8
1:B:26:LYS:C	1:B:27:LEU:HD13	0.52	2.29	12	3
1:B:81:THR:HA	1:B:85:HIS:HB2	0.52	1.80	11	1
1:B:7:MET:HE1	1:B:74:MET:CE	0.52	2.34	15	1
1:A:83:ALA:HB2	2:C:6:ASP:CB	0.52	2.31	8	2
1:A:7:MET:HE1	1:A:74:MET:CE	0.52	2.34	15	1
1:A:77:VAL:HG13	1:B:7:MET:SD	0.52	2.45	4	1
1:B:19:GLY:CA	1:B:24:LYS:HB2	0.52	2.35	7	1
1:B:82:THR:O	1:B:86:GLU:HB2	0.52	2.05	13	2
1:B:76:PHE:O	1:B:80:VAL:HG23	0.52	2.04	16	1
1:B:17:TYR:HD2	1:B:35:LEU:HD11	0.52	1.60	17	1
1:B:5:LYS:O	1:B:9:ALA:HB2	0.52	2.04	16	11
1:B:85:HIS:C	1:B:87:PHE:H	0.52	2.13	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:HD13	1:A:76:PHE:CD2	0.52	2.40	14	1
2:C:7:TRP:CE2	2:C:11:LEU:HD11	0.52	2.40	1	2
1:B:29:LYS:N	1:B:57:MET:HE1	0.52	2.20	15	2
1:A:85:HIS:CD2	1:B:70:PHE:CE2	0.51	2.99	3	3
1:B:76:PHE:CZ	1:B:80:VAL:HG21	0.51	2.40	5	3
1:B:80:VAL:HA	2:D:5:ILE:O	0.51	2.04	5	1
1:A:6:ALA:HB1	1:B:6:ALA:HB1	0.51	1.82	7	5
1:A:29:LYS:N	1:A:57:MET:HE1	0.51	2.20	15	2
1:A:81:THR:HG21	1:B:74:MET:CE	0.51	2.34	5	1
1:B:59:THR:CG2	2:D:8:ASN:HB2	0.51	2.35	1	2
2:D:7:TRP:CE2	2:D:11:LEU:HD11	0.51	2.40	1	2
1:B:77:VAL:O	1:B:81:THR:CG2	0.51	2.57	12	6
1:A:85:HIS:C	1:A:87:PHE:H	0.51	2.13	6	1
1:B:83:ALA:HB2	2:D:6:ASP:CB	0.51	2.32	8	1
1:A:32:LEU:HD13	1:A:32:LEU:C	0.51	2.30	15	1
1:B:75:ALA:O	1:B:79:MET:N	0.51	2.43	2	6
2:C:3:THR:O	2:C:5:ILE:HD13	0.51	2.05	2	2
2:C:10:ILE:HG23	2:C:11:LEU:CD2	0.51	2.36	11	6
1:A:18:SER:HB2	1:A:27:LEU:HD11	0.51	1.83	13	2
1:A:83:ALA:HB1	2:C:5:ILE:HA	0.51	1.82	13	2
1:A:13:VAL:HG22	1:B:2:GLU:OE2	0.51	2.06	12	1
1:A:14:PHE:CD2	1:A:18:SER:CB	0.51	2.94	17	2
1:B:14:PHE:CD2	1:B:18:SER:CB	0.51	2.94	17	2
1:A:82:THR:O	1:A:86:GLU:HB2	0.51	2.05	13	2
1:A:81:THR:HG21	1:B:74:MET:HE2	0.51	1.82	8	3
2:D:10:ILE:HG23	2:D:11:LEU:CD2	0.51	2.35	11	5
1:B:55:LYS:O	1:B:59:THR:N	0.51	2.43	9	7
2:C:10:ILE:HD12	2:C:11:LEU:HD22	0.51	1.82	14	1
1:A:19:GLY:HA2	1:A:24:LYS:HB3	0.51	1.83	17	1
1:B:60:LEU:HD23	1:B:79:MET:HE2	0.51	1.83	1	1
1:B:81:THR:HG23	1:B:85:HIS:CB	0.51	2.36	10	3
1:A:57:MET:HA	1:A:60:LEU:HD12	0.51	1.83	11	1
1:B:60:LEU:HD13	1:B:76:PHE:CD2	0.51	2.40	14	1
1:A:14:PHE:CE2	1:A:70:PHE:CB	0.51	2.94	2	4
1:A:74:MET:HE2	1:B:81:THR:HG21	0.51	1.82	8	3
1:B:7:MET:O	1:B:11:ILE:HG13	0.51	2.06	13	3
1:A:88:PHE:CE2	2:C:3:THR:HG23	0.51	2.41	11	1
1:B:14:PHE:CD1	1:B:14:PHE:C	0.50	2.89	2	2
1:A:32:LEU:HD23	1:A:68:CYS:CB	0.50	2.37	8	1
1:A:7:MET:O	1:A:11:ILE:HG13	0.50	2.06	13	3
1:B:88:PHE:CE2	2:D:3:THR:HG23	0.50	2.41	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:CYS:O	1:A:88:PHE:N	0.50	2.44	12	2
2:D:5:ILE:HD13	2:D:7:TRP:H	0.50	1.66	12	1
1:B:83:ALA:CB	2:D:5:ILE:HG22	0.50	2.36	13	1
1:B:32:LEU:HD23	1:B:68:CYS:HB3	0.50	1.83	9	2
1:A:75:ALA:O	1:A:79:MET:N	0.50	2.43	14	6
1:A:77:VAL:O	1:A:81:THR:CG2	0.50	2.57	12	6
2:D:7:TRP:CD2	2:D:11:LEU:CD2	0.50	2.95	14	2
2:C:4:LYS:CE	2:C:6:ASP:HA	0.50	2.37	5	1
1:A:70:PHE:CZ	1:B:85:HIS:CD2	0.50	2.99	6	2
1:B:32:LEU:HD23	1:B:68:CYS:CB	0.50	2.37	8	1
1:B:19:GLY:HA2	1:B:24:LYS:HB3	0.50	1.83	17	1
1:B:79:MET:HG3	1:B:80:VAL:N	0.50	2.21	15	5
2:C:7:TRP:CE3	2:C:10:ILE:CG2	0.50	2.94	2	8
1:B:70:PHE:CE2	1:B:74:MET:HE2	0.50	2.40	3	1
1:A:3:LEU:HD22	1:B:40:LEU:HD21	0.50	1.82	4	1
2:D:4:LYS:CE	2:D:6:ASP:HA	0.50	2.36	5	1
2:D:10:ILE:HD12	2:D:11:LEU:HD22	0.50	1.82	14	1
1:A:55:LYS:O	1:A:59:THR:N	0.50	2.43	9	7
1:B:83:ALA:HB1	2:D:5:ILE:HA	0.50	1.82	13	2
1:B:14:PHE:CD1	1:B:15:HIS:N	0.50	2.80	2	12
1:B:14:PHE:CE2	1:B:70:PHE:CB	0.50	2.94	2	3
1:A:81:THR:HG23	1:A:85:HIS:CB	0.50	2.37	4	3
1:B:18:SER:HB3	1:B:27:LEU:HD11	0.50	1.84	2	1
2:D:7:TRP:CE3	2:D:10:ILE:CG2	0.50	2.94	2	8
1:A:2:GLU:OE2	1:B:13:VAL:HG22	0.50	2.06	12	1
2:C:5:ILE:HD13	2:C:7:TRP:H	0.50	1.66	12	1
1:A:14:PHE:CD1	1:A:15:HIS:N	0.49	2.80	2	12
2:C:7:TRP:CD2	2:C:11:LEU:CD2	0.49	2.95	14	2
1:B:18:SER:HB2	1:B:27:LEU:HD11	0.49	1.83	13	2
1:B:60:LEU:HD22	1:B:68:CYS:SG	0.49	2.47	9	1
1:B:84:CYS:O	1:B:88:PHE:N	0.49	2.44	12	2
1:A:83:ALA:CB	2:C:5:ILE:C	0.49	2.85	12	7
1:B:27:LEU:CD2	1:B:68:CYS:O	0.49	2.61	16	8
1:A:8:VAL:CA	1:A:11:ILE:HG13	0.49	2.36	3	1
1:B:60:LEU:HD21	1:B:76:PHE:CG	0.49	2.42	9	1
