Full wwPDB NMR Structure Validation Report (i)

Feb 14, 2022 – 06:51 AM EST

PDB ID	:	1JM7
Title	:	Solution structure of the BRCA1/BARD1 RING-domain heterodimer
Authors	:	Brzovic, P.S.; Rajagopal, P.; Hoyt, D.W.; King, M.-C.; Klevit, R.E.
Deposited on	:	2001-07-17

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:

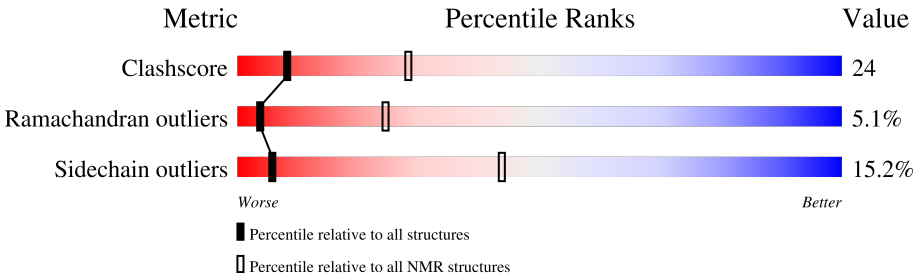
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	112	44% 43% • • 8%
2	B	117	40% 30% • 10% 17%

2 Ensemble composition and analysis (i)

This entry contains 14 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 2 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:3-A:101, B:33-B:117 (184)	0.62	13

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

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

The models can be grouped into 4 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 4, 8, 11, 12
2	7, 13, 14
3	1, 3, 9
4	5, 6, 10

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3162 atoms, of which 1589 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	103	1665	517	849	136	152	11	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	GLY	-	cloning artifact	UNP P38398
A	112	LYS	-	cloning artifact	UNP P38398

- Molecule 2 is a protein called BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	97	1493	461	740	140	140	12	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	141	GLY	-	cloning artifact	UNP Q99728
B	142	LYS	-	cloning artifact	UNP Q99728

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
3	A	2	2	2
3	B	2	2	2

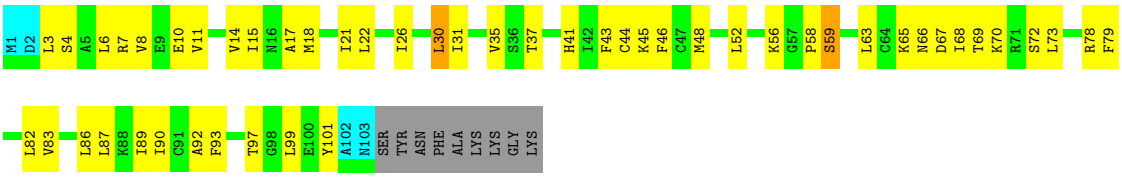
4 Residue-property plots (i)

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.

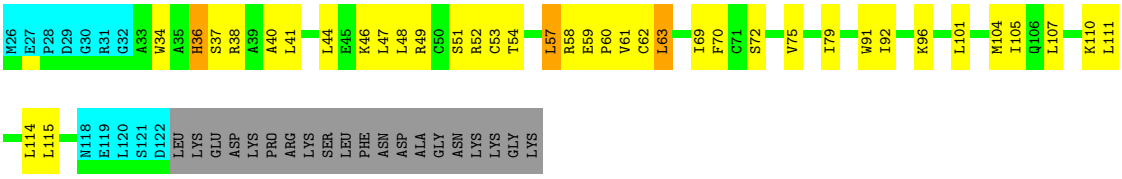
• Molecule 1: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN

Chain A: 44% 43% • • 8%



• Molecule 2: BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1

Chain B: 40% 30% • 10% 17%



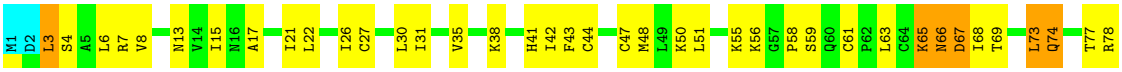
4.2 Scores per residue for each member of the ensemble

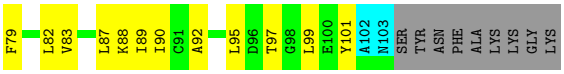
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN

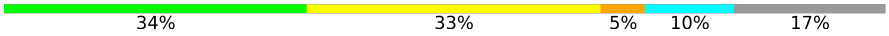
Chain A: 43% 40% 5% • 8%

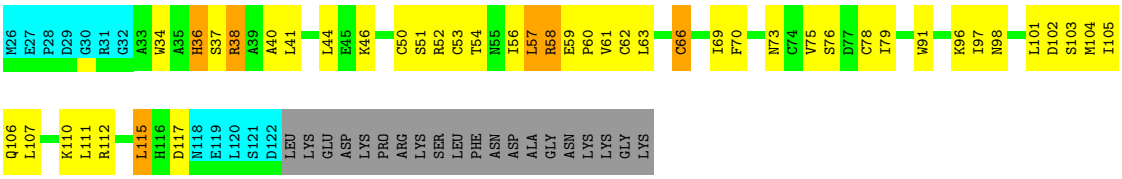




• Molecule 2: BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1

Chain B:

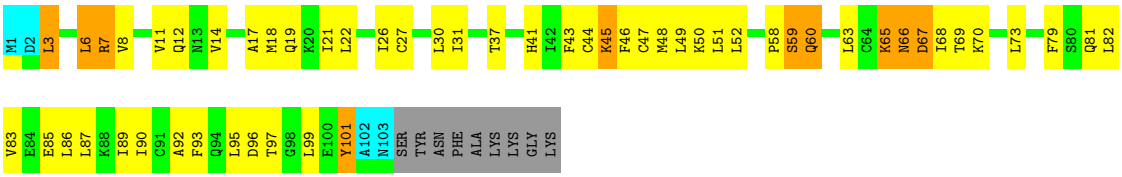




4.2.2 Score per residue for model 2

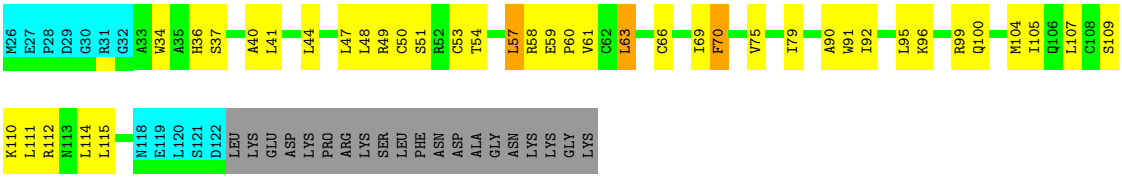
• Molecule 1: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN

Chain A:



• Molecule 2: BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1

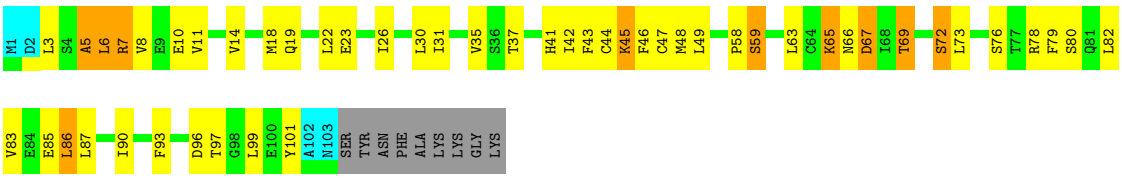
Chain B:



4.2.3 Score per residue for model 3

• Molecule 1: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN

Chain A:



• Molecule 2: BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1

Chain B: 41% 26% • • 10% 17%

M26 E27 P28 D29 G30 R31 G32 A33 W34 A35 H36 S37 L41 D42 R43 L44 E45 K46 L47 L48 S51 R52 I56 L57 R58 E59 P60 V61 C62 L63 G64 G65 H68 I69 F70 V75 I79 T88 W91 K96 L101 M104 I105 Q106 L107 C108 S109 K110 L111

L114 L115 H116 D117 N118 E119 L120 S121 D122 LEU LYS GLU ASP LYS PRO ARG LYS SER LEU PHE ASN ASP ALA GLY ASN LYS LYS GLY LYS

4.2.4 Score per residue for model 4

- Molecule 1: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN

Chain A: 38% 41% 8% • • 8%

M1 D2 L3 S4 A5 L6 R7 V8 E9 E10 V11 V14 A17 M18 I21 L22 I26 C27 L30 I31 K32 V35 S36 T37 H41 I42 F43 C44 K45 F46 C47 M48 L49 K50 L51 L52 K55 K56 G57 P58 S59 Q60 L63 C64 K65 N66 D67 I68 T69 K70 R71

S72 L73 T77 R78 F79 L82 V83 L86 I89 I90 C91 A92 T97 G98 L99 E100 Y101 A102 N103 SER TYR ASN PHE ALA LYS LYS GLY LYS

- Molecule 2: BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1

Chain B: 38% 28% 7% 10% 17%

M26 E27 P28 D29 G30 R31 G32 A33 W34 A35 H36 S37 R38 L41 L44 L47 L48 R49 C50 S51 R52 C53 T54 L57 R58 E59 P60 V61 C62 L63 I69 F70 N73 C74 V75 I79 I92 K96 I97 N98 R99 S103 M104 I105 Q106 L107 C108 S109 K110 L111

L114 L115 H116 D117 N118 E119 L120 S121 D122 LEU LYS GLU ASP LYS PRO ARG LYS SER LEU PHE ASN ASP ALA GLY ASN LYS LYS GLY LYS

