Full wwPDB NMR Structure Validation Report (i)

Feb 8, 2022 – 02:56 PM EST

PDB ID	:	1CIR
Title	:	COMPLEX OF TWO FRAGMENTS OF CI2 [(1-40)(DOT)(41-64)]
Authors	:	Davis, B.J.; Fersht, A.R.
Deposited on	:	1995-10-02

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

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

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

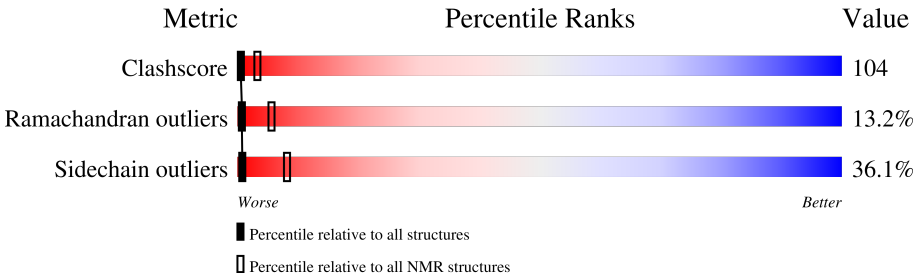
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	40	
2	B	24	

2 Ensemble composition and analysis (i)

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 11 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:3-A:32, B:43-B:63 (51)	0.29	11

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1047 atoms, of which 542 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CHYMOTRYPSIN INHIBITOR 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	39	632	197	330	47	57	1	0

- Molecule 2 is a protein called CHYMOTRYPSIN INHIBITOR 2.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	24	415	128	212	39	36	0

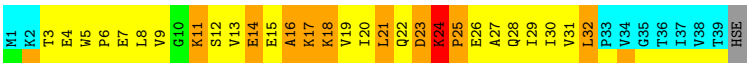
4 Residue-property plots

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: CHYMOTRYPSIN INHIBITOR 2

Chain A:



• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

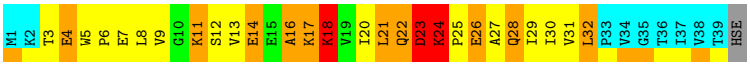
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:



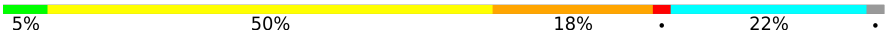
• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

4.2.2 Score per residue for model 2

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:



• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

4.2.3 Score per residue for model 3

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:

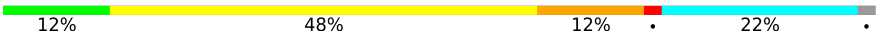
• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

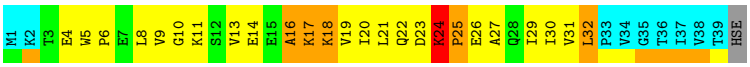
Chain B:

4.2.4 Score per residue for model 4

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:





• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

4.2.5 Score per residue for model 5

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:

• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

4.2.6 Score per residue for model 6

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:

• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

4.2.7 Score per residue for model 7

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:

• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

4.2.8 Score per residue for model 8

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:

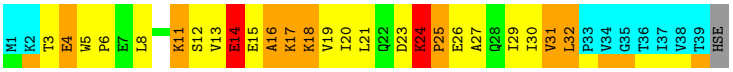
• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

4.2.9 Score per residue for model 9

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:



• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

4.2.10 Score per residue for model 10

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:

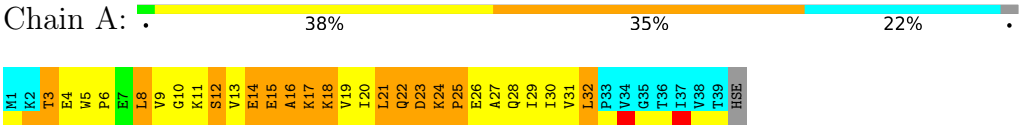
• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

4.2.11 Score per residue for model 11 (medoid)

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:



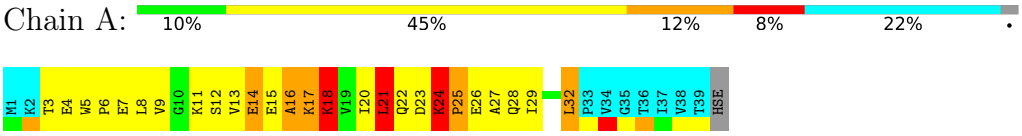
• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

4.2.12 Score per residue for model 12

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:



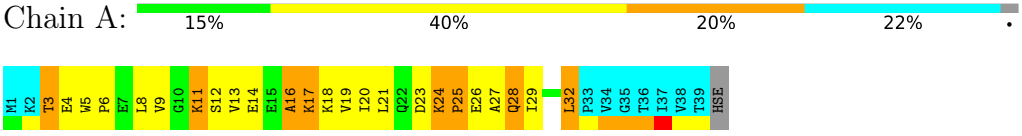
• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

4.2.13 Score per residue for model 13

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:



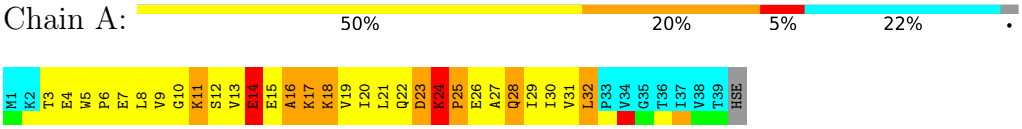
• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

4.2.14 Score per residue for model 14

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:



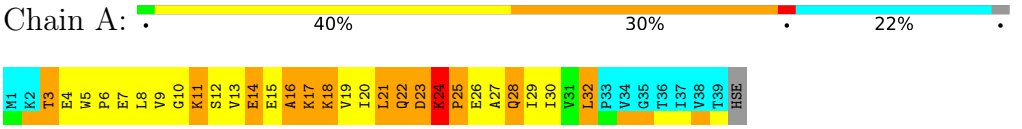
• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

4.2.15 Score per residue for model 15

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:



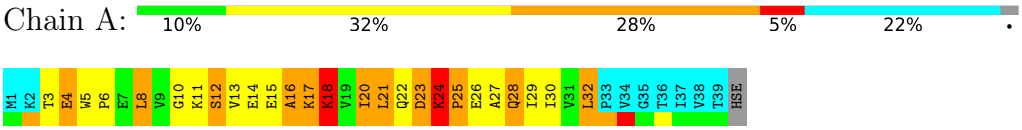
• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

4.2.16 Score per residue for model 16

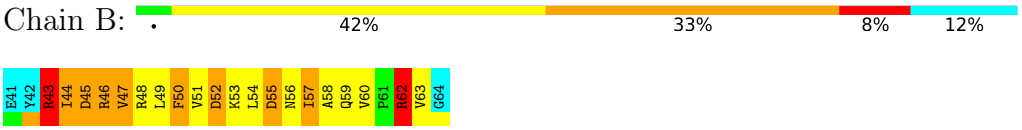
• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:



• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

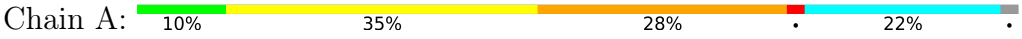
Chain B:



4.2.17 Score per residue for model 17

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:



• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

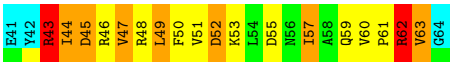
4.2.18 Score per residue for model 18

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:

• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

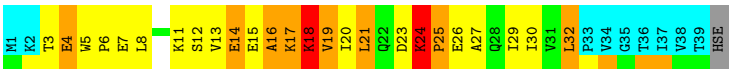
Chain B:



4.2.19 Score per residue for model 19

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:



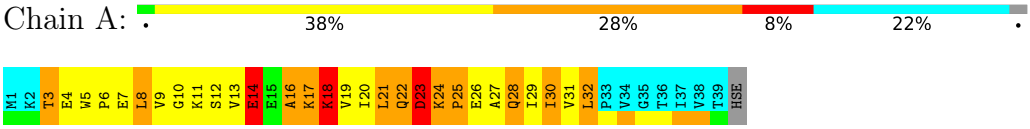
• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

4.2.20 Score per residue for model 20

• Molecule 1: CHYMOTRYPSIN INHIBITOR 2

Chain A:



• Molecule 2: CHYMOTRYPSIN INHIBITOR 2

Chain B:

5 Refinement protocol and experimental data overview

Of the ? calculated structures, 20 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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
2	B	0.0±0.0	3.8±0.4
All	All	0	76

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)
2	B	43	ARG	Sidechain	20
2	B	46	ARG	Sidechain	19
2	B	48	ARG	Sidechain	19
2	B	62	ARG	Sidechain	18

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	238	253	253	68±7
2	B	177	192	192	47±8
All	All	8300	8900	8900	1789

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 104.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LEU:HD11	2:B:50:PHE:CE1	1.05	1.86	19	14
1:A:32:LEU:HD22	2:B:50:PHE:CD1	1.03	1.87	18	1
2:B:47:VAL:CG2	2:B:63:VAL:HG23	1.03	1.83	12	19
2:B:47:VAL:HG23	2:B:63:VAL:HG23	0.98	1.34	14	6
1:A:13:VAL:HG22	2:B:49:LEU:HD21	0.97	1.36	17	3
1:A:8:LEU:HD22	1:A:8:LEU:O	0.96	1.58	10	1
1:A:8:LEU:HD23	1:A:9:VAL:N	0.95	1.77	3	1
1:A:32:LEU:HD21	2:B:50:PHE:CE1	0.95	1.97	20	9
1:A:31:VAL:HG22	2:B:49:LEU:HD23	0.94	1.36	11	4
2:B:49:LEU:HD11	2:B:57:ILE:HD12	0.93	1.39	10	4
1:A:8:LEU:HD21	2:B:57:ILE:HG21	0.92	1.40	6	5
1:A:3:THR:HG22	1:A:24:LYS:CD	0.91	1.95	10	8
1:A:32:LEU:HD23	1:A:32:LEU:N	0.90	1.80	17	9
1:A:5:TRP:O	1:A:8:LEU:HD12	0.89	1.66	10	1
1:A:16:ALA:HB2	2:B:57:ILE:HD11	0.87	1.42	9	11
1:A:20:ILE:HG21	1:A:29:ILE:HB	0.87	1.46	16	19
1:A:30:ILE:HG22	1:A:32:LEU:HD22	0.86	1.45	6	6
1:A:3:THR:HG22	1:A:24:LYS:HD2	0.86	1.48	10	8
1:A:32:LEU:HD21	2:B:50:PHE:CD1	0.86	2.06	4	10
1:A:27:ALA:HB1	2:B:63:VAL:HG21	0.86	1.46	14	14
1:A:32:LEU:HD12	2:B:50:PHE:CE1	0.86	2.06	6	3
1:A:31:VAL:HG13	2:B:49:LEU:HD12	0.85	1.48	20	1
1:A:23:ASP:OD1	1:A:27:ALA:HB3	0.85	1.71	18	2
1:A:32:LEU:O	2:B:51:VAL:HG22	0.84	1.72	12	8
1:A:31:VAL:C	1:A:32:LEU:HD23	0.84	1.93	17	5
1:A:31:VAL:HG13	2:B:49:LEU:HD13	0.82	1.47	7	1
1:A:12:SER:O	1:A:16:ALA:HB2	0.82	1.75	3	1
2:B:47:VAL:HG21	2:B:63:VAL:HG23	0.81	1.50	15	7
1:A:8:LEU:HD21	1:A:16:ALA:HB2	0.81	1.50	13	3
1:A:32:LEU:HD11	2:B:50:PHE:CD1	0.80	2.11	8	9
2:B:47:VAL:HG11	2:B:61:PRO:HB2	0.80	1.54	4	9
1:A:8:LEU:HD13	1:A:9:VAL:N	0.79	1.92	10	1
2:B:47:VAL:HG11	2:B:61:PRO:CB	0.79	2.08	1	6
1:A:8:LEU:HD13	1:A:8:LEU:C	0.79	1.97	10	1
1:A:32:LEU:HD11	2:B:50:PHE:CZ	0.78	2.13	13	2
1:A:16:ALA:C	1:A:20:ILE:HD12	0.78	1.98	19	13
1:A:20:ILE:HD13	1:A:29:ILE:HD13	0.78	1.56	4	13
1:A:24:LYS:HB2	1:A:25:PRO:HD3	0.76	1.57	8	8
1:A:3:THR:HG22	2:B:63:VAL:O	0.76	1.79	17	2
1:A:31:VAL:HG13	2:B:49:LEU:HG	0.76	1.57	4	2
1:A:24:LYS:CB	1:A:25:PRO:CD	0.75	2.65	11	20
1:A:32:LEU:HD12	2:B:50:PHE:CZ	0.75	2.16	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LEU:HD13	2:B:50:PHE:CE1	0.75	2.16	18	1
1:A:16:ALA:HB2	2:B:57:ILE:CD1	0.75	2.11	9	10
1:A:5:TRP:NE1	1:A:20:ILE:HD12	0.74	1.98	18	3
1:A:32:LEU:HD11	2:B:50:PHE:HE1	0.74	1.43	16	7
1:A:32:LEU:HD21	2:B:49:LEU:N	0.74	1.98	14	1
2:B:54:LEU:HD23	2:B:54:LEU:O	0.73	1.83	15	2
2:B:47:VAL:HG22	2:B:63:VAL:HG23	0.73	1.59	18	11
1:A:13:VAL:HG22	2:B:49:LEU:CD2	0.72	2.14	17	4
1:A:13:VAL:HG23	2:B:51:VAL:HG11	0.72	1.61	5	2
1:A:30:ILE:HG22	1:A:32:LEU:CD2	0.72	2.14	6	3
1:A:5:TRP:O	1:A:8:LEU:HD22	0.71	1.85	3	3
1:A:31:VAL:HG22	2:B:49:LEU:HB3	0.71	1.59	20	1
1:A:16:ALA:CA	1:A:20:ILE:HD12	0.71	2.16	13	7
2:B:54:LEU:HD22	2:B:54:LEU:N	0.70	2.02	10	1
1:A:8:LEU:HD11	2:B:57:ILE:HD13	0.70	1.64	11	3
1:A:16:ALA:HB1	2:B:49:LEU:CD2	0.70	2.15	9	3
1:A:8:LEU:HD21	1:A:16:ALA:CB	0.69	2.17	13	2
1:A:32:LEU:CD1	2:B:50:PHE:CE1	0.69	2.76	5	19
1:A:8:LEU:HD21	1:A:16:ALA:HA	0.69	1.65	19	4
1:A:32:LEU:CD2	2:B:50:PHE:CD1	0.69	2.73	18	3
1:A:3:THR:HG22	1:A:24:LYS:CG	0.68	2.17	10	2
2:B:49:LEU:C	2:B:49:LEU:HD13	0.68	2.10	20	2
1:A:13:VAL:HG23	2:B:51:VAL:CG1	0.67	2.20	5	1
1:A:24:LYS:HB3	1:A:25:PRO:HD2	0.67	1.67	2	2
1:A:32:LEU:CD2	2:B:50:PHE:CE1	0.67	2.75	20	3
1:A:32:LEU:N	1:A:32:LEU:CD2	0.66	2.58	5	9
1:A:9:VAL:HG23	2:B:60:VAL:CG2	0.66	2.21	20	10