1:B:79:MET:HE3	1:B:80:VAL:CG2	0.49	2.37	9	2
1:A:70:PHE:CE2	1:A:74:MET:HE2	0.49	2.41	3	1
1:B:11:ILE:HD12	1:B:70:PHE:CD1	0.49	2.42	6	2
1:A:10:LEU:HB3	1:A:73:PHE:CE1	0.49	2.43	11	2
1:A:60:LEU:HD22	1:A:68:CYS:SG	0.49	2.47	9	1
1:B:60:LEU:HD22	1:B:76:PHE:CD2	0.49	2.42	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:HD23	1:A:79:MET:HE2	0.49	1.83	1	1
1:B:13:VAL:CG1	1:B:35:LEU:HD11	0.49	2.37	10	2
1:A:27:LEU:CD2	1:A:68:CYS:O	0.49	2.61	16	8
1:A:85:HIS:CD2	1:B:70:PHE:CZ	0.49	3.00	6	2
1:A:81:THR:HG1	1:B:74:MET:HE3	0.49	1.67	7	1
1:A:79:MET:HE3	1:A:80:VAL:CG2	0.49	2.37	9	2
1:A:60:LEU:HD22	1:A:76:PHE:CD2	0.49	2.42	14	1
1:A:59:THR:CG2	2:C:8:ASN:HB2	0.49	2.35	1	3
1:B:83:ALA:CB	2:D:5:ILE:C	0.49	2.85	12	7
2:C:5:ILE:HG13	2:C:11:LEU:HG	0.49	1.84	2	3
1:A:70:PHE:CE2	1:B:85:HIS:CD2	0.49	3.00	10	3
1:A:7:MET:SD	1:B:77:VAL:HG13	0.49	2.47	4	1
1:B:57:MET:HA	1:B:60:LEU:HD12	0.49	1.83	11	1
2:D:5:ILE:HG13	2:D:11:LEU:HG	0.49	1.83	2	3
1:A:7:MET:HE2	1:B:77:VAL:HG23	0.49	1.83	8	2
1:A:32:LEU:HD23	1:A:68:CYS:HB3	0.49	1.83	9	2
2:D:10:ILE:HG13	2:D:11:LEU:HD23	0.49	1.84	12	1
1:A:60:LEU:HD21	1:A:76:PHE:CG	0.49	2.42	9	1
1:A:7:MET:CE	1:B:77:VAL:HG13	0.49	2.37	16	1
1:B:8:VAL:CA	1:B:11:ILE:HG13	0.49	2.36	3	1
1:A:11:ILE:HD12	1:A:70:PHE:CD1	0.49	2.43	6	2
1:B:35:LEU:HD22	1:B:35:LEU:H	0.49	1.67	5	8
2:C:10:ILE:HG13	2:C:11:LEU:HD23	0.49	1.84	12	1
1:A:77:VAL:HG23	1:B:7:MET:HE2	0.48	1.84	8	2
1:B:70:PHE:HA	1:B:73:PHE:CE2	0.48	2.43	11	1
1:A:3:LEU:HD13	1:B:40:LEU:HD11	0.48	1.85	14	1
1:A:18:SER:HB3	1:A:27:LEU:HD11	0.48	1.84	2	1
1:A:81:THR:OG1	1:A:85:HIS:CB	0.48	2.62	8	4
1:B:10:LEU:HB3	1:B:73:PHE:CE1	0.48	2.43	11	2
1:B:14:PHE:O	1:B:18:SER:CB	0.48	2.61	8	1
1:A:83:ALA:CB	2:C:5:ILE:HG22	0.48	2.36	13	1
1:A:35:LEU:O	1:A:39:GLU:N	0.48	2.45	14	5
1:A:59:THR:CG2	2:C:8:ASN:CB	0.48	2.91	15	1
1:B:59:THR:CG2	2:D:8:ASN:CB	0.48	2.91	15	2
1:A:34:GLU:O	1:A:38:ASN:N	0.48	2.47	5	6
2:D:5:ILE:CG1	2:D:11:LEU:CD1	0.48	2.92	10	3
1:A:35:LEU:HD22	1:A:35:LEU:H	0.48	1.67	5	8
2:D:4:LYS:O	2:D:6:ASP:N	0.48	2.46	16	6
2:D:4:LYS:O	2:D:5:ILE:C	0.48	2.57	17	5
1:A:70:PHE:HA	1:A:73:PHE:CE2	0.48	2.43	11	1
1:A:60:LEU:HD11	1:A:76:PHE:CE1	0.48	2.44	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:7:TRP:CB	2:D:11:LEU:HB2	0.48	2.39	15	1
1:A:14:PHE:CE2	1:A:70:PHE:HB2	0.48	2.44	7	11
1:B:49:GLU:O	1:B:53:VAL:CG2	0.48	2.62	1	4
1:A:14:PHE:O	1:A:18:SER:CB	0.48	2.61	8	1
1:B:13:VAL:HG12	1:B:35:LEU:CG	0.48	2.38	13	2
1:B:34:GLU:O	1:B:38:ASN:N	0.48	2.47	17	6
1:B:76:PHE:CE1	1:B:80:VAL:CG2	0.48	2.97	7	2
1:A:36:ILE:HG12	1:A:40:LEU:HD12	0.48	1.86	11	1
1:A:39:GLU:OE2	1:B:3:LEU:HD13	0.48	2.09	12	1
1:B:8:VAL:HA	1:B:11:ILE:CG2	0.48	2.39	4	1
1:A:28:LYS:HA	1:A:57:MET:HE1	0.48	1.86	3	1
1:A:8:VAL:HA	1:A:11:ILE:CG2	0.48	2.39	4	1
1:A:81:THR:HG21	1:B:74:MET:SD	0.48	2.49	13	1
1:B:27:LEU:CD1	1:B:68:CYS:O	0.47	2.62	15	7
1:B:10:LEU:HD11	1:B:74:MET:CE	0.47	2.39	6	1
1:A:3:LEU:HD13	1:B:39:GLU:OE2	0.47	2.09	12	1
1:A:10:LEU:HD12	1:A:74:MET:HE3	0.47	1.86	14	1
1:A:40:LEU:HD21	1:B:3:LEU:HD22	0.47	1.86	4	1
1:A:10:LEU:HD11	1:A:74:MET:CE	0.47	2.39	6	1
1:A:10:LEU:CB	1:A:73:PHE:CE1	0.47	2.98	11	2
1:A:84:CYS:HB2	2:C:5:ILE:HG22	0.47	1.85	2	1
2:C:4:LYS:O	2:C:6:ASP:N	0.47	2.46	16	6
1:A:27:LEU:CD1	1:A:68:CYS:O	0.47	2.62	15	6
2:C:5:ILE:CG1	2:C:11:LEU:CD1	0.47	2.92	10	3
1:A:14:PHE:CE2	1:A:27:LEU:HD13	0.47	2.43	11	1
1:B:14:PHE:CE2	1:B:70:PHE:HB2	0.47	2.44	7	10
1:A:17:TYR:CE2	1:A:34:GLU:CB	0.47	2.98	2	2
1:B:81:THR:CG2	1:B:82:THR:N	0.47	2.78	16	5
1:B:10:LEU:HD12	1:B:74:MET:HE3	0.47	1.86	14	1
1:A:40:LEU:HD21	1:B:3:LEU:HB2	0.47	1.85	17	1
1:B:81:THR:OG1	1:B:85:HIS:CB	0.47	2.62	8	4
1:B:70:PHE:CD1	1:B:70:PHE:C	0.47	2.93	7	2
1:B:14:PHE:CE2	1:B:27:LEU:HD13	0.47	2.43	11	1
2:D:6:ASP:O	2:D:7:TRP:C	0.47	2.58	14	1
2:C:10:ILE:CD1	2:C:11:LEU:HD22	0.47	2.40	2	1
2:D:10:ILE:HD13	2:D:11:LEU:HD22	0.47	1.87	2	1
1:A:56:VAL:HG13	1:A:57:MET:N	0.47	2.24	14	2
1:A:13:VAL:HG12	1:A:35:LEU:CG	0.47	2.39	17	2
2:C:7:TRP:CB	2:C:11:LEU:HB2	0.47	2.39	15	1
1:A:49:GLU:O	1:A:53:VAL:CG2	0.47	2.62	1	6