4.2.5 Score per residue for model 5

- Molecule 1: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN

Chain A: 43% 38% 7% • • 8%

M1 D2 L3 S4 A5 L6 E10 V11 V14 I15 N16 A17 M18 I21 L22 I26 C27 L30 I31 K32 V35 S36 T37 K38 C39 D40 H41 I42 F43 C44 K45 F46 C47 L52 N53 Q54 S59 L63 C64 K65 N66 D67 I68 T69 K70 R71 R78 F79 S80 Q81

L82 V83 L86 L87 K88 I89 I90 C91 A92 F93 T97 A102 N103 SER TYR ASN PHE ALA LYS LYS GLY LYS

- Molecule 2: BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1

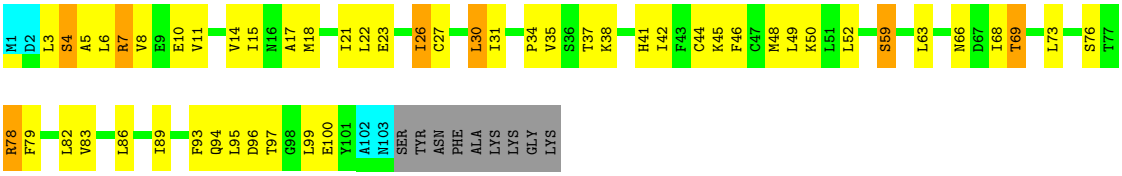
Chain B: 32% 36% • 10% 17%

M26 E27 P28 D29 G30 R31 G32 A33 W34 A35 H36 S37 R38 A39 A40 L41 L44 L47 L48 S51 R52 C53 T54 N55 I56 L57 R58 E59 P60 V61 C62 L63 G64 G65 H68 I69 F70 C71 S72 C78 I79 G80 T81 W91 I92 Q93 D94 L95 K96 I97 L101 D102 S103

4.2.6 Score per residue for model 6

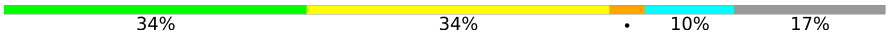
• Molecule 1: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN

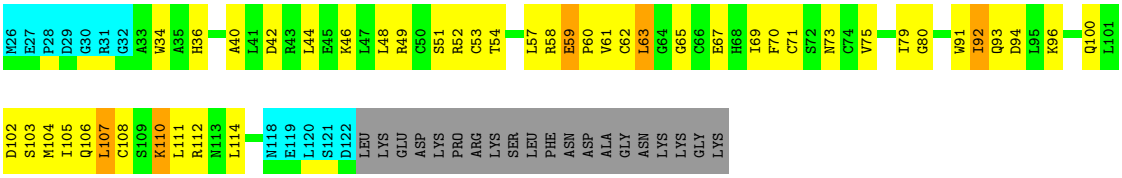
Chain A:



• Molecule 2: BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1

Chain B:

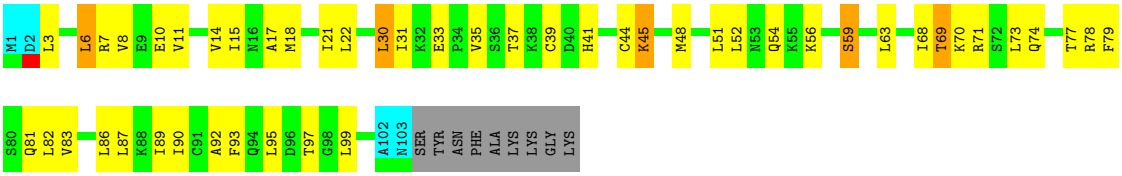




4.2.7 Score per residue for model 7

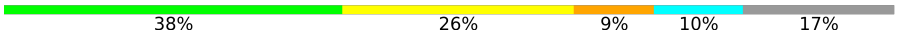
• Molecule 1: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN

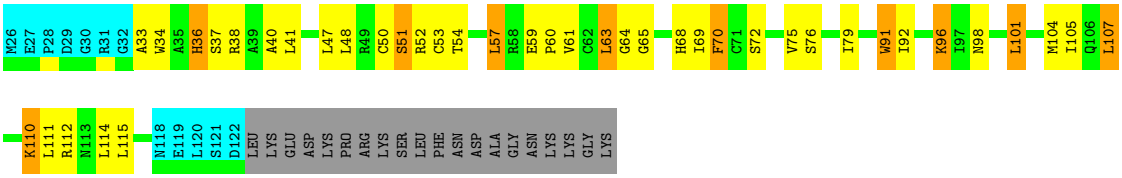
Chain A:



• Molecule 2: BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1

Chain B:

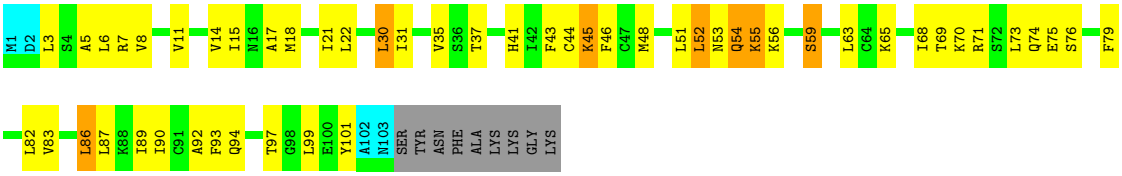




4.2.8 Score per residue for model 8

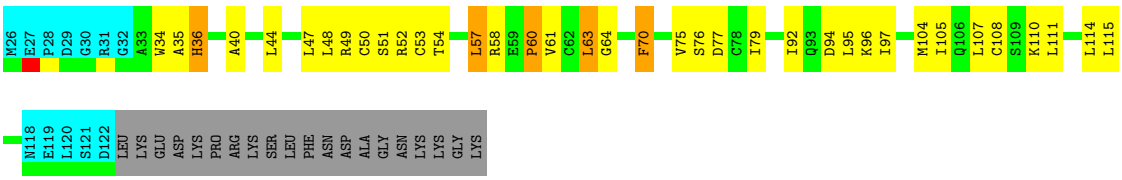
- Molecule 1: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN

Chain A: 42% 40% 6% • 8%



- Molecule 2: BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1

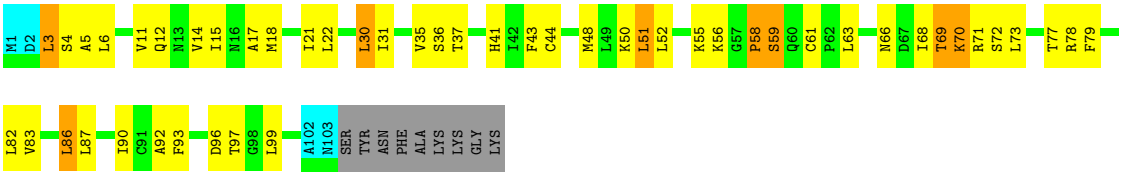
Chain B: 41% 27% • 10% 17%



4.2.9 Score per residue for model 9

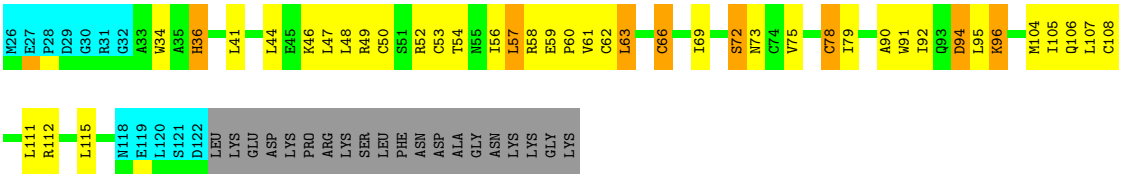
- Molecule 1: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN

Chain A: 44% 38% 7% • 8%



- Molecule 2: BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1

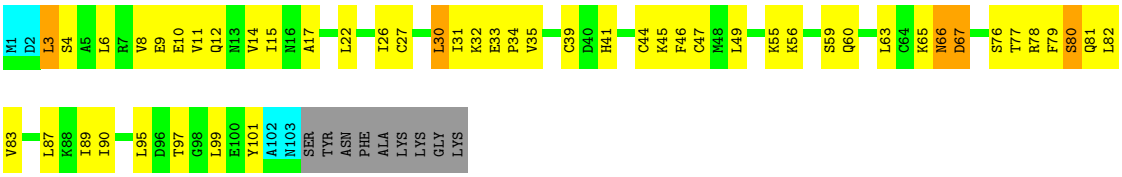
Chain B: 38% 28% 7% 10% 17%



4.2.10 Score per residue for model 10

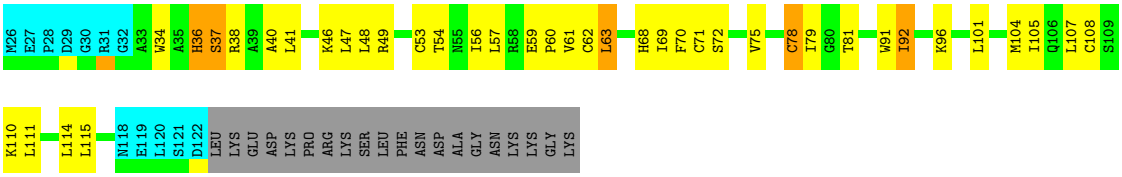
- Molecule 1: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN

Chain A: 44% 40% • • 8%



• Molecule 2: BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1

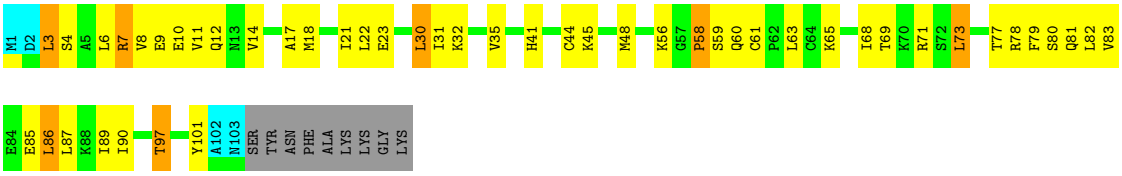
Chain B: 38% 30% • 10% 17%



4.2.11 Score per residue for model 11

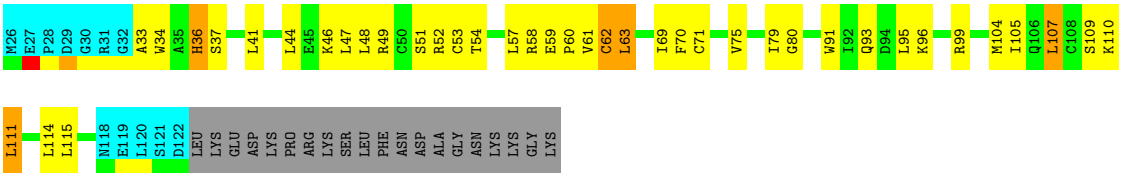
• Molecule 1: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN

Chain A: 46% 37% 6% • 8%



• Molecule 2: BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1

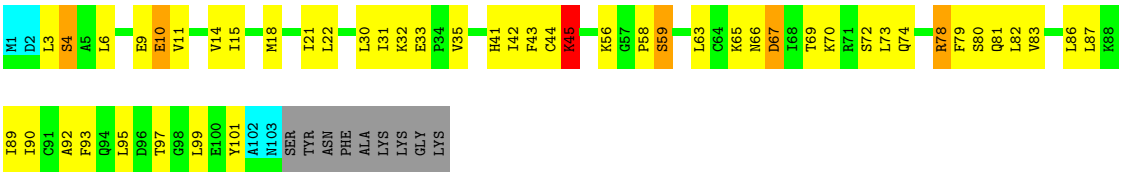
Chain B: 38% 30% • 10% 17%



4.2.12 Score per residue for model 12

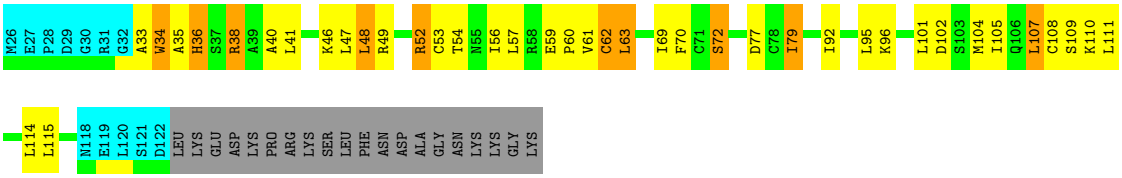
• Molecule 1: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN

Chain A: 45% 38% • • • 8%



• Molecule 2: BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1

Chain B: 38% 26% 9% 10% 17%



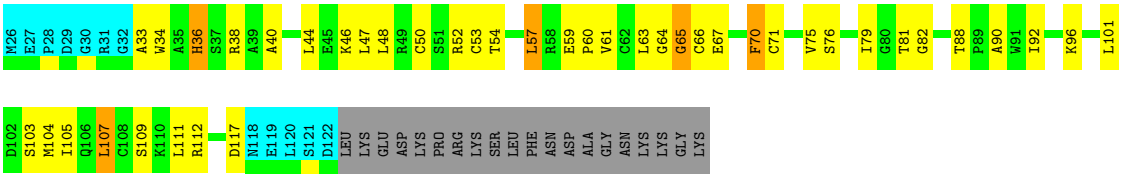
4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN

Chain A: 48% 35% • • • 8%

• Molecule 2: BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1

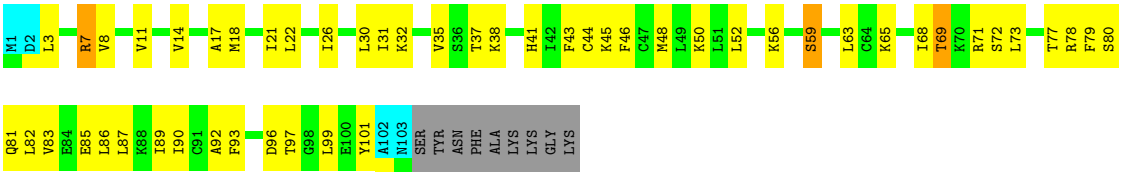
Chain B: 37% 32% • 10% 17%



4.2.14 Score per residue for model 14

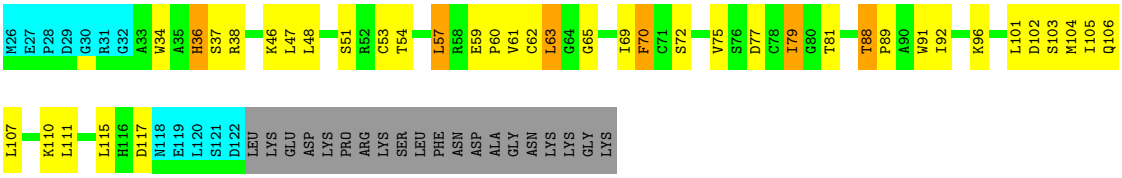
• Molecule 1: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN

Chain A: 43% 43% • • 8%



• Molecule 2: BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1

Chain B: 38% 29% 5% 10% 17%


M26
E27
P28
D29
G30
R31
G32
A33
W34
A35
H36
S37
R38
K46
L47
L48
S51
R52
C53
T54
L57
R58
E59
P60
V61
C62
L63
G64
G65
I69
F70
C71
S72
V75
S76
D77
C78
I79
G80
T81
T88
P89
A90
W91
I92
K96
L101
D102
S103
M104
I105
Q106
L107
K110
L111
L115
H116
D117
N118
E119
L120
S121
D122
LEU
LYS
GLU
ASP
LYS
PRO
ARG
LYS
SER
LEU
PHE
ASN
ASP
ALA
GLY
ASN
LYS
LYS
GLY
LYS

5 Refinement protocol and experimental data overview (i)

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

Of the 25 calculated structures, 14 were deposited, based on the following criterion: *structures with the least restraint violations, 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	1.0
CNS	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

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 (i)

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	787	823	823	48±6
2	B	663	661	661	40±6
All	All	20356	20776	20776	1007