1:A:24:LYS:CB	1:A:25:PRO:HD3	0.66	2.21	4	15
1:A:16:ALA:HB1	2:B:49:LEU:HD23	0.65	1.66	9	1
1:A:3:THR:HG22	1:A:24:LYS:CE	0.65	2.20	20	3
1:A:19:VAL:HG12	1:A:23:ASP:OD2	0.65	1.92	3	3
2:B:52:ASP:CB	2:B:58:ALA:HB2	0.65	2.21	19	3
1:A:31:VAL:HG12	2:B:49:LEU:HD12	0.65	1.69	9	1
1:A:5:TRP:N	1:A:6:PRO:CD	0.64	2.61	17	20
2:B:49:LEU:C	2:B:49:LEU:HD12	0.64	2.12	6	14
1:A:24:LYS:HB2	1:A:25:PRO:CD	0.64	2.23	7	13
1:A:24:LYS:CG	1:A:25:PRO:CD	0.64	2.76	15	9
2:B:47:VAL:HG22	2:B:63:VAL:CG2	0.63	2.23	17	9
1:A:32:LEU:CD1	2:B:50:PHE:CZ	0.63	2.80	13	4
1:A:5:TRP:CE2	1:A:20:ILE:HG12	0.63	2.28	13	16
1:A:9:VAL:CG2	2:B:60:VAL:CG2	0.63	2.76	11	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LEU:HD23	1:A:32:LEU:H	0.63	1.53	5	4
1:A:30:ILE:HD12	2:B:46:ARG:HD3	0.62	1.70	19	1
1:A:19:VAL:HG12	1:A:23:ASP:CG	0.62	2.15	2	2
1:A:9:VAL:HG22	2:B:60:VAL:CG2	0.62	2.25	1	5
1:A:16:ALA:CB	2:B:49:LEU:HD21	0.62	2.25	9	2
1:A:31:VAL:HG22	2:B:49:LEU:CB	0.61	2.24	20	1
1:A:5:TRP:N	1:A:6:PRO:HD3	0.61	2.10	1	20
1:A:16:ALA:HB1	1:A:20:ILE:HD12	0.61	1.73	10	5
1:A:24:LYS:CB	1:A:25:PRO:HD2	0.61	2.26	3	5
1:A:11:LYS:HB3	2:B:57:ILE:HD12	0.61	1.73	7	1
1:A:12:SER:O	1:A:16:ALA:CB	0.61	2.48	3	1
1:A:32:LEU:HD21	2:B:49:LEU:H	0.61	1.54	14	1
1:A:3:THR:HG22	1:A:24:LYS:HE3	0.61	1.71	20	2
1:A:8:LEU:HD12	1:A:11:LYS:CB	0.60	2.26	9	2
1:A:5:TRP:CE2	1:A:20:ILE:CG1	0.60	2.83	13	2
1:A:5:TRP:CZ2	1:A:23:ASP:OD2	0.60	2.54	4	1
1:A:30:ILE:HD13	2:B:46:ARG:CG	0.60	2.27	11	3
1:A:24:LYS:HB3	1:A:25:PRO:HD3	0.60	1.72	11	9
1:A:20:ILE:HD13	1:A:29:ILE:CD1	0.60	2.27	14	9
1:A:9:VAL:CG2	2:B:60:VAL:HG22	0.60	2.26	7	3
1:A:13:VAL:CG2	2:B:49:LEU:HD21	0.60	2.23	17	1
1:A:32:LEU:HD21	2:B:48:ARG:HG3	0.60	1.72	19	4
1:A:20:ILE:CD1	1:A:20:ILE:N	0.59	2.64	18	3
1:A:8:LEU:HD23	1:A:8:LEU:C	0.59	2.17	3	1
1:A:29:ILE:CD1	2:B:61:PRO:CG	0.59	2.81	2	1
1:A:24:LYS:CG	1:A:25:PRO:HD2	0.59	2.26	19	5
1:A:24:LYS:HB2	1:A:25:PRO:HD2	0.59	1.75	17	10
2:B:56:ASN:O	2:B:58:ALA:N	0.59	2.36	2	19
1:A:4:GLU:O	1:A:5:TRP:CG	0.59	2.55	16	1
1:A:13:VAL:CG2	1:A:31:VAL:HG11	0.59	2.28	4	2
1:A:24:LYS:HG3	1:A:25:PRO:CD	0.58	2.27	15	5
1:A:13:VAL:HG22	2:B:49:LEU:HD13	0.58	1.75	8	1
2:B:43:ARG:CG	2:B:43:ARG:O	0.58	2.51	4	19
1:A:16:ALA:CB	2:B:49:LEU:CD2	0.58	2.81	9	7
1:A:27:ALA:HA	2:B:45:ASP:HA	0.58	1.75	17	18
1:A:17:LYS:HE2	1:A:21:LEU:HD12	0.58	1.75	3	1
1:A:19:VAL:HG12	1:A:23:ASP:OD1	0.58	1.97	3	2
1:A:5:TRP:O	2:B:60:VAL:HG21	0.58	1.97	9	1
1:A:22:GLN:O	1:A:24:LYS:N	0.58	2.37	10	4
1:A:16:ALA:CB	2:B:49:LEU:HD11	0.58	2.28	12	2
1:A:20:ILE:HG21	1:A:29:ILE:CB	0.57	2.28	18	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:HD23	1:A:22:GLN:HB2	0.57	1.76	6	3
1:A:24:LYS:HB3	1:A:25:PRO:CD	0.57	2.29	18	4
1:A:3:THR:HG23	1:A:24:LYS:CD	0.57	2.30	6	3
2:B:49:LEU:HD11	2:B:57:ILE:CD1	0.57	2.29	4	2
2:B:52:ASP:CG	2:B:53:LYS:N	0.57	2.58	12	20
1:A:31:VAL:O	1:A:31:VAL:HG13	0.57	1.99	1	2
1:A:29:ILE:HD11	2:B:61:PRO:HG3	0.56	1.78	9	2
1:A:32:LEU:CD2	2:B:50:PHE:HA	0.56	2.30	18	1
2:B:54:LEU:O	2:B:55:ASP:CB	0.56	2.54	15	4
2:B:49:LEU:C	2:B:49:LEU:CD1	0.56	2.74	9	3
2:B:49:LEU:CD2	2:B:49:LEU:C	0.56	2.73	7	4
1:A:4:GLU:O	2:B:60:VAL:CG1	0.56	2.54	17	9
2:B:47:VAL:HG13	2:B:62:ARG:O	0.56	2.01	19	7
2:B:47:VAL:CG2	2:B:63:VAL:CG2	0.56	2.79	15	5
1:A:4:GLU:HB3	1:A:6:PRO:HD3	0.56	1.78	16	1
1:A:13:VAL:HG21	2:B:55:ASP:O	0.55	2.02	3	1
2:B:49:LEU:HD21	2:B:57:ILE:HD12	0.55	1.77	20	1
1:A:32:LEU:HD22	2:B:48:ARG:HD2	0.55	1.78	8	1
1:A:20:ILE:HA	1:A:23:ASP:OD2	0.55	2.02	1	2
1:A:14:GLU:O	1:A:18:LYS:CB	0.55	2.54	2	18
1:A:16:ALA:CB	2:B:49:LEU:HD22	0.55	2.32	6	3
1:A:19:VAL:HG12	1:A:23:ASP:HB2	0.55	1.79	17	1
1:A:12:SER:O	2:B:57:ILE:HD11	0.55	2.02	3	2
1:A:14:GLU:O	1:A:18:LYS:CG	0.55	2.55	5	3
1:A:20:ILE:O	1:A:22:GLN:N	0.55	2.40	17	12
1:A:21:LEU:C	1:A:21:LEU:HD23	0.54	2.22	2	1
1:A:13:VAL:HG21	1:A:31:VAL:HG21	0.54	1.79	10	3
1:A:32:LEU:CD2	2:B:50:PHE:CG	0.54	2.91	18	1
1:A:20:ILE:O	1:A:27:ALA:O	0.54	2.26	20	20
2:B:47:VAL:HG12	2:B:48:ARG:N	0.54	2.17	12	5
2:B:44:ILE:HG23	2:B:63:VAL:HG22	0.54	1.78	13	1
2:B:52:ASP:OD2	2:B:56:ASN:CB	0.54	2.56	11	2
2:B:52:ASP:OD1	2:B:55:ASP:N	0.54	2.40	1	4
1:A:32:LEU:HG	2:B:50:PHE:CD1	0.54	2.37	5	6
1:A:30:ILE:HD13	2:B:46:ARG:HG2	0.54	1.79	6	3
1:A:16:ALA:HA	1:A:20:ILE:HD12	0.54	1.79	11	1