1:A:77:VAL:O	1:A:81:THR:CB	0.47	2.63	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:77:VAL:O	1:B:81:THR:CB	0.47	2.63	10	4
1:B:80:VAL:CG1	2:D:7:TRP:CZ2	0.47	2.97	1	2
1:A:81:THR:CG2	1:A:82:THR:N	0.47	2.78	16	5
2:C:5:ILE:N	2:C:5:ILE:CD1	0.47	2.73	5	2
1:A:11:ILE:CD1	1:A:70:PHE:CG	0.47	2.98	7	1
1:B:7:MET:HG3	1:B:8:VAL:N	0.47	2.25	8	1
1:B:35:LEU:HD22	1:B:35:LEU:N	0.47	2.24	14	2
2:C:6:ASP:O	2:C:7:TRP:C	0.47	2.58	14	1
1:A:60:LEU:CD1	1:A:76:PHE:CD1	0.47	2.98	3	2
1:B:80:VAL:HG13	2:D:7:TRP:CE2	0.47	2.45	17	4
1:B:84:CYS:HB2	2:D:5:ILE:HG22	0.47	1.86	2	1
1:B:28:LYS:HA	1:B:57:MET:HE1	0.47	1.86	3	1
1:A:27:LEU:HD12	1:A:31:GLU:HB3	0.47	1.86	4	2
1:A:7:MET:HE3	1:B:77:VAL:CG1	0.47	2.36	5	1
1:A:76:PHE:CD1	1:A:80:VAL:CG2	0.47	2.98	7	1
1:A:76:PHE:CE1	1:A:80:VAL:CG2	0.47	2.97	7	2
1:B:10:LEU:CB	1:B:73:PHE:CE1	0.47	2.97	11	2
1:A:7:MET:HG3	1:A:8:VAL:N	0.47	2.24	8	1
1:A:59:THR:HG21	2:C:10:ILE:CG2	0.47	2.39	12	2
1:A:74:MET:SD	1:B:81:THR:HG21	0.47	2.49	13	1
1:A:77:VAL:O	1:A:81:THR:HB	0.47	2.09	4	5
1:B:17:TYR:CE2	1:B:34:GLU:CB	0.47	2.97	2	2
2:C:4:LYS:O	2:C:5:ILE:C	0.47	2.57	17	5
1:B:11:ILE:CD1	1:B:70:PHE:CG	0.47	2.98	7	1
1:A:40:LEU:HD11	1:B:3:LEU:HD13	0.47	1.85	14	1
1:B:27:LEU:HD12	1:B:31:GLU:HB3	0.47	1.86	4	1
1:B:11:ILE:CD1	1:B:70:PHE:CE1	0.47	2.98	17	3
1:B:56:VAL:HG13	1:B:57:MET:N	0.47	2.24	14	2
1:B:85:HIS:C	1:B:87:PHE:N	0.47	2.72	6	1
1:A:7:MET:HE2	1:B:77:VAL:CG1	0.47	2.39	7	1
2:D:5:ILE:C	2:D:5:ILE:HD13	0.47	2.35	13	1
1:A:80:VAL:CG1	2:C:7:TRP:CZ2	0.46	2.97	1	2
1:B:77:VAL:O	1:B:81:THR:HB	0.46	2.10	10	5
2:C:10:ILE:HD13	2:C:11:LEU:HD22	0.46	1.87	2	1
2:C:5:ILE:C	2:C:5:ILE:HD13	0.46	2.36	13	1
1:B:52:VAL:HB	2:D:10:ILE:HD11	0.46	1.87	16	1
1:A:13:VAL:CG1	1:A:35:LEU:HD11	0.46	2.38	1	2
1:A:35:LEU:HD22	1:A:35:LEU:N	0.46	2.24	14	2
1:A:3:LEU:HB2	1:B:40:LEU:HD21	0.46	1.85	17	1
1:B:35:LEU:O	1:B:39:GLU:N	0.46	2.49	2	6
1:B:10:LEU:CD1	1:B:11:ILE:HD13	0.46	2.40	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LYS:CG	1:A:53:VAL:CG1	0.46	2.93	11	1
1:B:17:TYR:CD1	1:B:35:LEU:CD2	0.46	2.99	15	2
1:A:80:VAL:HG13	2:C:7:TRP:CE2	0.46	2.45	17	3
1:A:11:ILE:CD1	1:A:70:PHE:CE1	0.46	2.98	17	3
1:A:70:PHE:CD1	1:A:70:PHE:C	0.46	2.93	7	1
1:B:60:LEU:HD11	1:B:76:PHE:CE1	0.46	2.44	15	1
1:A:70:PHE:CD1	1:A:70:PHE:O	0.46	2.69	7	2
1:A:85:HIS:C	1:A:87:PHE:N	0.46	2.72	6	1
1:B:70:PHE:CD1	1:B:70:PHE:O	0.46	2.69	7	2
1:A:10:LEU:CD1	1:A:11:ILE:HD13	0.46	2.40	8	1
1:A:74:MET:HE3	1:A:74:MET:HA	0.46	1.87	8	2
1:A:85:HIS:CD2	1:B:11:ILE:CD1	0.46	2.99	12	1
1:B:10:LEU:HD12	1:B:74:MET:CE	0.46	2.40	14	1
1:A:36:ILE:O	1:A:40:LEU:N	0.46	2.49	17	4
2:D:10:ILE:CD1	2:D:11:LEU:HD22	0.46	2.40	2	1
1:B:76:PHE:CD1	1:B:80:VAL:CG2	0.46	2.98	7	1
1:A:74:MET:HG3	1:B:82:THR:HG23	0.46	1.88	8	1
1:A:39:GLU:OE1	1:B:3:LEU:HD13	0.46	2.11	12	1
1:B:36:ILE:O	1:B:40:LEU:N	0.46	2.47	1	4
1:A:70:PHE:CE2	1:A:74:MET:HG3	0.46	2.46	2	1
1:B:70:PHE:CE2	1:B:74:MET:HG3	0.46	2.46	2	1
1:A:60:LEU:HD21	1:A:76:PHE:CB	0.46	2.40	9	1
1:B:60:LEU:HD21	1:B:76:PHE:CB	0.46	2.40	9	1
2:D:4:LYS:CE	2:D:12:SER:OXT	0.46	2.64	17	2
1:A:60:LEU:HD11	1:A:79:MET:CE	0.46	2.41	14	1
1:B:17:TYR:CE1	1:B:35:LEU:CD1	0.46	2.99	14	2
1:B:60:LEU:CD1	1:B:76:PHE:CD1	0.46	2.98	3	2
1:B:74:MET:HE3	1:B:74:MET:HA	0.46	1.87	8	2
1:B:36:ILE:HG12	1:B:40:LEU:HD12	0.46	1.86	11	1
1:A:36:ILE:HG22	1:A:37:ASN:N	0.46	2.26	13	1
1:B:60:LEU:HD11	1:B:79:MET:CE	0.46	2.41	14	1
1:B:19:GLY:N	1:B:24:LYS:CB	0.46	2.79	7	1
2:C:5:ILE:HD12	2:C:6:ASP:N	0.46	2.26	7	1
1:A:8:VAL:HG12	1:A:12:ASP:OD1	0.46	2.10	11	1
1:B:8:VAL:HG12	1:B:12:ASP:OD1	0.46	2.10	11	1
1:A:17:TYR:CD1	1:A:35:LEU:CD2	0.46	2.99	15	2
1:A:59:THR:OG1	2:C:10:ILE:HB	0.46	2.11	17	1
1:B:56:VAL:CG1	1:B:76:PHE:CZ	0.46	2.99	1	1
2:D:5:ILE:N	2:D:5:ILE:CD1	0.46	2.73	5	1
1:A:60:LEU:CD1	1:A:76:PHE:CE2	0.46	2.99	14	1
1:A:52:VAL:HB	2:C:10:ILE:HD11	0.46	1.87	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:LEU:HD13	1:B:39:GLU:CD	0.45	2.36	12	1
1:A:11:ILE:CD1	1:B:85:HIS:CD2	0.45	2.99	12	1
2:C:4:LYS:CE	2:C:12:SER:OXT	0.45	2.64	17	2
1:B:60:LEU:CD1	1:B:76:PHE:CE2	0.45	2.99	14	1