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LEU:HD12	1:A:83:VAL:HG13	0.96	1.35	4	1
2:B:75:VAL:HG22	2:B:79:ILE:HD11	0.93	1.35	11	5
2:B:79:ILE:HD11	2:B:92:ILE:HD11	0.91	1.42	5	1
1:A:14:VAL:HG13	2:B:107:LEU:HD23	0.87	1.47	11	2
1:A:41:HIS:ND1	1:A:63:LEU:HD22	0.85	1.85	10	13
1:A:92:ALA:HB1	2:B:36:HIS:CG	0.83	2.08	5	5
2:B:57:LEU:HD12	2:B:105:ILE:HD11	0.83	1.51	7	2
2:B:75:VAL:HG22	2:B:79:ILE:CD1	0.81	2.05	2	6
2:B:107:LEU:HD13	2:B:110:LYS:CE	0.80	2.06	2	3
1:A:17:ALA:HB3	2:B:107:LEU:HD11	0.80	1.54	4	8
1:A:3:LEU:HD23	2:B:33:ALA:HB1	0.79	1.54	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:PHE:O	1:A:83:VAL:HG23	0.78	1.78	10	12
1:A:3:LEU:O	1:A:6:LEU:HD23	0.76	1.81	7	2
1:A:3:LEU:HD11	2:B:34:TRP:CZ2	0.76	2.15	2	2
2:B:61:VAL:HG13	2:B:96:LYS:O	0.76	1.81	3	11
1:A:21:ILE:HG21	2:B:104:MET:CG	0.75	2.10	1	3
1:A:22:LEU:HD22	1:A:79:PHE:CD1	0.75	2.16	10	3
2:B:61:VAL:HG22	2:B:97:ILE:HD13	0.75	1.59	5	2
1:A:18:MET:HE2	2:B:107:LEU:HD12	0.75	1.59	7	1
1:A:82:LEU:HD22	2:B:104:MET:SD	0.74	2.22	10	10
2:B:57:LEU:HD12	2:B:105:ILE:CD1	0.74	2.12	7	2
1:A:92:ALA:HB1	2:B:36:HIS:CD2	0.74	2.18	8	6
1:A:31:ILE:HG22	1:A:44:CYS:SG	0.74	2.23	8	10
1:A:11:VAL:HG22	2:B:114:LEU:HD13	0.74	1.58	5	2
1:A:78:ARG:CD	2:B:69:ILE:HD11	0.74	2.12	5	2
1:A:6:LEU:HD21	2:B:33:ALA:HB2	0.74	1.60	11	1
2:B:57:LEU:O	2:B:105:ILE:HG21	0.73	1.84	3	7
2:B:57:LEU:O	2:B:105:ILE:HD13	0.73	1.84	2	5
2:B:78:CYS:O	2:B:81:THR:HG22	0.73	1.84	5	1
1:A:17:ALA:HB3	2:B:107:LEU:HD21	0.72	1.59	1	3
1:A:22:LEU:HD12	1:A:83:VAL:CG2	0.72	2.15	12	5
1:A:8:VAL:CG1	1:A:99:LEU:HD22	0.72	2.14	6	4
2:B:63:LEU:HD23	2:B:75:VAL:HG21	0.72	1.60	3	1
1:A:22:LEU:HD12	1:A:83:VAL:HG22	0.72	1.59	12	5
2:B:63:LEU:HD22	2:B:75:VAL:HG23	0.72	1.61	13	3
2:B:44:LEU:HD23	2:B:44:LEU:O	0.72	1.85	1	3
2:B:107:LEU:HD13	2:B:110:LYS:HE2	0.71	1.61	14	5
1:A:90:ILE:HD13	1:A:101:TYR:CE2	0.71	2.19	4	2
1:A:22:LEU:HD21	2:B:104:MET:CE	0.71	2.16	6	1
1:A:78:ARG:HG2	2:B:69:ILE:HD11	0.70	1.61	3	4
2:B:48:LEU:HD12	2:B:105:ILE:HD13	0.70	1.62	7	2
2:B:75:VAL:HG22	2:B:79:ILE:HD13	0.70	1.63	1	3
1:A:31:ILE:HG22	1:A:44:CYS:HB3	0.70	1.61	12	4
1:A:92:ALA:HB1	2:B:36:HIS:ND1	0.70	2.00	2	1
1:A:11:VAL:HG13	2:B:111:LEU:CD2	0.70	2.16	7	5
1:A:11:VAL:HG12	1:A:15:ILE:HD11	0.69	1.64	10	6
2:B:63:LEU:HD23	2:B:70:PHE:CE1	0.69	2.23	8	4
1:A:22:LEU:HD21	2:B:104:MET:SD	0.68	2.29	3	6
1:A:18:MET:CG	1:A:86:LEU:HD21	0.68	2.18	5	4
1:A:26:ILE:HD11	1:A:47:CYS:SG	0.68	2.29	4	4
1:A:7:ARG:O	1:A:11:VAL:HG23	0.68	1.89	8	2
1:A:22:LEU:HB3	1:A:83:VAL:HG22	0.68	1.63	9	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ILE:HD13	1:A:42:ILE:CG2	0.68	2.19	6	1
2:B:57:LEU:CD1	2:B:105:ILE:HD11	0.68	2.19	7	1
1:A:78:ARG:CG	2:B:69:ILE:HD11	0.68	2.19	7	4
1:A:26:ILE:HD11	1:A:47:CYS:HA	0.67	1.64	5	3
2:B:75:VAL:HG22	2:B:79:ILE:HG12	0.67	1.66	14	1
2:B:65:GLY:O	2:B:88:THR:HG21	0.67	1.88	14	3
1:A:87:LEU:HA	1:A:90:ILE:HD12	0.67	1.65	14	9
1:A:41:HIS:CG	1:A:63:LEU:HD13	0.67	2.25	10	1
1:A:5:ALA:O	1:A:8:VAL:HG23	0.66	1.90	3	1
2:B:48:LEU:HD13	2:B:101:LEU:CD1	0.66	2.20	7	1
1:A:6:LEU:HD11	2:B:33:ALA:CB	0.66	2.20	11	1
1:A:22:LEU:HD23	1:A:83:VAL:HG22	0.66	1.67	11	1
1:A:89:ILE:HG12	2:B:40:ALA:HB1	0.66	1.65	8	9
1:A:41:HIS:CE1	1:A:63:LEU:HD22	0.66	2.26	2	7
2:B:63:LEU:CD2	2:B:75:VAL:HG21	0.66	2.19	3	1
2:B:57:LEU:HD22	2:B:60:PRO:CG	0.66	2.20	6	1
1:A:15:ILE:HD12	1:A:89:ILE:HG22	0.66	1.65	13	1
2:B:48:LEU:HD12	2:B:105:ILE:CD1	0.66	2.20	7	2
2:B:48:LEU:HD13	2:B:105:ILE:HD13	0.66	1.66	10	1
1:A:48:MET:HE1	1:A:68:ILE:HD13	0.66	1.66	2	2
1:A:51:LEU:HD23	1:A:59:SER:OG	0.66	1.91	1	1
1:A:90:ILE:HG21	1:A:101:TYR:CD2	0.66	2.26	2	7
2:B:50:CYS:HB2	2:B:57:LEU:HD23	0.65	1.67	9	6
1:A:22:LEU:HD22	1:A:79:PHE:CD2	0.65	2.27	3	1
2:B:57:LEU:HD13	2:B:60:PRO:CG	0.65	2.21	8	1
1:A:22:LEU:HD23	1:A:83:VAL:CG2	0.65	2.22	11	1
1:A:26:ILE:HD12	1:A:27:CYS:N	0.65	2.07	2	4
1:A:30:LEU:CD2	1:A:87:LEU:HD21	0.65	2.22	11	5
1:A:35:VAL:HG21	1:A:45:LYS:HA	0.65	1.69	12	4
2:B:75:VAL:HG23	2:B:79:ILE:HD11	0.65	1.67	9	1
1:A:37:THR:HG22	1:A:73:LEU:HD23	0.64	1.68	14	2
1:A:48:MET:CE	1:A:68:ILE:HD13	0.64	2.22	2	3
2:B:111:LEU:HA	2:B:114:LEU:HD12	0.64	1.68	12	4
1:A:21:ILE:HD13	2:B:104:MET:HG2	0.64	1.70	12	4
2:B:63:LEU:CD2	2:B:75:VAL:HG23	0.64	2.22	11	3
1:A:3:LEU:HD22	2:B:34:TRP:CZ3	0.64	2.28	13	1
2:B:41:LEU:HD22	2:B:115:LEU:CD1	0.64	2.22	11	3
2:B:107:LEU:HD23	2:B:110:LYS:CE	0.64	2.23	1	2
2:B:41:LEU:HD22	2:B:115:LEU:HD12	0.64	1.69	7	1
1:A:22:LEU:HD23	1:A:79:PHE:CD2	0.63	2.28	5	1
1:A:18:MET:SD	1:A:86:LEU:HD11	0.63	2.33	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:THR:HG23	1:A:80:SER:OG	0.63	1.94	10	3
1:A:58:PRO:HB3	1:A:69:THR:HG22	0.63	1.67	12	4
1:A:97:THR:HB	1:A:99:LEU:HD23	0.63	1.69	8	1
1:A:8:VAL:HG11	1:A:99:LEU:HD11	0.63	1.69	4	2
2:B:79:ILE:HD11	2:B:92:ILE:CD1	0.63	2.23	5	3
1:A:22:LEU:HD21	1:A:82:LEU:CB	0.63	2.24	11	2
1:A:6:LEU:HD12	1:A:7:ARG:HB2	0.62	1.71	6	2
2:B:34:TRP:HB3	2:B:115:LEU:HD23	0.62	1.71	4	6
1:A:18:MET:HG2	1:A:86:LEU:HD21	0.62	1.69	11	2
1:A:3:LEU:HD21	2:B:34:TRP:CH2	0.62	2.29	6	1
1:A:37:THR:HG22	1:A:73:LEU:CD2	0.62	2.24	14	2
1:A:14:VAL:CG1	2:B:107:LEU:HD23	0.62	2.21	11	1
1:A:4:SER:HB2	1:A:6:LEU:HD23	0.62	1.71	1	2
1:A:48:MET:O	1:A:52:LEU:HD12	0.62	1.94	2	4
2:B:48:LEU:HA	2:B:57:LEU:HD12	0.62	1.69	6	1
1:A:48:MET:HG3	1:A:73:LEU:HD13	0.62	1.70	1	1
1:A:6:LEU:HD12	1:A:6:LEU:O	0.62	1.94	11	5
1:A:3:LEU:HD21	1:A:97:THR:HG22	0.62	1.71	2	1
1:A:6:LEU:HD21	2:B:33:ALA:CB	0.62	2.24	11	1
1:A:30:LEU:HD11	1:A:83:VAL:HG13	0.62	1.70	5	1
2:B:61:VAL:HG11	2:B:95:LEU:HB3	0.62	1.71	8	1
1:A:48:MET:SD	1:A:73:LEU:HD22	0.62	2.34	11	1
1:A:18:MET:SD	2:B:44:LEU:HD13	0.61	2.35	13	4
1:A:78:ARG:HB2	2:B:69:ILE:HD11	0.61	1.72	9	2
1:A:46:PHE:HA	1:A:49:LEU:HD12	0.61	1.72	4	1
1:A:35:VAL:HG21	1:A:45:LYS:CA	0.61	2.25	7	3
1:A:51:LEU:HD23	1:A:59:SER:HB3	0.61	1.71	8	2
1:A:82:LEU:HG	2:B:47:LEU:HD22	0.61	1.71	7	2
1:A:30:LEU:HD12	1:A:83:VAL:CG1	0.61	2.19	4	1
2:B:102:ASP:HA	2:B:105:ILE:HD12	0.61	1.71	6	5
1:A:93:PHE:CE1	1:A:97:THR:HG21	0.61	2.30	12	4
1:A:33:GLU:O	1:A:35:VAL:HG23	0.61	1.95	10	3
2:B:61:VAL:O	2:B:69:ILE:HG23	0.61	1.96	3	2
1:A:51:LEU:HD23	1:A:59:SER:HB2	0.61	1.71	7	2
1:A:10:GLU:HB3	2:B:114:LEU:HD21	0.60	1.73	3	4
1:A:78:ARG:HD2	2:B:69:ILE:HD11	0.60	1.72	5	2
2:B:79:ILE:HD11	2:B:92:ILE:HD12	0.60	1.74	12	2
2:B:57:LEU:HD13	2:B:60:PRO:HG3	0.60	1.72	8	6
2:B:110:LYS:O	2:B:114:LEU:HD13	0.60	1.95	10	3
1:A:52:LEU:HD23	1:A:59:SER:N	0.60	2.11	14	3
1:A:99:LEU:HD12	1:A:99:LEU:N	0.60	2.12	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:LEU:HD21	2:B:47:LEU:CB	0.60	2.27	9	4
1:A:86:LEU:HD12	1:A:90:ILE:HD11	0.59	1.72	3	5
1:A:17:ALA:CB	2:B:107:LEU:HD11	0.59	2.27	11	2
2:B:63:LEU:HD22	2:B:75:VAL:CG2	0.59	2.27	13	4
1:A:10:GLU:O	1:A:14:VAL:HG23	0.59	1.97	5	6
1:A:3:LEU:HD22	1:A:97:THR:HG22	0.59	1.72	6	1
1:A:48:MET:SD	1:A:73:LEU:HD11	0.59	2.37	9	3
1:A:31:ILE:HD13	1:A:42:ILE:HG21	0.59	1.74	6	1
2:B:63:LEU:HD21	2:B:79:ILE:HG23	0.59	1.74	9	1
1:A:86:LEU:HA	1:A:89:ILE:HD12	0.59	1.75	4	7
1:A:31:ILE:O	1:A:83:VAL:HG11	0.59	1.97	12	5
1:A:18:MET:HE3	2:B:107:LEU:HD12	0.58	1.73	6	1
1:A:22:LEU:HD21	2:B:104:MET:HE2	0.58	1.75	6	1
1:A:35:VAL:HG11	1:A:48:MET:SD	0.58	2.38	13	1
1:A:17:ALA:HB1	2:B:107:LEU:HD11	0.58	1.74	11	2
1:A:18:MET:HB3	1:A:86:LEU:HD21	0.58	1.73	9	2
2:B:75:VAL:O	2:B:79:ILE:HD11	0.58	1.97	13	1
1:A:21:ILE:HG21	2:B:104:MET:HG3	0.58	1.75	12	3
2:B:75:VAL:HG22	2:B:79:ILE:CG1	0.58	2.29	14	1
2:B:44:LEU:HD13	2:B:108:CYS:SG	0.58	2.39	8	1
1:A:11:VAL:HG13	2:B:111:LEU:HD23	0.58	1.76	4	2
1:A:8:VAL:HG12	1:A:99:LEU:HD22	0.58	1.76	1	5
1:A:37:THR:HG23	1:A:41:HIS:O	0.57	1.98	14	2
1:A:18:MET:HB3	1:A:86:LEU:HD11	0.57	1.76	5	1
2:B:44:LEU:HD22	2:B:108:CYS:SG	0.57	2.39	8	1
1:A:72:SER:C	1:A:73:LEU:HD22	0.57	2.19	4	3
2:B:63:LEU:HD23	2:B:79:ILE:HD13	0.57	1.77	10	1
1:A:78:ARG:HD3	2:B:69:ILE:HD11	0.57	1.77	12	2
1:A:11:VAL:HG13	2:B:111:LEU:HD11	0.57	1.77	10	1
1:A:6:LEU:HD12	2:B:34:TRP:CZ2	0.57	2.35	11	1
1:A:14:VAL:HG22	2:B:110:LYS:HE3	0.57	1.76	11	3