2:B:52:ASP:HB3	2:B:58:ALA:HB2	0.54	1.78	14	3
1:A:9:VAL:HG22	2:B:60:VAL:HG23	0.54	1.79	5	4
1:A:5:TRP:CD1	1:A:8:LEU:HD11	0.54	2.37	7	1
1:A:24:LYS:CE	1:A:25:PRO:HD3	0.54	2.33	8	2
2:B:47:VAL:CG1	2:B:62:ARG:O	0.53	2.56	11	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:54:LEU:O	2:B:55:ASP:OD1	0.53	2.26	11	4
1:A:24:LYS:CD	1:A:25:PRO:HD3	0.53	2.33	14	2
1:A:25:PRO:C	1:A:26:GLU:CG	0.53	2.75	1	19
1:A:16:ALA:HB1	2:B:49:LEU:HD22	0.53	1.80	16	7
1:A:24:LYS:HG3	1:A:25:PRO:HD2	0.53	1.80	8	6
1:A:5:TRP:O	1:A:8:LEU:CD2	0.53	2.57	11	2
1:A:29:ILE:HD11	2:B:61:PRO:CB	0.53	2.34	10	4
2:B:52:ASP:OD1	2:B:53:LYS:N	0.53	2.41	11	5
1:A:5:TRP:O	2:B:60:VAL:CG1	0.53	2.56	19	3
2:B:51:VAL:HG12	2:B:55:ASP:HA	0.53	1.80	19	1
1:A:23:ASP:OD2	1:A:24:LYS:CG	0.53	2.57	16	3
1:A:13:VAL:HA	2:B:49:LEU:HD21	0.53	1.79	6	5
1:A:4:GLU:HB2	1:A:6:PRO:HD3	0.53	1.80	5	7
1:A:25:PRO:O	1:A:26:GLU:CG	0.53	2.57	13	16
1:A:13:VAL:CG2	2:B:51:VAL:CG1	0.53	2.87	20	2
1:A:3:THR:HG23	1:A:24:LYS:HE2	0.53	1.79	13	2
1:A:5:TRP:CD1	1:A:8:LEU:CD1	0.53	2.92	7	1
1:A:5:TRP:O	2:B:60:VAL:CG2	0.53	2.57	16	2
1:A:13:VAL:CG2	2:B:51:VAL:HG11	0.53	2.34	12	3
2:B:48:ARG:HB3	2:B:50:PHE:CE2	0.53	2.39	20	2
1:A:8:LEU:HD12	1:A:11:LYS:HB3	0.53	1.81	9	1
2:B:55:ASP:OD1	2:B:55:ASP:O	0.53	2.27	11	2
1:A:24:LYS:HG2	1:A:25:PRO:HD2	0.53	1.81	19	2
2:B:43:ARG:HD3	2:B:63:VAL:CG1	0.52	2.35	20	1
1:A:32:LEU:HG	2:B:50:PHE:CE1	0.52	2.39	5	2
2:B:54:LEU:O	2:B:54:LEU:CD2	0.52	2.57	13	1
1:A:28:GLN:CB	2:B:45:ASP:O	0.52	2.56	10	10
2:B:52:ASP:OD1	2:B:54:LEU:N	0.52	2.42	5	10
1:A:19:VAL:O	1:A:23:ASP:N	0.52	2.43	5	6
1:A:20:ILE:H	1:A:20:ILE:HD13	0.52	1.63	5	2
2:B:62:ARG:O	2:B:63:VAL:CB	0.52	2.57	14	2
1:A:12:SER:O	2:B:57:ILE:CD1	0.52	2.58	3	1
1:A:24:LYS:CG	1:A:25:PRO:HD3	0.52	2.34	4	6
1:A:8:LEU:HD21	2:B:57:ILE:CG2	0.52	2.29	10	2
2:B:54:LEU:N	2:B:54:LEU:CD2	0.52	2.71	10	1
2:B:47:VAL:O	2:B:49:LEU:N	0.52	2.43	1	1
2:B:47:VAL:CG1	2:B:61:PRO:CB	0.52	2.86	14	6
1:A:4:GLU:CB	1:A:6:PRO:HD3	0.52	2.35	3	14
1:A:9:VAL:HG23	2:B:60:VAL:HG22	0.52	1.80	3	5
1:A:23:ASP:O	1:A:24:LYS:O	0.52	2.28	10	4
1:A:4:GLU:OE1	2:B:62:ARG:NH1	0.52	2.43	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:55:ASP:O	2:B:55:ASP:CG	0.52	2.47	15	2
1:A:20:ILE:O	1:A:23:ASP:OD1	0.52	2.27	20	5
1:A:8:LEU:HD22	1:A:8:LEU:C	0.52	2.24	10	1
1:A:24:LYS:HG3	1:A:25:PRO:HD3	0.52	1.82	15	1
2:B:47:VAL:CG1	2:B:61:PRO:HB2	0.51	2.34	12	6
1:A:21:LEU:CD1	1:A:28:GLN:OE1	0.51	2.58	14	1
2:B:44:ILE:HG22	2:B:63:VAL:O	0.51	2.04	13	1
2:B:52:ASP:OD1	2:B:52:ASP:C	0.51	2.47	15	17
1:A:8:LEU:CD1	2:B:57:ILE:CD1	0.51	2.88	3	1
2:B:47:VAL:CG1	2:B:62:ARG:C	0.51	2.79	5	3
1:A:5:TRP:O	2:B:60:VAL:HG11	0.51	2.04	18	2
2:B:43:ARG:CD	2:B:63:VAL:CG1	0.51	2.88	20	1
1:A:32:LEU:CG	2:B:50:PHE:CE1	0.51	2.93	5	1
1:A:3:THR:HG22	1:A:24:LYS:HD3	0.51	1.83	9	3
1:A:14:GLU:O	1:A:18:LYS:CD	0.51	2.59	1	1
1:A:24:LYS:CE	1:A:25:PRO:CD	0.51	2.89	8	1
1:A:24:LYS:HD3	1:A:25:PRO:CD	0.51	2.35	12	2
1:A:12:SER:CB	1:A:14:GLU:OE2	0.51	2.59	14	4
1:A:10:GLY:O	2:B:56:ASN:OD1	0.51	2.29	3	1
1:A:3:THR:HG23	1:A:24:LYS:HE3	0.51	1.81	11	1
1:A:29:ILE:CD1	2:B:61:PRO:HG3	0.51	2.35	2	1
1:A:8:LEU:HD11	2:B:57:ILE:CD1	0.51	2.35	11	1
1:A:4:GLU:O	2:B:61:PRO:O	0.51	2.27	14	2
1:A:8:LEU:CD1	1:A:11:LYS:HB3	0.51	2.36	9	2
1:A:19:VAL:O	1:A:20:ILE:C	0.51	2.50	2	7
1:A:23:ASP:OD2	1:A:24:LYS:HG2	0.51	2.06	16	3
1:A:5:TRP:CZ2	1:A:24:LYS:HE2	0.50	2.41	19	1
1:A:8:LEU:CD1	2:B:60:VAL:HG22	0.50	2.37	10	1
1:A:19:VAL:O	1:A:23:ASP:OD1	0.50	2.30	20	2
1:A:29:ILE:CG1	2:B:49:LEU:HB2	0.50	2.37	1	1
1:A:32:LEU:HD22	2:B:50:PHE:CE1	0.50	2.41	18	1
1:A:20:ILE:O	1:A:21:LEU:C	0.50	2.49	17	16
1:A:5:TRP:NE1	1:A:20:ILE:CD1	0.50	2.74	18	3
1:A:22:GLN:O	1:A:23:ASP:C	0.50	2.50	1	5
1:A:16:ALA:O	1:A:20:ILE:HD12	0.50	2.05	3	2
1:A:5:TRP:O	2:B:60:VAL:HG13	0.50	2.07	20	1
1:A:20:ILE:HD13	1:A:29:ILE:HD12	0.50	1.84	14	2
1:A:28:GLN:O	2:B:47:VAL:HG23	0.50	2.07	20	3
1:A:8:LEU:HB2	1:A:12:SER:CB	0.50	2.37	3	1
1:A:29:ILE:CD1	2:B:61:PRO:CB	0.49	2.89	2	3
1:A:14:GLU:O	1:A:18:LYS:HB2	0.49	2.08	12	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:PRO:O	1:A:26:GLU:HG2	0.49	2.06	16	18
2:B:47:VAL:HG12	2:B:62:ARG:H	0.49	1.67	5	1
2:B:44:ILE:HG13	2:B:45:ASP:N	0.49	2.23	11	17