1:B:79:MET:CE	1:B:80:VAL:HG23	0.45	2.41	14	1
1:A:56:VAL:CG1	1:A:76:PHE:CZ	0.45	2.99	1	1
1:A:53:VAL:O	1:A:57:MET:HB2	0.45	2.11	6	1
1:A:19:GLY:N	1:A:24:LYS:CB	0.45	2.80	7	1
1:B:56:VAL:HG12	1:B:60:LEU:HD11	0.45	1.88	10	1
1:A:3:LEU:HD22	1:B:40:LEU:CD2	0.45	2.40	11	1
1:A:40:LEU:CD2	1:B:3:LEU:HD22	0.45	2.41	11	1
1:A:10:LEU:HD12	1:A:74:MET:CE	0.45	2.41	14	1
1:A:60:LEU:CD1	1:A:76:PHE:CD2	0.45	3.00	14	1
1:B:26:LYS:CG	1:B:67:GLU:HB3	0.45	2.42	3	1
1:B:27:LEU:O	1:B:67:GLU:CG	0.45	2.65	17	5
1:A:36:ILE:HA	1:A:40:LEU:HG	0.45	1.88	5	1
1:B:52:VAL:O	1:B:56:VAL:N	0.45	2.49	17	3
2:D:5:ILE:HD12	2:D:6:ASP:N	0.45	2.26	7	1
1:B:11:ILE:CD1	1:B:70:PHE:CD1	0.45	3.00	11	1
1:A:81:THR:HG21	1:B:74:MET:HG3	0.45	1.88	3	1
1:A:75:ALA:O	1:A:79:MET:CB	0.45	2.65	9	2
1:B:69:ASP:OD1	1:B:69:ASP:N	0.45	2.50	8	3
1:B:59:THR:HG21	2:D:10:ILE:CG2	0.45	2.39	12	1
1:B:59:THR:HG22	2:D:8:ASN:HB3	0.45	1.88	4	1
1:A:52:VAL:O	1:A:56:VAL:N	0.45	2.46	11	3
1:B:88:PHE:O	1:B:88:PHE:CD2	0.45	2.70	6	1
2:D:5:ILE:HD12	2:D:5:ILE:N	0.45	2.27	12	1
1:A:74:MET:HB2	1:B:82:THR:HG22	0.45	1.88	14	1
1:A:27:LEU:O	1:A:67:GLU:CG	0.45	2.65	17	5
1:A:59:THR:HG22	2:C:8:ASN:HB3	0.45	1.88	4	1
1:A:88:PHE:O	1:A:88:PHE:CD2	0.45	2.70	6	1
1:A:11:ILE:CD1	1:A:70:PHE:CD1	0.45	3.00	11	1
1:B:83:ALA:HA	2:D:1:THR:O	0.45	2.12	13	1
1:A:17:TYR:CE1	1:A:35:LEU:CD1	0.45	2.99	14	2
1:A:69:ASP:OD1	1:A:69:ASP:N	0.45	2.50	8	4
1:A:36:ILE:O	1:A:40:LEU:HB3	0.45	2.12	13	1
1:A:79:MET:CE	1:A:80:VAL:HG23	0.45	2.41	14	1
1:A:76:PHE:CD1	1:A:80:VAL:HG21	0.45	2.47	4	1
1:B:74:MET:HE3	1:B:74:MET:CA	0.45	2.41	11	1
1:A:3:LEU:HD13	1:B:39:GLU:OE1	0.45	2.11	12	1
1:A:39:GLU:CD	1:B:3:LEU:HD13	0.45	2.36	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:THR:HG22	2:C:7:TRP:O	0.45	2.11	12	1
1:B:19:GLY:HA2	1:B:24:LYS:CB	0.45	2.42	17	1
2:D:5:ILE:O	2:D:7:TRP:N	0.45	2.50	3	2
1:A:86:GLU:O	1:A:87:PHE:HB2	0.45	2.12	6	1
1:B:75:ALA:O	1:B:79:MET:CB	0.45	2.65	9	2
1:B:33:LYS:CG	1:B:53:VAL:CG1	0.45	2.93	11	1
2:D:5:ILE:O	2:D:5:ILE:CG1	0.45	2.65	13	1
1:B:59:THR:OG1	2:D:10:ILE:HB	0.45	2.11	17	1
1:B:25:HIS:O	1:B:69:ASP:CB	0.44	2.65	7	6
1:A:10:LEU:O	1:A:73:PHE:CE2	0.44	2.70	3	1
1:B:10:LEU:O	1:B:73:PHE:CE2	0.44	2.70	3	1
2:C:5:ILE:O	2:C:7:TRP:N	0.44	2.50	3	2
1:B:76:PHE:CD1	1:B:80:VAL:HG21	0.44	2.47	4	1
1:A:74:MET:HE3	1:A:74:MET:CA	0.44	2.41	11	1
1:B:60:LEU:HD22	1:B:76:PHE:HB2	0.44	1.89	12	1
2:C:4:LYS:HG2	2:C:5:ILE:HD12	0.44	1.88	12	1
1:B:60:LEU:CD1	1:B:76:PHE:CD2	0.44	3.00	14	1
1:A:77:VAL:HG13	1:B:7:MET:CE	0.44	2.37	16	1
1:A:19:GLY:HA2	1:A:24:LYS:CB	0.44	2.42	17	1
2:D:4:LYS:C	2:D:6:ASP:N	0.44	2.75	16	6
1:A:26:LYS:CG	1:A:67:GLU:HB3	0.44	2.42	3	1
1:B:74:MET:O	1:B:78:ALA:CB	0.44	2.65	17	7
1:B:32:LEU:HD12	1:B:53:VAL:HG11	0.44	1.89	8	1
2:C:4:LYS:C	2:C:6:ASP:N	0.44	2.75	16	6
1:A:74:MET:O	1:A:78:ALA:CB	0.44	2.65	17	7
1:A:29:LYS:N	1:A:57:MET:HE3	0.44	2.27	5	1
1:A:14:PHE:CB	1:A:73:PHE:CE2	0.44	3.00	16	3
1:A:70:PHE:CZ	1:B:82:THR:HA	0.44	2.48	9	1
1:B:59:THR:HG22	2:D:7:TRP:O	0.44	2.12	12	1
1:B:36:ILE:O	1:B:40:LEU:HB3	0.44	2.12	13	1
2:C:5:ILE:HG13	2:C:11:LEU:HD12	0.44	1.90	16	1
2:C:7:TRP:CE2	2:C:11:LEU:CD1	0.44	3.00	1	1
1:B:36:ILE:HG22	1:B:37:ASN:N	0.44	2.26	13	1
1:B:53:VAL:O	1:B:57:MET:HB2	0.44	2.11	6	1
2:D:4:LYS:HD3	2:D:6:ASP:HB3	0.44	1.90	6	1
1:A:82:THR:HA	1:B:70:PHE:CZ	0.44	2.48	9	1
1:B:79:MET:HE1	2:D:7:TRP:HA	0.44	1.90	14	1
1:A:25:HIS:O	1:A:69:ASP:CB	0.44	2.65	7	5
1:B:33:LYS:HD2	1:B:53:VAL:HB	0.44	1.90	8	1
2:D:4:LYS:HG2	2:D:5:ILE:HD12	0.44	1.89	12	1
1:A:56:VAL:HG22	2:C:10:ILE:HG12	0.44	1.89	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:10:ILE:HD12	2:C:11:LEU:CD2	0.44	2.43	2	1
1:A:10:LEU:HD12	1:A:73:PHE:CD2	0.44	2.48	8	1
1:A:82:THR:HG23	1:B:74:MET:CG	0.44	2.42	8	1
1:B:14:PHE:CB	1:B:73:PHE:CE2	0.44	3.00	16	3
1:B:60:LEU:CD2	1:B:76:PHE:HB2	0.44	2.42	9	1
1:A:56:VAL:HG12	1:A:60:LEU:HD11	0.44	1.89	10	1
1:A:29:LYS:O	1:A:33:LYS:CB	0.44	2.66	14	1
1:B:56:VAL:O	1:B:60:LEU:HG	0.44	2.13	17	1
2:D:7:TRP:CE2	2:D:11:LEU:CD1	0.44	3.00	1	1
1:A:13:VAL:CG1	1:A:35:LEU:HD21	0.44	2.42	3	2