1:A:8:VAL:CG1	1:A:99:LEU:HD11	0.57	2.30	4	1
2:B:48:LEU:HD11	2:B:104:MET:HB2	0.57	1.77	7	2
1:A:35:VAL:HG11	1:A:73:LEU:HD12	0.57	1.75	11	1
2:B:58:ARG:HA	2:B:105:ILE:HD13	0.56	1.77	1	2
1:A:81:GLN:HB2	2:B:47:LEU:HD22	0.56	1.77	14	2
2:B:69:ILE:HG21	2:B:101:LEU:HD13	0.56	1.76	3	1
1:A:30:LEU:HD21	1:A:87:LEU:HD21	0.56	1.77	13	3
1:A:97:THR:HB	1:A:99:LEU:HD13	0.56	1.78	10	8
1:A:81:GLN:CB	2:B:47:LEU:HD21	0.56	2.31	5	1
1:A:3:LEU:HD13	1:A:96:ASP:O	0.56	2.01	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LEU:CD2	1:A:87:LEU:HD11	0.56	2.31	7	3
1:A:45:LYS:NZ	1:A:73:LEU:HD11	0.55	2.16	2	1
2:B:69:ILE:HD13	2:B:101:LEU:HD11	0.55	1.78	1	1
2:B:75:VAL:HG12	2:B:75:VAL:O	0.55	2.01	6	1
1:A:3:LEU:CD2	2:B:33:ALA:HB1	0.55	2.28	7	1
1:A:82:LEU:HD21	2:B:48:LEU:CD2	0.55	2.31	7	1
2:B:57:LEU:HD22	2:B:60:PRO:HG3	0.55	1.78	6	1
1:A:11:VAL:HG12	1:A:15:ILE:CD1	0.55	2.31	9	2
2:B:57:LEU:HD22	2:B:60:PRO:HB3	0.55	1.79	10	4
1:A:93:PHE:CZ	1:A:97:THR:HG21	0.55	2.37	12	3
2:B:48:LEU:HD23	2:B:105:ILE:CG1	0.55	2.30	3	1
1:A:3:LEU:CD1	2:B:33:ALA:HB1	0.54	2.32	12	1
1:A:4:SER:OG	1:A:6:LEU:HD23	0.54	2.02	12	1
2:B:41:LEU:HD21	2:B:108:CYS:SG	0.54	2.42	12	2
1:A:11:VAL:HG22	2:B:114:LEU:CD1	0.54	2.30	5	1
1:A:22:LEU:HD21	1:A:82:LEU:HB3	0.54	1.77	11	3
1:A:41:HIS:CG	1:A:63:LEU:HD22	0.54	2.36	6	5
2:B:48:LEU:HD22	2:B:105:ILE:HG13	0.54	1.77	14	1
1:A:11:VAL:CG2	2:B:114:LEU:HD13	0.54	2.30	5	1
1:A:3:LEU:HD23	2:B:34:TRP:CZ2	0.54	2.37	10	2
2:B:107:LEU:HD23	2:B:110:LYS:HE2	0.54	1.78	1	2
2:B:50:CYS:CA	2:B:57:LEU:HD23	0.54	2.33	13	1
2:B:61:VAL:HG22	2:B:96:LYS:O	0.54	2.02	2	2
1:A:35:VAL:HG21	1:A:45:LYS:CE	0.54	2.33	4	1
1:A:14:VAL:O	2:B:107:LEU:HD12	0.54	2.03	4	4
1:A:3:LEU:HD21	2:B:34:TRP:HB2	0.54	1.78	12	1
1:A:70:LYS:HA	1:A:73:LEU:HD23	0.54	1.79	13	1
1:A:3:LEU:HD11	2:B:34:TRP:CE2	0.53	2.39	2	1
1:A:37:THR:HG21	1:A:43:PHE:CE2	0.53	2.38	5	1
1:A:82:LEU:HD23	2:B:47:LEU:HD12	0.53	1.80	14	2
1:A:22:LEU:O	1:A:30:LEU:HD13	0.53	2.03	4	1
1:A:3:LEU:HD12	1:A:3:LEU:N	0.53	2.18	13	1
1:A:15:ILE:HG22	1:A:101:TYR:CE1	0.53	2.39	1	1
2:B:41:LEU:CD2	2:B:115:LEU:HD12	0.53	2.34	7	1
1:A:52:LEU:HD21	1:A:69:THR:O	0.53	2.04	4	1
2:B:63:LEU:HD13	2:B:63:LEU:O	0.53	2.04	6	2
1:A:3:LEU:HD12	1:A:6:LEU:HD21	0.53	1.80	2	1
1:A:46:PHE:HA	1:A:49:LEU:HD13	0.53	1.79	10	1
1:A:3:LEU:HD11	2:B:33:ALA:HB1	0.53	1.79	12	1
1:A:15:ILE:HD12	1:A:89:ILE:CG2	0.53	2.33	13	1
1:A:81:GLN:HB2	2:B:47:LEU:HD11	0.53	1.80	11	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LEU:HD23	1:A:87:LEU:HD11	0.53	1.79	10	2
1:A:51:LEU:HD23	1:A:59:SER:CB	0.53	2.33	2	3
1:A:31:ILE:HD12	1:A:34:PRO:HB3	0.53	1.80	6	1
2:B:63:LEU:CD2	2:B:79:ILE:HG23	0.52	2.34	9	1
1:A:22:LEU:HD23	1:A:79:PHE:CG	0.52	2.39	5	1
1:A:30:LEU:HD23	1:A:83:VAL:CG1	0.52	2.35	6	1
1:A:22:LEU:HD21	2:B:104:MET:HE3	0.52	1.80	2	1
1:A:11:VAL:HG22	2:B:114:LEU:HD23	0.52	1.82	3	2
1:A:37:THR:HG21	1:A:43:PHE:CE1	0.52	2.39	13	3
1:A:79:PHE:HA	1:A:82:LEU:HD12	0.52	1.82	3	4
2:B:92:ILE:HD12	2:B:94:ASP:O	0.52	2.05	9	2
2:B:61:VAL:HG11	2:B:95:LEU:CD1	0.52	2.35	12	1
2:B:111:LEU:HD12	2:B:114:LEU:HD12	0.52	1.82	12	1
1:A:3:LEU:HD11	1:A:96:ASP:OD2	0.52	2.05	14	2
2:B:103:SER:O	2:B:107:LEU:HD23	0.52	2.05	14	2
2:B:48:LEU:HD12	2:B:105:ILE:CG1	0.52	2.35	6	2
2:B:63:LEU:HD23	2:B:70:PHE:HE1	0.51	1.64	8	1
2:B:63:LEU:HD22	2:B:92:ILE:HD11	0.51	1.82	2	1
2:B:41:LEU:HD12	2:B:111:LEU:HB3	0.51	1.82	5	1
1:A:11:VAL:HG21	2:B:34:TRP:CZ3	0.51	2.40	11	2
1:A:18:MET:HA	1:A:21:ILE:HD12	0.51	1.82	4	8
2:B:61:VAL:HG23	2:B:96:LYS:O	0.51	2.06	1	1
1:A:35:VAL:HG21	1:A:45:LYS:HE2	0.51	1.82	4	1
1:A:18:MET:HG2	1:A:86:LEU:HD13	0.51	1.82	12	2
2:B:63:LEU:CD2	2:B:92:ILE:HD11	0.51	2.36	2	1
1:A:26:ILE:HD11	1:A:47:CYS:CB	0.51	2.36	3	2
1:A:46:PHE:CD1	1:A:49:LEU:HD22	0.51	2.40	6	1
1:A:77:THR:HG22	1:A:77:THR:O	0.50	2.06	9	4
1:A:78:ARG:CB	2:B:69:ILE:HD11	0.50	2.36	10	2
1:A:11:VAL:HG13	2:B:111:LEU:CD1	0.50	2.36	10	1
1:A:6:LEU:HD11	2:B:33:ALA:HB1	0.50	1.81	11	1
1:A:31:ILE:HG13	1:A:83:VAL:HG21	0.50	1.83	12	2
2:B:44:LEU:HD11	2:B:104:MET:CE	0.50	2.36	11	2
1:A:17:ALA:O	1:A:21:ILE:HD12	0.50	2.07	7	2
2:B:41:LEU:HD13	2:B:111:LEU:CB	0.50	2.36	11	4
2:B:61:VAL:HG11	2:B:95:LEU:HD13	0.50	1.82	5	2
2:B:112:ARG:HA	2:B:115:LEU:HD12	0.50	1.83	5	1
2:B:41:LEU:HD22	2:B:115:LEU:HD11	0.50	1.82	11	1
1:A:3:LEU:HD22	2:B:34:TRP:CZ2	0.50	2.41	5	1
1:A:30:LEU:HD22	1:A:87:LEU:HD21	0.50	1.82	11	1
1:A:14:VAL:CG1	2:B:111:LEU:HD13	0.50	2.37	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:111:LEU:O	2:B:115:LEU:HD13	0.50	2.06	12	1
1:A:82:LEU:HD21	2:B:47:LEU:HB2	0.50	1.83	9	1
2:B:61:VAL:HG21	2:B:95:LEU:HG	0.50	1.82	9	1
2:B:59:GLU:CG	2:B:97:ILE:HG21	0.50	2.37	5	1
2:B:75:VAL:HG23	2:B:79:ILE:HG13	0.50	1.82	10	1
2:B:75:VAL:HG23	2:B:79:ILE:CD1	0.50	2.35	9	1
1:A:52:LEU:HD12	1:A:59:SER:HB3	0.49	1.84	4	1
1:A:31:ILE:O	1:A:83:VAL:HG21	0.49	2.06	4	1
2:B:62:CYS:O	2:B:92:ILE:HD11	0.49	2.07	12	1
1:A:5:ALA:HA	1:A:8:VAL:HG23	0.49	1.85	4	2
1:A:37:THR:HG21	1:A:43:PHE:CD1	0.49	2.42	9	4
2:B:82:GLY:HA2	2:B:90:ALA:HB2	0.49	1.84	13	1
2:B:61:VAL:HG23	2:B:72:SER:HA	0.49	1.84	12	5
2:B:38:ARG:HD2	2:B:115:LEU:HD13	0.49	1.84	1	1
2:B:44:LEU:HD23	2:B:48:LEU:HD23	0.49	1.85	6	1
2:B:48:LEU:HD12	2:B:105:ILE:HD11	0.49	1.84	9	1
2:B:69:ILE:HG21	2:B:101:LEU:CD1	0.49	2.36	14	2
2:B:48:LEU:HD22	2:B:105:ILE:CG1	0.49	2.37	14	1
1:A:3:LEU:HD13	1:A:97:THR:HG22	0.49	1.85	4	2
2:B:63:LEU:O	2:B:92:ILE:HD11	0.49	2.08	13	2
1:A:97:THR:CB	1:A:99:LEU:HD13	0.48	2.38	3	6
2:B:37:SER:OG	2:B:115:LEU:HD21	0.48	2.08	2	1
1:A:26:ILE:HD11	1:A:47:CYS:CA	0.48	2.38	5	1
1:A:97:THR:CB	1:A:99:LEU:HD23	0.48	2.36	8	1
1:A:22:LEU:CD2	2:B:104:MET:HE3	0.48	2.39	13	1
2:B:48:LEU:HD23	2:B:105:ILE:HG12	0.48	1.85	2	1
1:A:82:LEU:HG	2:B:47:LEU:HD23	0.48	1.85	5	1
1:A:79:PHE:CD1	1:A:82:LEU:CD1	0.48	2.96	14	1
1:A:8:VAL:HG22	2:B:34:TRP:CH2	0.48	2.44	3	1
1:A:81:GLN:CB	2:B:47:LEU:HD22	0.48	2.38	10	2
1:A:8:VAL:HG11	1:A:99:LEU:HD22	0.48	1.85	6	1
2:B:38:ARG:HA	2:B:115:LEU:HD21	0.48	1.85	12	1
2:B:48:LEU:HD21	2:B:104:MET:HG3	0.48	1.86	14	1
2:B:70:PHE:N	2:B:70:PHE:CD1	0.48	2.82	13	4
1:A:31:ILE:CD1	1:A:42:ILE:HG21	0.48	2.38	6	1
2:B:91:TRP:O	2:B:92:ILE:HG23	0.48	2.09	7	1
2:B:88:THR:HG22	2:B:89:PRO:HD2	0.48	1.85	14	1
1:A:37:THR:HA	1:A:73:LEU:HD13	0.48	1.86	6	1
2:B:48:LEU:CA	2:B:57:LEU:HD12	0.48	2.38	6	1
2:B:44:LEU:HD11	2:B:104:MET:HE2	0.48	1.84	11	1
2:B:50:CYS:CB	2:B:57:LEU:HD23	0.48	2.38	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ILE:HG22	1:A:44:CYS:CB	0.48	2.38	12	1
1:A:18:MET:CB	1:A:86:LEU:HD21	0.47	2.39	9	3
1:A:3:LEU:HD22	1:A:97:THR:HG23	0.47	1.85	11	1
1:A:52:LEU:HD13	1:A:70:LYS:HB3	0.47	1.84	9	1
1:A:11:VAL:CG2	2:B:114:LEU:HD23	0.47	2.39	3	2
1:A:11:VAL:O	1:A:15:ILE:HD12	0.47	2.09	12	1
2:B:111:LEU:O	2:B:115:LEU:HD12	0.47	2.10	14	4
1:A:30:LEU:HD11	1:A:83:VAL:CG1	0.47	2.40	5	1
2:B:48:LEU:HD12	2:B:105:ILE:HG12	0.47	1.86	13	2
1:A:81:GLN:HB2	2:B:47:LEU:HD21	0.47	1.86	7	2
2:B:48:LEU:HD11	2:B:101:LEU:CD2	0.47	2.40	5	1
1:A:85:GLU:OE1	2:B:47:LEU:HD13	0.47	2.10	13	1
1:A:42:ILE:HD11	1:A:78:ARG:HH22	0.47	1.69	1	1
1:A:90:ILE:HG23	1:A:101:TYR:CD2	0.47	2.45	8	1
1:A:37:THR:HG21	1:A:48:MET:HE3	0.47	1.87	6	1
1:A:68:ILE:CG2	1:A:73:LEU:HD21	0.47	2.40	13	1
1:A:82:LEU:HD21	2:B:47:LEU:HB3	0.47	1.87	13	1
1:A:90:ILE:HG21	1:A:101:TYR:CE2	0.46	2.45	4	1
1:A:14:VAL:HG21	2:B:114:LEU:CD1	0.46	2.40	7	1
2:B:92:ILE:HG22	2:B:96:LYS:HD2	0.46	1.87	4	1
2:B:57:LEU:HD22	2:B:60:PRO:CB	0.46	2.40	6	2
1:A:3:LEU:HD22	2:B:34:TRP:CH2	0.46	2.45	7	1
1:A:35:VAL:HG21	1:A:45:LYS:HE3	0.46	1.85	8	1
1:A:61:CYS:HB2	1:A:68:ILE:HD11	0.46	1.86	9	1
2:B:62:CYS:O	2:B:75:VAL:HG21	0.46	2.10	11	1
2:B:75:VAL:CG2	2:B:79:ILE:HD11	0.46	2.25	11	1
2:B:44:LEU:HD21	2:B:104:MET:SD	0.46	2.51	2	1
1:A:7:ARG:O	1:A:9:GLU:N	0.46	2.48	11	2
1:A:14:VAL:HG11	2:B:111:LEU:HD13	0.46	1.85	12	1
1:A:22:LEU:CD2	1:A:79:PHE:CE1	0.46	2.99	10	3
1:A:58:PRO:HB3	1:A:69:THR:HG23	0.46	1.86	9	1
1:A:79:PHE:CD1	1:A:82:LEU:HD12	0.46	2.46	14	1
1:A:3:LEU:HD22	1:A:96:ASP:OD2	0.46	2.11	2	1
2:B:56:ILE:CG2	2:B:105:ILE:HG23	0.46	2.40	10	3