1:A:31:VAL:CG1	2:B:49:LEU:HD12	0.49	2.37	9	1
2:B:52:ASP:HB2	2:B:58:ALA:CB	0.49	2.38	19	2
1:A:31:VAL:HG13	2:B:49:LEU:CG	0.49	2.38	3	2
1:A:30:ILE:CG2	1:A:32:LEU:HD22	0.49	2.38	7	2
1:A:8:LEU:HD11	2:B:57:ILE:HD12	0.49	1.85	9	1
1:A:9:VAL:CG2	2:B:60:VAL:HG23	0.49	2.38	20	3
2:B:53:LYS:HB2	2:B:54:LEU:HD22	0.49	1.83	10	1
2:B:51:VAL:HG23	2:B:52:ASP:N	0.49	2.22	6	1
1:A:15:GLU:O	1:A:19:VAL:HG23	0.49	2.07	11	1
1:A:5:TRP:CE2	1:A:23:ASP:OD2	0.49	2.65	4	1
1:A:3:THR:O	1:A:5:TRP:CZ3	0.49	2.66	6	3
2:B:60:VAL:HB	2:B:62:ARG:NH1	0.49	2.23	7	1
1:A:32:LEU:HD21	2:B:50:PHE:HD1	0.49	1.65	8	1
1:A:21:LEU:HD12	1:A:28:GLN:OE1	0.49	2.07	14	1
1:A:3:THR:CG2	2:B:63:VAL:O	0.49	2.60	18	2
1:A:21:LEU:CD1	1:A:28:GLN:HG3	0.49	2.37	1	1
1:A:17:LYS:HA	1:A:29:ILE:CG2	0.49	2.38	14	5
2:B:54:LEU:O	2:B:55:ASP:CG	0.49	2.52	11	4
1:A:32:LEU:CD1	2:B:50:PHE:CD1	0.48	2.95	14	7
2:B:52:ASP:CB	2:B:58:ALA:CB	0.48	2.91	17	2
1:A:23:ASP:HB3	1:A:24:LYS:CE	0.48	2.38	19	1
1:A:29:ILE:HD11	2:B:61:PRO:HB3	0.48	1.84	20	2
2:B:43:ARG:O	2:B:43:ARG:HG3	0.48	2.08	19	9
1:A:29:ILE:HD11	2:B:61:PRO:CG	0.48	2.38	9	3
1:A:8:LEU:C	1:A:8:LEU:HD23	0.48	2.28	6	2
1:A:22:GLN:O	1:A:23:ASP:OD1	0.48	2.31	1	1
1:A:24:LYS:HG2	1:A:25:PRO:HD3	0.48	1.85	2	1
2:B:49:LEU:CD1	2:B:57:ILE:HD12	0.48	2.37	4	1
2:B:46:ARG:HG2	2:B:47:VAL:N	0.48	2.23	9	1
1:A:8:LEU:HD21	2:B:57:ILE:CD1	0.48	2.38	18	1
1:A:32:LEU:HD21	2:B:50:PHE:CZ	0.48	2.39	20	1
1:A:20:ILE:N	1:A:20:ILE:HD13	0.48	2.23	5	2
2:B:44:ILE:O	2:B:63:VAL:HG22	0.48	2.08	7	1
1:A:24:LYS:HE2	1:A:25:PRO:CD	0.48	2.38	8	1
2:B:43:ARG:O	2:B:44:ILE:C	0.48	2.51	10	19
1:A:3:THR:HG23	1:A:24:LYS:CE	0.48	2.38	13	2
1:A:3:THR:CA	1:A:24:LYS:HD3	0.48	2.39	17	2
1:A:23:ASP:OD1	1:A:24:LYS:HD2	0.48	2.09	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ILE:O	1:A:32:LEU:CD2	0.48	2.61	17	1
1:A:3:THR:CG2	1:A:24:LYS:HD2	0.48	2.39	3	2
1:A:31:VAL:CA	1:A:32:LEU:HD23	0.48	2.39	17	2
1:A:8:LEU:O	1:A:8:LEU:HG	0.48	2.08	8	5
1:A:5:TRP:CZ2	1:A:20:ILE:HG23	0.48	2.44	10	1
2:B:57:ILE:N	2:B:57:ILE:HD13	0.48	2.22	15	1
1:A:30:ILE:O	2:B:49:LEU:HB3	0.48	2.09	20	6
1:A:3:THR:CG2	1:A:24:LYS:HE2	0.48	2.39	6	2
2:B:48:ARG:HG3	2:B:50:PHE:CE2	0.48	2.44	13	1
2:B:47:VAL:HG11	2:B:62:ARG:N	0.48	2.23	15	1
2:B:47:VAL:CG1	2:B:63:VAL:HG23	0.48	2.39	16	1
1:A:32:LEU:HD22	2:B:50:PHE:CG	0.48	2.39	18	1
1:A:5:TRP:CZ2	1:A:24:LYS:CE	0.48	2.97	19	1
2:B:47:VAL:HG11	2:B:61:PRO:CA	0.48	2.39	1	1
1:A:30:ILE:CD1	2:B:46:ARG:HG2	0.48	2.39	6	1
1:A:31:VAL:CG2	2:B:49:LEU:HD23	0.47	2.37	17	3
1:A:3:THR:OG1	1:A:24:LYS:CD	0.47	2.62	5	2
1:A:3:THR:CG2	1:A:24:LYS:HE3	0.47	2.39	15	3
1:A:20:ILE:HG21	1:A:29:ILE:CG2	0.47	2.38	18	1
1:A:8:LEU:C	1:A:8:LEU:CD2	0.47	2.82	3	1
1:A:6:PRO:HA	2:B:60:VAL:HG21	0.47	1.87	20	2
2:B:55:ASP:OD1	2:B:55:ASP:C	0.47	2.52	19	4
1:A:32:LEU:HD13	2:B:50:PHE:CZ	0.47	2.44	18	1
2:B:55:ASP:N	2:B:55:ASP:OD1	0.47	2.47	9	2
1:A:32:LEU:O	2:B:50:PHE:HA	0.47	2.08	7	4
1:A:3:THR:O	2:B:62:ARG:O	0.47	2.32	1	2
1:A:9:VAL:HG23	2:B:60:VAL:HG21	0.47	1.85	12	6
2:B:51:VAL:CG1	2:B:55:ASP:HA	0.47	2.40	11	3
1:A:16:ALA:O	1:A:20:ILE:HB	0.47	2.10	18	7
2:B:62:ARG:O	2:B:63:VAL:HB	0.47	2.09	1	2
1:A:4:GLU:CB	2:B:62:ARG:HD2	0.47	2.40	12	4
1:A:13:VAL:HA	1:A:16:ALA:HB3	0.47	1.87	19	8
1:A:23:ASP:O	1:A:24:LYS:CB	0.47	2.60	3	1
1:A:29:ILE:CD1	2:B:49:LEU:HB2	0.47	2.40	20	11
1:A:3:THR:HA	1:A:23:ASP:OD2	0.47	2.10	12	1
1:A:17:LYS:O	1:A:21:LEU:CB	0.47	2.63	15	1
1:A:4:GLU:HA	2:B:62:ARG:CD	0.47	2.40	20	5
1:A:4:GLU:CA	2:B:62:ARG:HD2	0.47	2.40	10	2
1:A:27:ALA:HB1	2:B:63:VAL:CG2	0.47	2.31	14	1
2:B:45:ASP:O	2:B:45:ASP:CG	0.47	2.53	20	16
1:A:8:LEU:O	1:A:11:LYS:HB2	0.47	2.10	9	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:GLU:O	1:A:5:TRP:HB2	0.47	2.10	3	7
1:A:32:LEU:CD2	2:B:48:ARG:HD2	0.47	2.39	9	1
1:A:13:VAL:HG13	2:B:49:LEU:HD23	0.47	1.86	13	2
1:A:16:ALA:O	1:A:17:LYS:C	0.47	2.53	6	16
1:A:24:LYS:HG2	1:A:25:PRO:CD	0.47	2.40	2	2
1:A:5:TRP:O	1:A:8:LEU:HB2	0.47	2.10	20	1
1:A:18:LYS:HG2	1:A:19:VAL:N	0.46	2.25	3	1
1:A:23:ASP:O	1:A:24:LYS:HB2	0.46	2.09	3	1
2:B:47:VAL:HG12	2:B:48:ARG:H	0.46	1.70	3	1
1:A:17:LYS:HG2	1:A:29:ILE:HG23	0.46	1.85	20	2
1:A:30:ILE:CD1	2:B:46:ARG:HD2	0.46	2.40	4	1
2:B:49:LEU:HD12	2:B:50:PHE:N	0.46	2.25	6	1
2:B:45:ASP:O	2:B:45:ASP:OD1	0.46	2.32	9	1