1:A:82:THR:HG23	1:B:74:MET:HG3	0.44	1.88	8	1
1:B:10:LEU:HD12	1:B:73:PHE:CD2	0.44	2.48	8	1
2:C:5:ILE:O	2:C:5:ILE:CG1	0.44	2.65	13	1
1:B:13:VAL:CG1	1:B:35:LEU:HD21	0.44	2.42	3	2
1:A:6:ALA:HB2	1:B:9:ALA:HB3	0.44	1.89	5	1
1:A:77:VAL:CG1	1:B:7:MET:HE3	0.44	2.36	5	1
1:A:32:LEU:HD12	1:A:53:VAL:HG11	0.44	1.88	8	1
1:A:78:ALA:HB2	1:B:78:ALA:CB	0.44	2.43	8	1
1:B:60:LEU:CD2	1:B:76:PHE:CD2	0.44	3.01	14	1
1:A:60:LEU:HD22	1:A:76:PHE:HB2	0.43	1.90	12	1
1:A:7:MET:HE2	1:B:81:THR:OG1	0.43	2.13	17	1
2:C:11:LEU:O	2:C:12:SER:OXT	0.43	2.36	17	1
1:A:71:GLN:CA	1:B:82:THR:HG23	0.43	2.42	1	1
1:B:69:ASP:N	1:B:69:ASP:OD1	0.43	2.52	3	1
1:A:27:LEU:O	1:A:67:GLU:HG3	0.43	2.13	5	2
1:A:77:VAL:CG1	1:B:7:MET:HE2	0.43	2.39	7	1
1:A:74:MET:CG	1:B:82:THR:HG23	0.43	2.42	8	1
2:C:4:LYS:C	2:C:5:ILE:HD12	0.43	2.39	12	2
1:A:70:PHE:CZ	1:A:74:MET:HG3	0.43	2.48	5	2
1:B:29:LYS:N	1:B:57:MET:HE3	0.43	2.28	5	1
1:B:36:ILE:HA	1:B:40:LEU:HG	0.43	1.88	5	1
1:B:87:PHE:O	1:B:88:PHE:CD1	0.43	2.72	6	1
1:A:73:PHE:CD1	1:A:74:MET:N	0.43	2.86	7	1
1:B:24:LYS:O	1:B:25:HIS:CB	0.43	2.66	14	2
1:A:82:THR:HG22	1:B:74:MET:HB2	0.43	1.88	14	1
1:B:25:HIS:O	1:B:25:HIS:CD2	0.43	2.71	16	1
2:D:10:ILE:HD12	2:D:11:LEU:CD2	0.43	2.43	2	1
1:A:24:LYS:O	1:A:25:HIS:CB	0.43	2.66	14	2
1:A:84:CYS:O	1:A:88:PHE:HB2	0.43	2.14	10	1
2:C:5:ILE:HD12	2:C:5:ILE:N	0.43	2.27	12	1
1:A:60:LEU:CD2	1:A:76:PHE:CD2	0.43	3.01	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:29:LYS:O	1:B:33:LYS:CB	0.43	2.66	14	1
1:B:70:PHE:CZ	1:B:74:MET:HG3	0.43	2.48	5	2
1:A:8:VAL:HA	1:A:11:ILE:CD1	0.43	2.43	3	1
1:B:86:GLU:O	1:B:87:PHE:HB2	0.43	2.12	6	1
1:B:73:PHE:CD1	1:B:74:MET:N	0.43	2.86	7	1
2:D:5:ILE:HD12	2:D:5:ILE:C	0.43	2.39	9	2
1:A:26:LYS:HA	1:A:69:ASP:HB3	0.43	1.91	12	2
2:D:4:LYS:C	2:D:5:ILE:HD12	0.43	2.39	12	2
1:A:25:HIS:O	1:A:25:HIS:CD2	0.43	2.71	16	1
1:B:56:VAL:HG22	2:D:10:ILE:HG12	0.43	1.88	16	1
1:A:6:ALA:HB1	1:B:6:ALA:O	0.43	2.14	17	1
1:A:57:MET:HE2	1:A:68:CYS:SG	0.43	2.54	3	1
1:B:11:ILE:C	1:B:11:ILE:HD13	0.43	2.39	4	1
1:A:14:PHE:CE2	1:A:70:PHE:N	0.43	2.87	6	1
1:A:69:ASP:OD1	1:A:72:GLU:CG	0.43	2.67	11	2
1:A:79:MET:HE1	2:C:7:TRP:HA	0.43	1.90	14	1
1:A:69:ASP:OD1	1:A:71:GLN:CG	0.43	2.67	1	2
2:D:7:TRP:CZ2	2:D:11:LEU:HD11	0.43	2.49	1	1
1:A:78:ALA:CB	1:B:78:ALA:CB	0.43	2.96	14	4
1:A:11:ILE:C	1:A:11:ILE:HD13	0.43	2.39	4	1
1:A:9:ALA:HB3	1:B:6:ALA:HB2	0.43	1.88	5	1
1:B:11:ILE:HG12	1:B:70:PHE:CE2	0.43	2.49	5	1
1:B:27:LEU:O	1:B:67:GLU:HG3	0.43	2.13	5	2
1:A:33:LYS:HD3	1:A:53:VAL:HG11	0.43	1.90	13	1
2:D:11:LEU:O	2:D:12:SER:OXT	0.43	2.36	17	1
1:B:84:CYS:C	1:B:86:GLU:N	0.43	2.75	7	5
1:B:55:LYS:O	1:B:59:THR:OG1	0.43	2.37	8	3
1:A:11:ILE:HG12	1:A:70:PHE:CE2	0.43	2.49	5	1
1:B:17:TYR:CG	1:B:35:LEU:CD1	0.43	3.01	8	1
2:D:10:ILE:CD1	2:D:10:ILE:C	0.43	2.91	15	1
2:D:5:ILE:HG13	2:D:11:LEU:HD12	0.43	1.90	16	1
1:A:26:LYS:HA	1:A:69:ASP:HA	0.43	1.91	7	4
1:A:87:PHE:O	1:A:88:PHE:CD1	0.43	2.72	6	1
1:A:86:GLU:O	1:B:25:HIS:CE1	0.43	2.72	12	1
1:B:69:ASP:OD1	1:B:71:GLN:CG	0.42	2.67	1	2
1:B:57:MET:HE2	1:B:68:CYS:SG	0.42	2.54	3	1
1:A:17:TYR:CE2	1:A:34:GLU:OE2	0.42	2.72	17	1
1:A:75:ALA:O	1:A:79:MET:HG2	0.42	2.14	11	2
2:C:5:ILE:HD12	2:C:5:ILE:C	0.42	2.39	9	2
1:A:56:VAL:O	1:A:60:LEU:N	0.42	2.52	9	1
1:A:78:ALA:O	1:A:82:THR:OG1	0.42	2.38	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:60:LEU:CD2	1:B:76:PHE:CD1	0.42	3.00	9	1
1:A:14:PHE:CE2	1:A:25:HIS:CD2	0.42	3.07	12	1
1:B:33:LYS:HD3	1:B:53:VAL:HG11	0.42	1.90	13	1
1:A:25:HIS:O	1:A:69:ASP:HB3	0.42	2.14	14	1
1:A:26:LYS:HG3	1:A:67:GLU:HB3	0.42	1.91	8	1
1:A:30:SER:O	1:A:34:GLU:CG	0.42	2.68	10	1
1:A:52:VAL:CG2	1:A:53:VAL:N	0.42	2.82	13	2
2:D:8:ASN:O	2:D:12:SER:N	0.42	2.48	15	1
1:A:25:HIS:O	1:A:26:LYS:CG	0.42	2.68	16	1
1:B:31:GLU:O	1:B:35:LEU:HB2	0.42	2.15	1	1
1:B:75:ALA:O	1:B:79:MET:HG2	0.42	2.14	11	2
1:B:26:LYS:HA	1:B:69:ASP:HA	0.42	1.91	7	3
1:B:69:ASP:OD1	1:B:72:GLU:CG	0.42	2.67	11	2
2:D:6:ASP:HA	2:D:12:SER:O	0.42	2.14	11	1
1:A:14:PHE:CZ	1:A:25:HIS:CD2	0.42	3.06	12	1
1:B:25:HIS:O	1:B:69:ASP:HB3	0.42	2.14	14	1
1:A:6:ALA:O	1:B:6:ALA:HB1	0.42	2.14	17	1