1:A:22:LEU:HD11	1:A:79:PHE:CE1	0.46	2.46	11	1
1:A:35:VAL:CG1	1:A:73:LEU:HD12	0.46	2.41	11	1
2:B:63:LEU:HG	2:B:75:VAL:HG21	0.46	1.87	1	1
2:B:70:PHE:CD1	2:B:70:PHE:N	0.46	2.84	4	4
1:A:6:LEU:CD1	2:B:34:TRP:CZ2	0.45	2.98	11	1
1:A:8:VAL:HG11	1:A:99:LEU:HD13	0.45	1.88	6	1
1:A:82:LEU:CG	2:B:47:LEU:HD22	0.45	2.40	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:48:LEU:CD1	2:B:101:LEU:HD11	0.45	2.41	12	1
1:A:8:VAL:HG13	1:A:93:PHE:CZ	0.45	2.46	3	4
1:A:35:VAL:HG21	1:A:45:LYS:CB	0.45	2.41	7	2
1:A:41:HIS:CD2	1:A:63:LEU:HD13	0.45	2.46	10	1
2:B:52:ARG:CD	2:B:70:PHE:CD2	0.45	3.00	12	1
1:A:38:LYS:CE	2:B:91:TRP:CH2	0.45	3.00	1	1
2:B:51:SER:CB	2:B:70:PHE:CE2	0.45	3.00	4	2
2:B:47:LEU:HD12	2:B:47:LEU:N	0.45	2.27	5	1
1:A:37:THR:HG21	1:A:48:MET:CE	0.45	2.41	6	2
2:B:41:LEU:HD11	2:B:108:CYS:SG	0.45	2.52	10	1
2:B:52:ARG:NH1	2:B:70:PHE:CE1	0.45	2.85	11	1
1:A:14:VAL:CB	2:B:111:LEU:HD13	0.45	2.42	12	1
2:B:38:ARG:NH2	2:B:116:HIS:CE1	0.45	2.85	4	1
1:A:37:THR:CG2	1:A:43:PHE:CD1	0.45	2.99	14	3
1:A:48:MET:CE	1:A:73:LEU:HD21	0.45	2.40	14	1
2:B:48:LEU:HD11	2:B:101:LEU:HD22	0.45	1.88	5	1
1:A:21:ILE:HG21	2:B:100:GLN:O	0.45	2.12	2	2
2:B:41:LEU:HD13	2:B:111:LEU:HD23	0.45	1.89	10	1
1:A:41:HIS:O	1:A:42:ILE:HD13	0.45	2.12	12	1
2:B:59:GLU:N	2:B:60:PRO:CD	0.45	2.80	11	12
1:A:3:LEU:CD1	2:B:34:TRP:CE2	0.45	3.00	2	1
1:A:37:THR:HG21	1:A:48:MET:HE1	0.45	1.89	3	1
1:A:42:ILE:HG22	1:A:43:PHE:N	0.45	2.27	3	1
1:A:73:LEU:HD22	1:A:73:LEU:N	0.45	2.27	13	1
1:A:89:ILE:CG1	2:B:40:ALA:HB1	0.45	2.42	13	1
1:A:3:LEU:CD2	2:B:34:TRP:CZ2	0.44	3.00	1	3
1:A:21:ILE:HG21	2:B:104:MET:HG2	0.44	1.87	7	2
1:A:3:LEU:CD2	2:B:34:TRP:CH2	0.44	3.00	10	1
1:A:43:PHE:CD1	1:A:48:MET:CE	0.44	2.99	13	1
2:B:48:LEU:O	2:B:57:LEU:HD11	0.44	2.11	8	3
1:A:4:SER:HA	1:A:8:VAL:HG21	0.44	1.89	6	1
1:A:37:THR:CG2	1:A:48:MET:HE3	0.44	2.42	6	1
2:B:61:VAL:HG13	2:B:75:VAL:HG11	0.44	1.90	6	1
1:A:26:ILE:HD12	1:A:27:CYS:HB3	0.44	1.88	2	1
1:A:18:MET:HG3	1:A:86:LEU:HD11	0.44	1.88	8	1
1:A:22:LEU:CD1	1:A:79:PHE:CD2	0.44	2.99	9	1
1:A:8:VAL:HG22	2:B:34:TRP:HH2	0.44	1.71	3	1
1:A:82:LEU:N	2:B:47:LEU:HD13	0.44	2.25	14	2
1:A:79:PHE:CZ	2:B:101:LEU:HD22	0.44	2.48	10	1
2:B:70:PHE:CD1	2:B:75:VAL:CG1	0.44	3.01	10	1
1:A:22:LEU:HD11	1:A:79:PHE:CD1	0.44	2.47	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:41:LEU:C	2:B:41:LEU:HD23	0.44	2.32	12	1
1:A:35:VAL:HG13	1:A:35:VAL:O	0.44	2.12	8	4
1:A:35:VAL:HG12	1:A:73:LEU:HD12	0.44	1.89	7	1
1:A:48:MET:O	1:A:52:LEU:HD13	0.44	2.12	4	1
2:B:41:LEU:HD13	2:B:111:LEU:HD13	0.44	1.87	11	1
2:B:44:LEU:HD23	2:B:48:LEU:CD2	0.44	2.43	4	1
1:A:14:VAL:HG13	2:B:107:LEU:CD2	0.44	2.42	5	1
1:A:68:ILE:HG22	1:A:69:THR:N	0.44	2.28	6	5
1:A:31:ILE:HD13	1:A:42:ILE:HG22	0.44	1.88	6	1
2:B:79:ILE:HG22	2:B:80:GLY:N	0.44	2.28	11	2
1:A:41:HIS:CE1	1:A:63:LEU:CB	0.44	3.00	13	1
1:A:3:LEU:HD21	2:B:33:ALA:HB1	0.44	1.89	5	1
1:A:99:LEU:N	1:A:99:LEU:CD1	0.44	2.80	6	1
2:B:71:CYS:O	2:B:75:VAL:HG23	0.43	2.13	6	1
1:A:86:LEU:O	1:A:90:ILE:HD12	0.43	2.13	9	1
2:B:38:ARG:HA	2:B:115:LEU:HD13	0.43	1.90	7	1
2:B:57:LEU:HD12	2:B:105:ILE:HD13	0.43	1.89	13	1
1:A:53:ASN:O	1:A:55:LYS:N	0.43	2.51	8	1
2:B:37:SER:CB	2:B:115:LEU:HD21	0.43	2.43	3	2
1:A:61:CYS:CB	1:A:68:ILE:HD11	0.43	2.44	1	2
1:A:30:LEU:HD21	1:A:87:LEU:CD2	0.43	2.43	9	1
1:A:66:ASN:O	1:A:67:ASP:CB	0.43	2.67	1	1
1:A:3:LEU:CD2	1:A:8:VAL:HG22	0.43	2.43	6	1
1:A:90:ILE:CD1	1:A:101:TYR:CE2	0.43	3.02	12	1
1:A:90:ILE:HG21	1:A:101:TYR:CG	0.43	2.49	13	1
2:B:48:LEU:HD12	2:B:105:ILE:HG13	0.43	1.90	8	2
2:B:75:VAL:HB	2:B:79:ILE:HD11	0.43	1.89	10	1
2:B:56:ILE:HD12	2:B:56:ILE:H	0.43	1.74	1	1
2:B:48:LEU:HD22	2:B:48:LEU:N	0.43	2.29	8	1
2:B:75:VAL:CG2	2:B:79:ILE:CD1	0.43	2.97	9	1
2:B:59:GLU:N	2:B:60:PRO:HD3	0.43	2.29	6	1
1:A:14:VAL:HG13	2:B:110:LYS:HE3	0.43	1.89	7	2
2:B:62:CYS:O	2:B:92:ILE:HD13	0.43	2.14	10	2
2:B:47:LEU:O	2:B:48:LEU:HD22	0.43	2.13	13	1
2:B:97:ILE:HG22	2:B:98:ASN:N	0.42	2.29	1	2
1:A:26:ILE:HG13	1:A:27:CYS:N	0.42	2.29	5	1
1:A:78:ARG:HB3	2:B:69:ILE:HD11	0.42	1.91	6	1
1:A:35:VAL:HG22	1:A:36:SER:N	0.42	2.29	9	1
1:A:11:VAL:HG21	2:B:34:TRP:CH2	0.42	2.48	12	2
1:A:3:LEU:HD23	1:A:96:ASP:HB3	0.42	1.91	9	1
1:A:92:ALA:HB1	2:B:36:HIS:HB2	0.42	1.90	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:ALA:O	1:A:7:ARG:N	0.42	2.53	3	1
1:A:3:LEU:N	1:A:3:LEU:HD23	0.42	2.29	2	1
2:B:110:LYS:C	2:B:114:LEU:HD12	0.42	2.35	2	1
2:B:59:GLU:HG2	2:B:97:ILE:HG21	0.42	1.91	5	1
2:B:71:CYS:O	2:B:75:VAL:HG12	0.42	2.14	11	1
1:A:21:ILE:HD13	2:B:104:MET:HA	0.42	1.91	14	1
2:B:63:LEU:HD23	2:B:75:VAL:CG1	0.42	2.45	4	1
1:A:14:VAL:HG11	2:B:111:LEU:HG	0.42	1.91	9	1
1:A:41:HIS:CE1	1:A:63:LEU:HB2	0.42	2.49	12	2
1:A:22:LEU:CB	1:A:83:VAL:HG22	0.42	2.45	5	1
2:B:56:ILE:HG22	2:B:57:LEU:N	0.42	2.28	12	1
1:A:18:MET:HE2	2:B:107:LEU:HB3	0.42	1.90	13	1
1:A:22:LEU:CD2	1:A:82:LEU:CB	0.42	2.98	5	1
1:A:6:LEU:HD11	2:B:34:TRP:HE1	0.42	1.73	8	1
2:B:48:LEU:O	2:B:57:LEU:HD12	0.42	2.14	6	2
2:B:63:LEU:HD21	2:B:79:ILE:HD11	0.42	1.91	6	1
2:B:38:ARG:N	2:B:115:LEU:HD21	0.42	2.29	10	1
2:B:61:VAL:HG22	2:B:62:CYS:N	0.42	2.29	6	1
2:B:53:CYS:O	2:B:54:THR:CG2	0.42	2.68	9	13
1:A:22:LEU:CD2	1:A:79:PHE:CE2	0.42	3.03	3	1
1:A:42:ILE:O	1:A:43:PHE:CD1	0.41	2.73	1	4
1:A:93:PHE:CE2	1:A:97:THR:HG21	0.41	2.50	13	1
1:A:15:ILE:HG22	1:A:90:ILE:HG12	0.41	1.91	13	1
1:A:49:LEU:HD12	1:A:49:LEU:N	0.41	2.31	3	1
2:B:57:LEU:HB2	2:B:105:ILE:HD11	0.41	1.91	10	1
1:A:92:ALA:O	2:B:36:HIS:CD2	0.41	2.74	13	5
2:B:61:VAL:CG1	2:B:75:VAL:HG11	0.41	2.45	1	1
1:A:3:LEU:HD11	2:B:34:TRP:CH2	0.41	2.51	2	1
1:A:39:CYS:HB3	1:A:41:HIS:CD2	0.41	2.51	10	3
1:A:22:LEU:CD2	2:B:104:MET:CE	0.41	2.99	13	1
1:A:3:LEU:HD22	2:B:34:TRP:CE3	0.41	2.51	13	1
2:B:36:HIS:ND1	2:B:37:SER:N	0.41	2.69	11	7
1:A:7:ARG:O	2:B:34:TRP:CZ2	0.41	2.74	6	2
2:B:47:LEU:N	2:B:47:LEU:CD1	0.41	2.84	5	1
2:B:48:LEU:O	2:B:57:LEU:HD21	0.41	2.16	9	1
1:A:26:ILE:HD12	1:A:27:CYS:CB	0.41	2.46	2	1
2:B:51:SER:HB2	2:B:70:PHE:CE2	0.41	2.51	4	1
1:A:37:THR:CG2	1:A:43:PHE:CD2	0.41	3.03	5	1
2:B:47:LEU:HD22	2:B:47:LEU:N	0.41	2.31	9	1
1:A:14:VAL:HG13	2:B:107:LEU:CD1	0.41	2.45	14	1
1:A:37:THR:HG22	1:A:73:LEU:HD11	0.41	1.93	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:69:ILE:O	2:B:70:PHE:CD1	0.41	2.74	6	1
1:A:11:VAL:HA	2:B:114:LEU:HD13	0.41	1.91	7	1
2:B:63:LEU:CD2	2:B:75:VAL:CG2	0.41	2.98	7	1
1:A:45:LYS:NZ	1:A:73:LEU:CD1	0.41	2.84	2	1
1:A:92:ALA:O	2:B:36:HIS:CE1	0.41	2.74	2	1
2:B:68:HIS:O	2:B:70:PHE:CE1	0.41	2.74	3	1
1:A:44:CYS:O	1:A:46:PHE:N	0.41	2.54	14	1
2:B:48:LEU:HD21	2:B:104:MET:CG	0.41	2.46	14	1
1:A:43:PHE:CZ	1:A:63:LEU:HD11	0.40	2.52	2	1
2:B:62:CYS:SG	2:B:92:ILE:HG21	0.40	2.57	6	1
1:A:31:ILE:O	1:A:31:ILE:HG13	0.40	2.16	11	1
1:A:11:VAL:HG22	2:B:114:LEU:CB	0.40	2.46	5	1
1:A:42:ILE:O	1:A:43:PHE:CD2	0.40	2.74	5	1
2:B:41:LEU:HD13	2:B:115:LEU:CD1	0.40	2.46	5	1
1:A:35:VAL:HG22	1:A:73:LEU:HD12	0.40	1.93	6	1
2:B:48:LEU:HD13	2:B:101:LEU:HD13	0.40	1.88	7	1
2:B:48:LEU:HD11	2:B:101:LEU:CD1	0.40	2.46	12	1
1:A:43:PHE:CD1	1:A:48:MET:HE1	0.40	2.51	13	1
2:B:50:CYS:HA	2:B:57:LEU:HD23	0.40	1.94	13	1
2:B:81:THR:HG23	2:B:82:GLY:N	0.40	2.32	13	1
1:A:3:LEU:CD1	2:B:34:TRP:CZ2	0.40	3.00	2	1
1:A:11:VAL:HG22	2:B:114:LEU:HB3	0.40	1.93	4	1
2:B:56:ILE:CG2	2:B:105:ILE:CG2	0.40	3.00	5	1
1:A:22:LEU:CD2	1:A:79:PHE:CD1	0.40	3.03	6	1
1:A:15:ILE:HG21	1:A:90:ILE:CG1	0.40	2.47	12	1
1:A:26:ILE:HG21	1:A:43:PHE:CE2	0.40	2.52	14	1
1:A:35:VAL:HG23	1:A:74:GLN:C	0.40	2.36	1	1
1:A:35:VAL:CG2	1:A:45:LYS:CD	0.40	2.99	5	1
1:A:37:THR:CG2	1:A:48:MET:CE	0.40	3.00	7	1
1:A:52:LEU:HD21	1:A:69:THR:HA	0.40	1.92	8	1
1:A:14:VAL:HB	2:B:111:LEU:HD13	0.40	1.92	12	1
1:A:81:GLN:HB3	2:B:47:LEU:HD21	0.40	1.93	5	1
1:A:4:SER:CB	1:A:6:LEU:HD23	0.40	2.47	12	1
1:A:22:LEU:CD1	1:A:83:VAL:HG22	0.40	2.41	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	99/112 (88%)	79±4 (80±4%)	14±3 (14±3%)	6±2 (7±2%)	2	18
2	B	85/117 (73%)	71±2 (83±2%)	11±2 (13±2%)	3±1 (3±2%)	6	36
All	All	2576/3206 (80%)	2094 (81%)	350 (14%)	132 (5%)	4	24