1:A:5:TRP:CD2	1:A:20:ILE:HG12	0.46	2.45	11	2
2:B:56:ASN:O	2:B:57:ILE:C	0.46	2.54	1	10
1:A:16:ALA:HB1	1:A:20:ILE:CD1	0.46	2.40	13	3
1:A:8:LEU:HD11	2:B:57:ILE:HG21	0.46	1.88	3	1
1:A:5:TRP:NE1	1:A:20:ILE:HG13	0.46	2.26	11	2
1:A:25:PRO:C	1:A:26:GLU:HG3	0.46	2.31	8	17
2:B:55:ASP:OD1	2:B:55:ASP:N	0.46	2.48	10	1
1:A:8:LEU:HG	2:B:57:ILE:HD12	0.46	1.86	19	4
2:B:61:PRO:O	2:B:62:ARG:CD	0.46	2.63	14	2
1:A:29:ILE:HG12	2:B:49:LEU:HB2	0.46	1.87	1	3
1:A:13:VAL:O	1:A:14:GLU:C	0.46	2.54	5	16
1:A:23:ASP:C	1:A:24:LYS:O	0.46	2.54	1	1
1:A:3:THR:OG1	1:A:24:LYS:HD2	0.46	2.11	5	3
1:A:21:LEU:HD23	1:A:22:GLN:N	0.46	2.25	6	1
1:A:24:LYS:NZ	2:B:63:VAL:CG1	0.46	2.79	9	1
1:A:5:TRP:CD1	1:A:20:ILE:CD1	0.46	2.98	18	1
1:A:8:LEU:CB	1:A:12:SER:CB	0.45	2.94	3	1
1:A:8:LEU:HA	1:A:12:SER:OG	0.45	2.11	3	1
1:A:28:GLN:HB3	2:B:45:ASP:O	0.45	2.11	7	2
1:A:19:VAL:C	1:A:23:ASP:OD2	0.45	2.55	3	2
2:B:43:ARG:O	2:B:43:ARG:HG2	0.45	2.10	13	2
2:B:61:PRO:O	2:B:62:ARG:HD3	0.45	2.12	18	8
2:B:63:VAL:O	2:B:63:VAL:HG12	0.45	2.11	10	1
1:A:5:TRP:CZ2	1:A:20:ILE:HA	0.45	2.45	15	1
1:A:32:LEU:HD21	2:B:48:ARG:HD2	0.45	1.87	9	1
1:A:4:GLU:CG	2:B:62:ARG:HD2	0.45	2.42	12	1
1:A:24:LYS:HD3	1:A:25:PRO:HD3	0.45	1.87	12	2
1:A:14:GLU:O	1:A:18:LYS:HG3	0.45	2.12	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:THR:HA	1:A:24:LYS:HD3	0.45	1.89	17	1
2:B:48:ARG:O	2:B:50:PHE:N	0.45	2.50	9	3
1:A:16:ALA:CB	1:A:20:ILE:HD12	0.45	2.42	10	1
2:B:52:ASP:OD2	2:B:56:ASN:HB2	0.45	2.11	15	2
1:A:12:SER:CA	2:B:57:ILE:HG13	0.45	2.41	12	1
1:A:23:ASP:OD1	1:A:24:LYS:HG2	0.45	2.12	14	1
2:B:47:VAL:CG2	2:B:62:ARG:O	0.45	2.65	15	1
2:B:52:ASP:HB2	2:B:58:ALA:HB2	0.45	1.85	19	1
1:A:16:ALA:O	1:A:20:ILE:HD13	0.45	2.11	18	2
1:A:9:VAL:HG22	2:B:60:VAL:HG22	0.45	1.88	7	1
1:A:13:VAL:HG22	2:B:49:LEU:HD11	0.45	1.88	9	1
1:A:5:TRP:C	2:B:60:VAL:HG11	0.45	2.31	17	1
1:A:23:ASP:N	1:A:23:ASP:OD1	0.45	2.50	5	1
1:A:9:VAL:HG23	2:B:60:VAL:HG23	0.45	1.86	20	1
1:A:20:ILE:CD1	1:A:29:ILE:HD13	0.44	2.41	15	1
2:B:52:ASP:OD2	2:B:56:ASN:HB3	0.44	2.12	11	3
1:A:30:ILE:HD13	2:B:46:ARG:HG3	0.44	1.90	11	1
2:B:43:ARG:HD2	2:B:63:VAL:HG11	0.44	1.88	20	1
2:B:49:LEU:CD2	2:B:57:ILE:HD12	0.44	2.42	20	1
1:A:28:GLN:HB2	2:B:45:ASP:O	0.44	2.12	10	4
1:A:32:LEU:O	2:B:51:VAL:CG2	0.44	2.64	3	2
1:A:29:ILE:HA	2:B:47:VAL:HG23	0.44	1.89	8	1
1:A:29:ILE:CD1	2:B:47:VAL:HB	0.44	2.42	17	4
1:A:21:LEU:HD23	1:A:22:GLN:CB	0.44	2.41	6	1
1:A:5:TRP:HB3	1:A:8:LEU:HB3	0.44	1.89	9	1
1:A:29:ILE:HD12	2:B:47:VAL:HB	0.44	1.89	19	3
2:B:48:ARG:CG	2:B:50:PHE:CE2	0.44	3.01	13	1
1:A:24:LYS:CD	1:A:25:PRO:CD	0.44	2.95	14	1
1:A:8:LEU:O	1:A:11:LYS:CB	0.44	2.65	19	1
1:A:22:GLN:C	1:A:23:ASP:OD1	0.44	2.56	10	2
2:B:56:ASN:OD1	2:B:56:ASN:C	0.44	2.56	14	1
1:A:20:ILE:CA	1:A:23:ASP:OD2	0.44	2.66	1	1
1:A:10:GLY:C	2:B:56:ASN:OD1	0.44	2.56	14	5
1:A:20:ILE:CG2	1:A:29:ILE:HB	0.44	2.36	13	2
1:A:5:TRP:HB2	2:B:60:VAL:HG13	0.44	1.89	16	1
1:A:32:LEU:HD21	2:B:50:PHE:HE1	0.44	1.70	19	1
1:A:25:PRO:O	1:A:26:GLU:HG3	0.44	2.12	1	1
1:A:3:THR:HG23	1:A:24:LYS:HG3	0.44	1.90	2	1
1:A:8:LEU:CD1	2:B:57:ILE:HD13	0.44	2.42	3	1
1:A:13:VAL:HG22	1:A:31:VAL:HG11	0.44	1.90	4	1
1:A:30:ILE:HD11	2:B:46:ARG:HD2	0.44	1.89	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ASP:O	1:A:24:LYS:C	0.44	2.56	18	1
1:A:8:LEU:HD21	1:A:16:ALA:CA	0.44	2.43	17	3
2:B:45:ASP:O	2:B:45:ASP:OD2	0.44	2.35	8	3
2:B:54:LEU:C	2:B:55:ASP:CG	0.43	2.77	5	8
1:A:32:LEU:CD1	2:B:50:PHE:HE1	0.43	2.27	2	1
2:B:49:LEU:HD21	2:B:57:ILE:CD1	0.43	2.43	20	1
1:A:4:GLU:HA	2:B:62:ARG:HD3	0.43	1.88	1	1
1:A:23:ASP:CG	1:A:24:LYS:N	0.43	2.71	17	1
1:A:26:GLU:O	2:B:45:ASP:HB2	0.43	2.13	1	1
1:A:17:LYS:HA	1:A:29:ILE:HG22	0.43	1.90	14	1
1:A:13:VAL:CG2	2:B:51:VAL:HG12	0.43	2.43	20	1
1:A:18:LYS:N	1:A:18:LYS:HD2	0.43	2.27	1	1
1:A:32:LEU:HD13	2:B:48:ARG:HH11	0.43	1.74	10	1
1:A:32:LEU:CD2	2:B:48:ARG:HG3	0.43	2.43	15	1
1:A:4:GLU:O	2:B:60:VAL:HG11	0.43	2.13	18	1
1:A:30:ILE:CG2	1:A:31:VAL:N	0.43	2.82	2	2
1:A:20:ILE:HA	1:A:23:ASP:OD1	0.43	2.14	6	2
1:A:20:ILE:C	1:A:23:ASP:OD1	0.43	2.57	10	1
1:A:23:ASP:OD1	1:A:23:ASP:C	0.43	2.56	12	1
1:A:10:GLY:HA2	2:B:56:ASN:OD1	0.43	2.14	20	2
1:A:5:TRP:HB3	1:A:8:LEU:HB2	0.43	1.91	16	1
2:B:43:ARG:HB2	2:B:43:ARG:CZ	0.43	2.42	20	1