1:B:8:VAL:HA	1:B:11:ILE:CD1	0.42	2.43	3	1
1:B:14:PHE:CE2	1:B:70:PHE:N	0.42	2.87	6	1
1:B:2:GLU:O	1:B:5:LYS:HD2	0.42	2.14	7	1
1:B:14:PHE:CZ	1:B:25:HIS:CD2	0.42	3.06	12	1
2:D:4:LYS:O	2:D:5:ILE:CB	0.42	2.67	12	1
1:A:11:ILE:HG12	1:A:70:PHE:CZ	0.42	2.50	13	1
2:D:4:LYS:C	2:D:5:ILE:CG2	0.42	2.90	13	1
2:C:7:TRP:CE3	2:C:11:LEU:HG	0.42	2.50	16	1
1:A:56:VAL:O	1:A:60:LEU:HG	0.42	2.13	17	1
1:A:84:CYS:C	1:A:86:GLU:N	0.42	2.75	7	6
2:D:5:ILE:CD1	2:D:11:LEU:HB2	0.42	2.45	1	1
1:B:70:PHE:CE1	1:B:74:MET:CG	0.42	3.03	7	2
1:B:14:PHE:CE2	1:B:25:HIS:CD2	0.42	3.07	12	1
1:A:80:VAL:HG13	2:C:7:TRP:CD1	0.42	2.50	15	1
1:B:70:PHE:CE2	1:B:74:MET:CG	0.42	3.03	2	1
2:C:4:LYS:HD3	2:C:6:ASP:HB3	0.42	1.90	6	1
1:B:56:VAL:O	1:B:60:LEU:N	0.42	2.52	9	1
1:B:84:CYS:O	1:B:88:PHE:HB2	0.42	2.14	10	1
1:B:81:THR:OG1	1:B:85:HIS:CD2	0.42	2.73	11	1
1:A:25:HIS:CE1	1:B:86:GLU:O	0.42	2.72	12	1
1:B:74:MET:HE2	1:B:74:MET:CA	0.42	2.44	13	1
2:D:5:ILE:HB	2:D:7:TRP:HD1	0.42	1.75	15	1
1:B:33:LYS:HD2	1:B:53:VAL:CG1	0.42	2.45	16	1
1:A:19:GLY:CA	1:A:24:LYS:O	0.42	2.68	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:VAL:HG13	2:C:7:TRP:CZ3	0.42	2.50	4	2
1:B:86:GLU:O	1:B:87:PHE:CB	0.42	2.68	6	1
1:A:2:GLU:O	1:A:5:LYS:HD2	0.42	2.14	7	1
1:A:17:TYR:CG	1:A:35:LEU:CD1	0.42	3.01	8	2
1:A:81:THR:O	1:A:85:HIS:HB3	0.42	2.14	9	1
1:A:73:PHE:C	1:A:73:PHE:HD1	0.42	2.23	11	1
2:D:5:ILE:HG13	2:D:11:LEU:CD1	0.42	2.45	17	1
1:A:31:GLU:O	1:A:35:LEU:HB2	0.42	2.15	1	1
1:A:35:LEU:C	1:A:35:LEU:CD2	0.42	2.93	3	2
1:B:35:LEU:C	1:B:35:LEU:CD2	0.42	2.93	3	2
2:C:5:ILE:CD1	2:C:11:LEU:HB2	0.42	2.45	1	1
1:A:2:GLU:OE2	1:A:3:LEU:HD23	0.42	2.15	2	1
1:A:60:LEU:O	1:A:62:ASN:N	0.42	2.53	4	1
1:B:26:LYS:HG3	1:B:67:GLU:HB3	0.42	1.91	8	2
1:A:33:LYS:HD2	1:A:53:VAL:HB	0.42	1.90	8	1
1:B:48:LYS:O	1:B:49:GLU:CB	0.42	2.68	9	1
1:B:30:SER:O	1:B:34:GLU:CG	0.42	2.67	10	1
2:C:6:ASP:HA	2:C:12:SER:O	0.42	2.14	11	1
1:B:80:VAL:HG13	2:D:7:TRP:CD1	0.42	2.50	15	1
2:C:5:ILE:HB	2:C:7:TRP:HD1	0.42	1.75	15	1
2:D:7:TRP:CE3	2:D:11:LEU:HG	0.42	2.50	16	1
1:A:4:GLU:HG3	1:A:5:LYS:N	0.42	2.30	1	1
1:B:4:GLU:HG3	1:B:5:LYS:N	0.42	2.30	1	1
1:B:25:HIS:O	1:B:25:HIS:CG	0.42	2.72	16	2
1:B:56:VAL:HG13	2:D:7:TRP:CZ3	0.42	2.50	4	2
1:A:70:PHE:CE1	1:A:74:MET:CG	0.42	3.03	9	2
1:B:26:LYS:HA	1:B:69:ASP:HB3	0.42	1.91	12	2
1:B:49:GLU:N	1:B:52:VAL:CG2	0.42	2.83	12	2
1:B:81:THR:O	1:B:85:HIS:HB3	0.42	2.14	9	1
1:B:11:ILE:HG12	1:B:70:PHE:CZ	0.42	2.50	13	1
2:C:10:ILE:C	2:C:10:ILE:CD1	0.42	2.93	14	1
1:A:17:TYR:CZ	1:A:34:GLU:HG2	0.42	2.50	17	1
2:C:7:TRP:CZ2	2:C:11:LEU:HD11	0.41	2.49	1	1
1:A:70:PHE:CE1	1:B:86:GLU:HA	0.41	2.49	8	1
1:A:78:ALA:CB	1:B:78:ALA:HB2	0.41	2.43	8	1
1:A:49:GLU:N	1:A:52:VAL:CG2	0.41	2.83	12	2
1:A:60:LEU:CD2	1:A:76:PHE:CD1	0.41	3.00	9	2
1:A:76:PHE:CD2	1:A:77:VAL:N	0.41	2.88	10	1
1:A:88:PHE:CZ	2:C:3:THR:CG2	0.41	3.00	11	1
1:B:81:THR:HG23	1:B:82:THR:N	0.41	2.30	11	1
2:C:4:LYS:O	2:C:5:ILE:CB	0.41	2.67	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:TYR:CE1	1:A:35:LEU:HD11	0.41	2.49	14	1
1:A:69:ASP:OD2	1:A:71:GLN:CG	0.41	2.68	14	1
1:B:17:TYR:CE2	1:B:34:GLU:OE2	0.41	2.72	17	1
1:A:82:THR:HG23	1:B:71:GLN:CA	0.41	2.42	1	1
1:B:53:VAL:C	1:B:56:VAL:HG12	0.41	2.40	6	1
1:B:78:ALA:O	1:B:82:THR:CG2	0.41	2.67	7	1
1:A:86:GLU:HA	1:B:70:PHE:CE1	0.41	2.49	8	1
1:B:17:TYR:O	1:B:18:SER:C	0.41	2.63	8	1
1:B:76:PHE:CD2	1:B:77:VAL:N	0.41	2.88	10	1
1:A:81:THR:HG23	1:A:82:THR:N	0.41	2.30	11	1
1:B:17:TYR:CE1	1:B:35:LEU:HD11	0.41	2.49	14	1
1:B:83:ALA:HB3	2:D:5:ILE:CA	0.41	2.45	5	1
1:A:83:ALA:O	2:C:2:ARG:O	0.41	2.38	6	1
1:A:75:ALA:O	1:A:79:MET:HB3	0.41	2.15	9	1
1:B:75:ALA:O	1:B:79:MET:HB3	0.41	2.15	9	1
1:B:52:VAL:CG2	1:B:53:VAL:N	0.41	2.83	11	2
1:A:85:HIS:NE2	1:B:11:ILE:CD1	0.41	2.84	13	1
1:B:76:PHE:CD1	1:B:76:PHE:C	0.41	2.99	14	1
1:A:5:LYS:O	1:A:9:ALA:N	0.41	2.53	15	1
1:B:25:HIS:O	1:B:26:LYS:CG	0.41	2.67	16	1
1:B:17:TYR:CZ	1:B:34:GLU:HG2	0.41	2.50	17	1
1:A:83:ALA:HB3	2:C:5:ILE:CA	0.41	2.45	5	1
1:A:70:PHE:CE2	1:B:86:GLU:HA	0.41	2.51	9	1
1:A:86:GLU:HA	1:B:70:PHE:CE2	0.41	2.51	9	1