All 42 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	30	LEU	14
1	A	65	LYS	8
1	A	66	ASN	8
1	A	7	ARG	8
1	A	67	ASP	7
2	B	117	ASP	5
1	A	58	PRO	4
1	A	70	LYS	4
1	A	59	SER	4
1	A	55	LYS	4
2	B	64	GLY	4
2	B	65	GLY	4
2	B	62	CYS	3
2	B	78	CYS	3
1	A	60	GLN	3
1	A	5	ALA	3
1	A	45	LYS	3
1	A	72	SER	3
1	A	56	LYS	3
2	B	76	SER	3
2	B	66	CYS	2
2	B	90	ALA	2
2	B	95	LEU	2
2	B	57	LEU	2
1	A	3	LEU	2
1	A	54	GLN	2
1	A	4	SER	2
2	B	67	GLU	2
1	A	71	ARG	2
2	B	71	CYS	2
2	B	81	THR	2
1	A	8	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	101	TYR	1
1	A	6	LEU	1
2	B	56	ILE	1
2	B	73	ASN	1
1	A	26	ILE	1
1	A	100	GLU	1
2	B	60	PRO	1
1	A	34	PRO	1
2	B	34	TRP	1
2	B	35	ALA	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	94/104 (90%)	82±2 (87±2%)	12±2 (13±2%)	7 48
2	B	76/103 (74%)	63±3 (82±4%)	13±3 (18±4%)	4 39
All	All	2380/2898 (82%)	2018 (85%)	362 (15%)	6 44