1:A:31:VAL:C	1:A:32:LEU:CD2	0.43	2.80	6	1
2:B:49:LEU:O	2:B:49:LEU:HG	0.43	2.13	17	2
1:A:4:GLU:HG3	2:B:62:ARG:CG	0.43	2.43	10	1
1:A:5:TRP:CH2	1:A:20:ILE:HG23	0.43	2.48	10	1
1:A:32:LEU:HD11	2:B:48:ARG:HD2	0.42	1.89	17	2
1:A:8:LEU:C	1:A:8:LEU:CD1	0.42	2.71	10	1
1:A:9:VAL:CG1	1:A:10:GLY:N	0.42	2.82	11	2
1:A:19:VAL:CG1	1:A:23:ASP:OD2	0.42	2.67	2	1
1:A:13:VAL:HG21	1:A:31:VAL:HG23	0.42	1.91	6	1
1:A:9:VAL:CG2	2:B:60:VAL:HG21	0.42	2.44	8	1
1:A:28:GLN:OE1	2:B:45:ASP:OD2	0.42	2.37	17	1
1:A:20:ILE:CD1	1:A:20:ILE:H	0.42	2.27	18	1
2:B:50:PHE:CB	2:B:59:GLN:HB2	0.42	2.44	18	1
1:A:21:LEU:HA	1:A:27:ALA:O	0.42	2.15	15	1
1:A:5:TRP:CD1	1:A:20:ILE:HD11	0.42	2.50	16	1
1:A:8:LEU:CG	2:B:57:ILE:HG21	0.42	2.44	3	1
2:B:54:LEU:O	2:B:55:ASP:C	0.42	2.58	3	2
2:B:59:GLN:O	2:B:60:VAL:C	0.42	2.57	19	2
1:A:20:ILE:HD13	1:A:20:ILE:H	0.42	1.74	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:60:VAL:HG13	2:B:61:PRO:HD2	0.42	1.92	17	1
1:A:4:GLU:O	1:A:5:TRP:C	0.42	2.57	18	1
2:B:47:VAL:CG1	2:B:48:ARG:N	0.42	2.82	7	2
2:B:61:PRO:O	2:B:62:ARG:HD2	0.42	2.15	15	1
1:A:17:LYS:O	1:A:21:LEU:HB2	0.42	2.15	15	5
1:A:23:ASP:OD1	1:A:24:LYS:CD	0.42	2.67	15	1
1:A:3:THR:O	2:B:62:ARG:HA	0.42	2.15	14	1
1:A:8:LEU:HD11	1:A:15:GLU:HB3	0.42	1.91	18	1
1:A:31:VAL:HA	2:B:49:LEU:O	0.42	2.15	20	1
1:A:22:GLN:C	1:A:23:ASP:CG	0.42	2.78	1	1
1:A:4:GLU:O	1:A:5:TRP:CB	0.42	2.65	3	1
1:A:5:TRP:O	1:A:8:LEU:HB3	0.41	2.15	9	2
1:A:30:ILE:HD12	2:B:46:ARG:HG3	0.41	1.91	2	1
2:B:46:ARG:HG3	2:B:46:ARG:NH1	0.41	2.28	2	1
1:A:13:VAL:HG21	1:A:31:VAL:CG2	0.41	2.45	6	1
1:A:3:THR:CA	1:A:23:ASP:OD2	0.41	2.68	12	1
1:A:23:ASP:OD2	1:A:24:LYS:HD2	0.41	2.15	12	1
1:A:30:ILE:HD12	2:B:46:ARG:HD2	0.41	1.91	16	1
1:A:17:LYS:HG2	1:A:29:ILE:CG2	0.41	2.45	4	3
1:A:29:ILE:HG13	2:B:47:VAL:O	0.41	2.15	14	4
2:B:54:LEU:O	2:B:54:LEU:HD12	0.41	2.15	4	1
2:B:47:VAL:CG2	2:B:63:VAL:CA	0.41	2.98	14	1
1:A:8:LEU:CD2	2:B:57:ILE:HG21	0.41	2.30	6	1
1:A:16:ALA:CB	2:B:57:ILE:HD11	0.41	2.31	9	1
1:A:24:LYS:NZ	2:B:63:VAL:HB	0.41	2.30	9	1
1:A:4:GLU:C	1:A:6:PRO:HD3	0.41	2.35	12	1
1:A:32:LEU:HD23	2:B:50:PHE:HA	0.41	1.92	18	1
1:A:4:GLU:HA	2:B:62:ARG:HD2	0.41	1.93	2	1
1:A:8:LEU:O	1:A:9:VAL:C	0.41	2.58	3	1
2:B:47:VAL:HG22	2:B:62:ARG:O	0.41	2.15	15	1
1:A:29:ILE:HG13	2:B:47:VAL:HB	0.41	1.92	17	2
1:A:31:VAL:HG22	2:B:49:LEU:CG	0.41	2.45	20	1
1:A:3:THR:CG2	1:A:24:LYS:CE	0.41	2.99	2	1
2:B:46:ARG:C	2:B:47:VAL:CG2	0.41	2.88	13	1
1:A:12:SER:O	1:A:13:VAL:C	0.41	2.58	7	1
1:A:16:ALA:HB1	2:B:49:LEU:HD21	0.41	1.92	20	1
1:A:14:GLU:O	1:A:18:LYS:HD2	0.41	2.15	1	1
2:B:50:PHE:CD2	2:B:59:GLN:OE1	0.41	2.73	3	1
1:A:8:LEU:O	1:A:8:LEU:CD2	0.41	2.50	10	1
1:A:12:SER:CA	2:B:57:ILE:HG12	0.41	2.45	16	1
2:B:52:ASP:OD1	2:B:53:LYS:CD	0.41	2.68	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LEU:CG	2:B:50:PHE:CD1	0.41	3.03	20	1
2:B:48:ARG:NH1	2:B:48:ARG:HG2	0.41	2.31	2	1
1:A:19:VAL:O	1:A:21:LEU:N	0.41	2.54	6	1
1:A:30:ILE:N	1:A:30:ILE:HD12	0.41	2.31	6	1
1:A:5:TRP:HB3	1:A:8:LEU:CG	0.41	2.46	7	1
2:B:56:ASN:O	2:B:56:ASN:CG	0.41	2.58	9	1
1:A:5:TRP:CE2	1:A:20:ILE:HG13	0.41	2.50	11	1
1:A:25:PRO:HB2	2:B:43:ARG:NH2	0.41	2.31	11	1
1:A:32:LEU:HD12	2:B:50:PHE:CD1	0.41	2.50	14	1
1:A:16:ALA:O	1:A:18:LYS:N	0.41	2.53	15	1
1:A:3:THR:CB	1:A:24:LYS:HD2	0.41	2.46	3	1
1:A:23:ASP:CG	1:A:24:LYS:HG2	0.41	2.36	14	1
1:A:20:ILE:C	1:A:22:GLN:N	0.41	2.74	20	1
2:B:54:LEU:CG	2:B:54:LEU:O	0.40	2.69	12	1
1:A:12:SER:HB2	1:A:14:GLU:OE2	0.40	2.16	2	1
2:B:44:ILE:CG1	2:B:45:ASP:N	0.40	2.85	2	1
1:A:16:ALA:O	1:A:20:ILE:CG1	0.40	2.69	5	1
2:B:53:LYS:CG	2:B:54:LEU:N	0.40	2.84	7	1
2:B:45:ASP:OD1	2:B:45:ASP:C	0.40	2.59	13	1
1:A:11:LYS:O	2:B:56:ASN:OD1	0.40	2.39	2	1
1:A:12:SER:CB	1:A:14:GLU:CD	0.40	2.90	2	1
1:A:13:VAL:HA	2:B:49:LEU:HD11	0.40	1.92	7	1
2:B:47:VAL:CG1	2:B:61:PRO:HB3	0.40	2.47	1	1
1:A:3:THR:OG1	1:A:24:LYS:HE3	0.40	2.16	18	1
1:A:8:LEU:HG	1:A:8:LEU:O	0.40	2.16	2	1
2:B:52:ASP:CG	2:B:56:ASN:CB	0.40	2.90	15	1
1:A:8:LEU:CD2	2:B:57:ILE:CD1	0.40	2.99	18	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	30/40 (75%)	18±1 (61±5%)	7±1 (22±4%)	5±1 (17±3%)	0 3
2	B	21/24 (88%)	12±2 (59±8%)	7±2 (33±8%)	2±1 (8±3%)	2 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1020/1280 (80%)	614 (60%)	271 (27%)	135 (13%)	1 5