1:B:55:LYS:O	1:B:59:THR:CB	0.41	2.69	9	1
1:A:70:PHE:HB2	1:A:73:PHE:CE2	0.41	2.50	11	1
1:A:81:THR:OG1	1:A:85:HIS:CD2	0.41	2.73	11	1
1:A:19:GLY:H	1:A:24:LYS:HG2	0.41	1.74	17	1
1:B:62:ASN:O	1:B:63:ASP:CB	0.41	2.68	2	1
1:A:81:THR:O	1:A:85:HIS:CB	0.41	2.68	5	1
1:A:78:ALA:O	1:A:82:THR:CG2	0.41	2.67	7	1
1:A:55:LYS:O	1:A:59:THR:CB	0.41	2.69	9	1
1:B:69:ASP:OD2	1:B:71:GLN:CG	0.41	2.68	14	1
1:B:19:GLY:CA	1:B:24:LYS:O	0.41	2.68	17	1
2:C:10:ILE:CD1	2:C:11:LEU:CD2	0.41	2.99	2	1
1:A:74:MET:O	1:A:78:ALA:HB3	0.41	2.16	4	2
1:B:60:LEU:O	1:B:62:ASN:N	0.41	2.53	4	1
1:A:29:LYS:HB2	1:A:33:LYS:HE2	0.41	1.93	8	1
2:D:5:ILE:CG1	2:D:11:LEU:CG	0.41	2.98	10	1
2:C:10:ILE:CD1	2:C:10:ILE:C	0.41	2.91	15	1
1:A:33:LYS:HD2	1:A:53:VAL:CG1	0.41	2.44	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:VAL:CG1	1:A:76:PHE:CE1	0.41	3.04	1	1
1:A:62:ASN:O	1:A:63:ASP:CB	0.41	2.68	2	1
1:A:70:PHE:CE2	1:A:74:MET:CG	0.41	3.03	2	1
1:B:80:VAL:HA	2:D:7:TRP:CD1	0.41	2.51	3	1
1:A:17:TYR:O	1:A:18:SER:C	0.41	2.63	8	1
1:B:27:LEU:HD23	1:B:31:GLU:CB	0.41	2.45	9	1
2:C:5:ILE:CG1	2:C:11:LEU:CG	0.41	2.99	10	1
1:B:70:PHE:HB2	1:B:73:PHE:CE2	0.41	2.50	11	1
1:B:75:ALA:O	1:B:79:MET:HE2	0.41	2.15	12	1
1:A:11:ILE:CD1	1:B:85:HIS:NE2	0.41	2.84	13	1
1:A:74:MET:HE2	1:A:74:MET:CA	0.41	2.44	13	1
1:B:19:GLY:H	1:B:24:LYS:HG2	0.41	1.75	17	1
2:C:4:LYS:HD3	2:C:6:ASP:CB	0.41	2.46	17	1
2:D:4:LYS:HD3	2:D:6:ASP:CB	0.41	2.46	17	1
1:A:55:LYS:O	1:A:59:THR:OG1	0.41	2.38	3	2
1:B:27:LEU:O	1:B:68:CYS:N	0.41	2.44	12	1
1:A:72:GLU:O	1:A:76:PHE:N	0.41	2.51	13	1
1:A:6:ALA:CA	1:B:6:ALA:HB1	0.41	2.45	17	1
1:B:83:ALA:CB	2:D:5:ILE:O	0.41	2.69	1	1
2:C:4:LYS:C	2:C:5:ILE:HG13	0.41	2.41	1	1
2:C:3:THR:O	2:C:5:ILE:CD1	0.41	2.69	2	1
1:A:8:VAL:O	1:A:11:ILE:CG2	0.41	2.69	4	1
1:A:70:PHE:O	1:A:74:MET:CG	0.41	2.69	5	1
1:B:77:VAL:O	1:B:81:THR:HG22	0.41	2.16	5	1
1:B:81:THR:O	1:B:85:HIS:CB	0.41	2.68	5	1
1:A:86:GLU:O	1:A:87:PHE:CB	0.41	2.68	6	1
2:D:4:LYS:O	2:D:4:LYS:CD	0.41	2.69	6	1
1:A:27:LEU:HD23	1:A:31:GLU:CB	0.41	2.45	9	1
1:A:48:LYS:O	1:A:49:GLU:CB	0.41	2.68	9	1
1:A:13:VAL:O	1:A:16:GLN:CG	0.41	2.69	11	1
1:A:76:PHE:CA	1:A:79:MET:HG2	0.41	2.43	11	1
1:A:81:THR:OG1	1:A:85:HIS:HB3	0.41	2.16	11	1
1:A:35:LEU:HA	1:A:38:ASN:HB3	0.41	1.93	13	1
1:B:53:VAL:O	1:B:56:VAL:CG1	0.41	2.68	13	1
1:A:76:PHE:O	1:A:79:MET:HG3	0.41	2.16	14	1
1:A:79:MET:O	2:C:6:ASP:HB3	0.41	2.16	15	1
1:B:5:LYS:O	1:B:9:ALA:N	0.41	2.53	15	1
1:B:19:GLY:HA2	1:B:24:LYS:C	0.41	2.41	17	1
2:C:5:ILE:HG13	2:C:11:LEU:CD1	0.41	2.45	17	1
1:B:19:GLY:N	1:B:24:LYS:CG	0.41	2.84	7	1
1:B:13:VAL:O	1:B:16:GLN:CG	0.41	2.69	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:5:ILE:HG12	2:D:5:ILE:O	0.41	2.16	13	1
1:A:76:PHE:C	1:A:76:PHE:CD1	0.41	2.99	14	1
1:B:79:MET:O	2:D:6:ASP:HB3	0.41	2.16	15	1
1:A:35:LEU:CD2	1:A:39:GLU:CG	0.41	2.99	16	1
1:B:35:LEU:CD2	1:B:39:GLU:CG	0.41	2.98	16	1
1:A:83:ALA:CB	2:C:5:ILE:O	0.40	2.69	1	1
1:B:2:GLU:OE2	1:B:3:LEU:HD23	0.40	2.15	2	1
1:B:3:LEU:HD23	1:B:3:LEU:H	0.40	1.77	2	1
1:B:8:VAL:O	1:B:11:ILE:CG2	0.40	2.69	4	1
1:B:83:ALA:O	2:D:2:ARG:O	0.40	2.38	6	1
1:B:32:LEU:CD2	1:B:68:CYS:HB2	0.40	2.47	14	1
2:D:3:THR:O	2:D:3:THR:HG22	0.40	2.16	1	1
2:D:10:ILE:CD1	2:D:11:LEU:CD2	0.40	2.99	2	1
1:B:69:ASP:O	1:B:72:GLU:HG3	0.40	2.17	10	1
1:B:72:GLU:O	1:B:76:PHE:N	0.40	2.51	10	1
1:A:75:ALA:O	1:A:79:MET:HE2	0.40	2.15	12	1
1:A:36:ILE:O	1:A:40:LEU:HD22	0.40	2.16	13	1
1:B:56:VAL:CG1	1:B:76:PHE:CE1	0.40	3.04	1	1
1:A:60:LEU:HD22	1:A:72:GLU:O	0.40	2.16	2	1
1:B:31:GLU:O	1:B:35:LEU:CD2	0.40	2.66	4	1
1:A:26:LYS:HG2	1:A:67:GLU:HB3	0.40	1.92	5	1
1:A:53:VAL:C	1:A:56:VAL:HG12	0.40	2.40	6	1
1:A:81:THR:HB	1:A:85:HIS:HB3	0.40	1.94	7	1
2:C:5:ILE:CD1	2:C:7:TRP:CD1	0.40	2.94	7	1
1:A:8:VAL:HA	1:A:11:ILE:HG12	0.40	1.93	8	1
1:B:25:HIS:O	1:B:69:ASP:HB2	0.40	2.17	8	1
1:A:53:VAL:O	1:A:56:VAL:CG1	0.40	2.69	13	1
1:A:19:GLY:HA2	1:A:24:LYS:C	0.40	2.41	17	1
2:C:3:THR:HG22	2:C:3:THR:O	0.40	2.17	1	1
1:A:77:VAL:O	1:A:81:THR:HG22	0.40	2.16	5	1
2:C:4:LYS:O	2:C:4:LYS:CD	0.40	2.69	6	1
1:A:25:HIS:O	1:A:69:ASP:HB2	0.40	2.17	8	1
1:B:81:THR:CA	1:B:85:HIS:HB3	0.40	2.46	10	1