All 93 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	59	SER	13
2	B	36	HIS	12
2	B	63	LEU	11
2	B	51	SER	10
2	B	52	ARG	10
2	B	46	LYS	9
2	B	58	ARG	9
1	A	69	THR	9
2	B	91	TRP	9
2	B	57	LEU	8
2	B	49	ARG	8
1	A	56	LYS	7
2	B	70	PHE	7
1	A	45	LYS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	86	LEU	7
2	B	107	LEU	7
1	A	32	LYS	7
1	A	3	LEU	6
1	A	50	LYS	6
1	A	65	LYS	6
1	A	95	LEU	6
2	B	38	ARG	6
2	B	112	ARG	6
1	A	46	PHE	6
1	A	67	ASP	6
2	B	106	GLN	5
1	A	6	LEU	5
2	B	109	SER	5
1	A	71	ARG	5
1	A	74	GLN	4
2	B	66	CYS	4
2	B	103	SER	4
1	A	12	GLN	4
1	A	66	ASN	4
1	A	85	GLU	4
1	A	76	SER	4
1	A	80	SER	4
2	B	111	LEU	4
1	A	70	LYS	4
2	B	79	ILE	4
2	B	72	SER	4
2	B	96	LYS	4
1	A	73	LEU	3
2	B	73	ASN	3
2	B	99	ARG	3
1	A	23	GLU	3
2	B	108	CYS	3
1	A	4	SER	3
1	A	54	GLN	3
2	B	68	HIS	3
2	B	94	ASP	3
1	A	78	ARG	3
1	A	94	GLN	3
2	B	77	ASP	3
1	A	9	GLU	3
1	A	7	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	55	LYS	2
1	A	19	GLN	2
1	A	60	GLN	2
2	B	42	ASP	2
1	A	79	PHE	2
2	B	62	CYS	2
1	A	38	LYS	2
2	B	92	ILE	2
2	B	93	GLN	2
2	B	110	LYS	2
2	B	101	LEU	2
2	B	78	CYS	2
2	B	37	SER	2
1	A	72	SER	2
1	A	13	ASN	1
1	A	88	LYS	1
2	B	76	SER	1
2	B	115	LEU	1
1	A	49	LEU	1
1	A	30	LEU	1
2	B	104	MET	1
1	A	91	CYS	1
1	A	26	ILE	1
1	A	27	CYS	1
1	A	82	LEU	1
2	B	59	GLU	1
2	B	98	ASN	1
1	A	52	LEU	1
1	A	75	GLU	1
1	A	51	LEU	1
1	A	97	THR	1
1	A	10	GLU	1
2	B	48	LEU	1
1	A	48	MET	1
1	A	63	LEU	1
1	A	93	PHE	1
2	B	88	THR	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 monosaccharides in this entry.

6.6 Ligand geometry (i)

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

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 (i)

No chemical shift data were provided