All 15 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	24	LYS	20
2	B	57	ILE	20
1	A	16	ALA	19
1	A	18	LYS	19
1	A	25	PRO	18
1	A	14	GLU	12
1	A	21	LEU	9
1	A	23	ASP	4
2	B	55	ASP	4
2	B	49	LEU	3
2	B	63	VAL	2
2	B	50	PHE	2
2	B	48	ARG	1
2	B	44	ILE	1
2	B	51	VAL	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	27/35 (77%)	18±2 (66±8%)	9±2 (34±8%)	1 11
2	B	20/22 (91%)	12±2 (60±9%)	8±2 (40±9%)	0 5
All	All	940/1140 (82%)	601 (64%)	339 (36%)	1 8

All 37 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	32	LEU	20
2	B	55	ASP	20

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Mol	Chain	Res	Type	Models (Total)
1	A	17	LYS	19
2	B	44	ILE	19
2	B	62	ARG	19
2	B	52	ASP	15
1	A	11	LYS	14
1	A	12	SER	14
1	A	22	GLN	13
1	A	7	GLU	12
1	A	24	LYS	12
1	A	15	GLU	11
1	A	28	GLN	10
2	B	43	ARG	10
2	B	47	VAL	10
2	B	54	LEU	10
1	A	23	ASP	9
2	B	46	ARG	9
2	B	45	ASP	9
1	A	18	LYS	8
2	B	48	ARG	8
2	B	59	GLN	8
2	B	63	VAL	7
1	A	3	THR	7
1	A	8	LEU	7
1	A	4	GLU	6
2	B	49	LEU	6
1	A	21	LEU	5
1	A	14	GLU	5
2	B	51	VAL	4
1	A	20	ILE	3
2	B	53	LYS	2
2	B	56	ASN	2
1	A	30	ILE	2
1	A	19	VAL	2
1	A	26	GLU	1
1	A	31	VAL	1

6.3.3 RNA

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 monosaccharides 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