1:B:81:THR:OG1	1:B:85:HIS:HB3	0.40	2.16	11	1
2:C:5:ILE:HG12	2:C:11:LEU:CG	0.40	2.47	11	1
1:A:3:LEU:HD23	1:A:3:LEU:H	0.40	1.76	2	1
1:B:18:SER:CB	1:B:27:LEU:HD11	0.40	2.46	2	1
1:B:70:PHE:O	1:B:74:MET:CG	0.40	2.69	5	1
1:B:81:THR:HB	1:B:85:HIS:HB3	0.40	1.94	7	1
1:A:31:GLU:O	1:A:34:GLU:HB2	0.40	2.17	9	1
1:A:49:GLU:O	1:A:52:VAL:CG2	0.40	2.70	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:32:LEU:HD21	1:B:57:MET:CB	0.40	2.47	14	1
1:B:76:PHE:O	1:B:79:MET:HG3	0.40	2.16	14	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	76/91 (84%)	60±3 (80±4%)	13±2 (17±3%)	3±1 (3±2%)	5	35
1	B	76/91 (84%)	61±3 (80±4%)	13±2 (17±3%)	3±1 (3±2%)	5	35
2	C	10/12 (83%)	5±1 (49±9%)	3±1 (30±9%)	2±0 (21±3%)	0	2
2	D	10/12 (83%)	5±1 (49±9%)	3±1 (29±9%)	2±0 (21±3%)	0	2
All	All	2924/3502 (83%)	2224 (76%)	542 (19%)	158 (5%)	2	22

All 26 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	C	8	ASN	17
2	D	8	ASN	17
1	A	61	ASP	12
1	B	61	ASP	12
2	C	5	ILE	12
2	D	5	ILE	12
1	A	63	ASP	9
1	B	63	ASP	9
2	C	6	ASP	7
2	D	6	ASP	7
1	A	25	HIS	6
1	B	25	HIS	6
1	A	65	ASP	5
1	B	65	ASP	5
1	A	24	LYS	4
1	B	24	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	49	GLU	3
1	B	49	GLU	3
1	A	76	PHE	1
1	A	87	PHE	1
1	B	76	PHE	1
1	B	87	PHE	1
1	A	39	GLU	1
1	B	39	GLU	1
1	A	19	GLY	1
1	B	19	GLY	1

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	69/82 (84%)	44±3 (64±4%)	25±3 (36±4%)	1	9
1	B	69/82 (84%)	44±3 (64±4%)	25±3 (36±4%)	1	9
2	C	11/12 (92%)	6±1 (58±8%)	5±1 (42±8%)	0	4
2	D	12/12 (100%)	6±1 (53±7%)	6±1 (47±7%)	0	2
All	All	2737/3196 (86%)	1727 (63%)	1010 (37%)	1	8

All 143 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	D	1	THR	17
1	A	14	PHE	16
1	A	26	LYS	16
1	A	36	ILE	16
1	A	73	PHE	16
1	B	14	PHE	16
1	B	26	LYS	16
1	B	36	ILE	16
1	B	73	PHE	16
2	C	10	ILE	16
2	D	10	ILE	16

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Mol	Chain	Res	Type	Models (Total)
1	A	87	PHE	14
1	B	87	PHE	14
2	C	9	LYS	14
2	D	9	LYS	14
1	A	5	LYS	13
1	A	48	LYS	13
1	B	5	LYS	13
1	B	48	LYS	13
1	A	67	GLU	13
1	B	67	GLU	13
2	C	5	ILE	13
2	D	5	ILE	13
1	A	57	MET	12
1	B	57	MET	12
2	C	4	LYS	12
2	D	4	LYS	12
1	A	3	LEU	11
1	B	3	LEU	11
1	A	58	GLU	11
1	A	60	LEU	11
1	B	58	GLU	11
1	B	60	LEU	11
1	A	35	LEU	10
1	B	35	LEU	10
1	A	29	LYS	10
1	B	29	LYS	10
1	A	68	CYS	10
1	B	68	CYS	10
1	A	12	ASP	9
1	A	16	GLN	9
1	B	12	ASP	9
1	B	16	GLN	9
1	A	34	GLU	9
1	B	34	GLU	9
1	A	24	LYS	8
1	A	69	ASP	8
1	B	24	LYS	8
1	B	69	ASP	8
1	A	28	LYS	8
1	B	28	LYS	8
1	A	49	GLU	8
1	B	49	GLU	8

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Mol	Chain	Res	Type	Models (Total)
1	A	10	LEU	8
1	B	10	LEU	8
1	A	53	VAL	7
1	A	63	ASP	7
1	A	84	CYS	7
1	B	53	VAL	7
1	B	63	ASP	7
1	B	84	CYS	7
2	C	11	LEU	7
2	D	11	LEU	7
1	A	15	HIS	6
1	A	33	LYS	6
1	A	55	LYS	6
1	B	15	HIS	6
1	B	33	LYS	6
1	B	55	LYS	6
2	C	8	ASN	6
2	D	8	ASN	6
1	A	7	MET	6
1	B	7	MET	6
1	A	4	GLU	5
1	B	4	GLU	5
1	A	11	ILE	5
1	A	30	SER	5
1	A	86	GLU	5
1	B	11	ILE	5
1	B	30	SER	5
1	B	86	GLU	5
1	A	72	GLU	5
1	B	72	GLU	5
1	A	1	SER	5
1	A	50	GLN	5
1	B	1	SER	5
1	B	50	GLN	5
2	C	2	ARG	5
2	D	2	ARG	5
1	A	31	GLU	5
1	B	31	GLU	5
1	A	40	LEU	4
1	A	77	VAL	4
1	B	2	GLU	4
1	B	40	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	B	77	VAL	4
1	A	39	GLU	4
1	A	51	GLU	4
1	A	70	PHE	4
1	A	79	MET	4
1	B	39	GLU	4
1	B	51	GLU	4
1	B	70	PHE	4
1	B	79	MET	4
1	A	59	THR	4
1	A	81	THR	4
1	B	59	THR	4
1	B	81	THR	4
1	A	18	SER	4
1	B	18	SER	4
1	A	65	ASP	4
1	B	65	ASP	4
1	A	32	LEU	4
1	B	32	LEU	4
1	A	61	ASP	3
1	A	74	MET	3
1	A	85	HIS	3
1	B	61	ASP	3
1	B	74	MET	3
1	B	85	HIS	3
1	A	27	LEU	3
1	A	54	ASP	3
1	B	27	LEU	3
1	B	54	ASP	3
2	C	3	THR	3
2	D	3	THR	3
1	A	71	GLN	3
1	B	71	GLN	3
1	A	2	GLU	3
1	A	62	ASN	3
1	B	62	ASN	3
1	A	52	VAL	2
1	B	52	VAL	2
2	C	12	SER	2
2	D	12	SER	2
1	A	88	PHE	1
1	B	88	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	76	PHE	1
1	B	76	PHE	1
1	A	82	THR	1
1	B	82	THR	1
1	A	37	ASN	1
1	B	37	ASN	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](#)

There are no ligands in this entry.

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