Full wwPDB NMR Structure Validation Report (i)

Jun 23, 2024 – 12:44 AM EDT

PDB ID	:	6GBD
BMRB ID	:	16879
Title	:	Murine Protein Tyrosine Phosphatase PTPN13 PDZ3 Domain
Authors	:	Kock, G.; Stoll, R.
Deposited on	:	2018-04-13

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 (i) symbol.

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

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

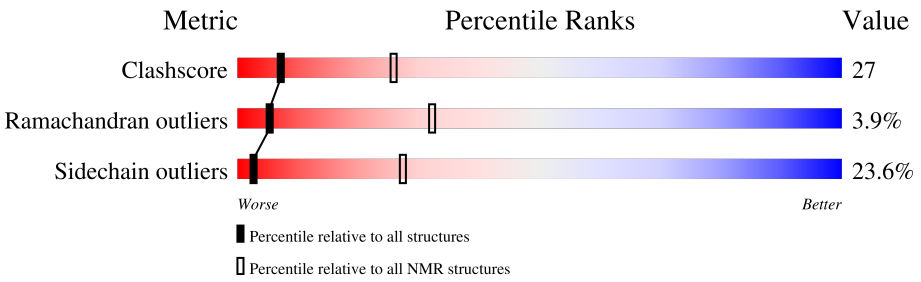
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 is 76%.

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	119	43% 38% • 15%

2 Ensemble composition and analysis (i)

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

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:9-A:109 (101)	1.01	1

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

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

The models can be grouped into 3 clusters and 5 single-model clusters were found.

Cluster number	Models
1	1, 4, 6, 7, 8, 11, 17, 20
2	2, 3, 12, 14, 16
3	10, 18
Single-model clusters	5; 9; 13; 15; 19

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1798 atoms, of which 905 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PDZ3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	119	1798	566	905	151	175	1	0

There are 5 discrepancies between the modelled and reference sequences:

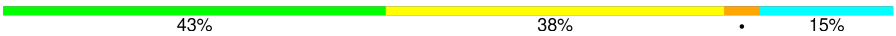
Chain	Residue	Modelled	Actual	Comment	Reference
A	115	PRO	-	expression tag	UNP Q64512
A	116	GLY	-	expression tag	UNP Q64512
A	117	ASN	-	expression tag	UNP Q64512
A	118	SER	-	expression tag	UNP Q64512
A	119	SER	-	expression tag	UNP Q64512

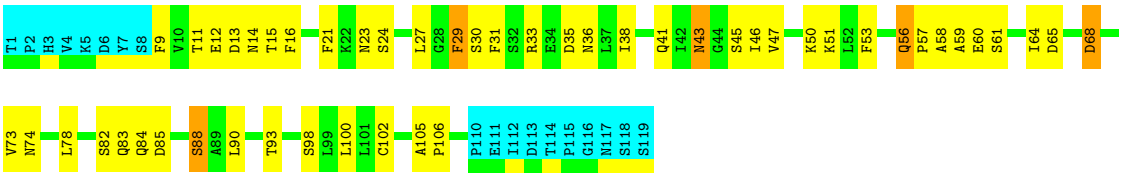
4 Residue-property plots (i)

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: PDZ3

Chain A: 

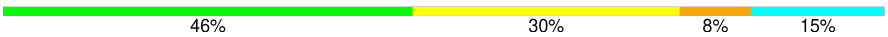


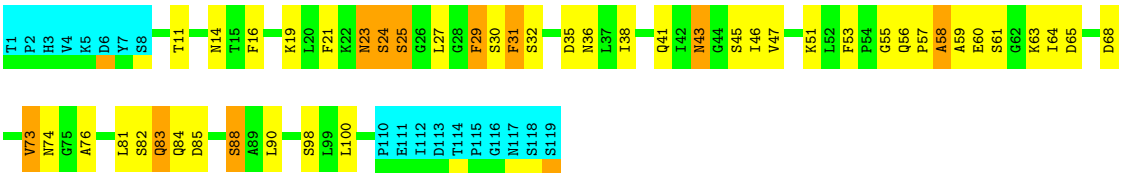
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

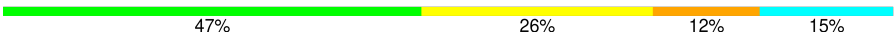
• Molecule 1: PDZ3

Chain A: 



4.2.2 Score per residue for model 2

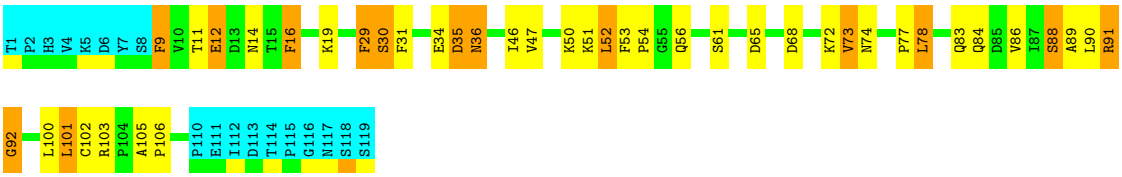
• Molecule 1: PDZ3

Chain A: 

4.2.3 Score per residue for model 3

- Molecule 1: PDZ3

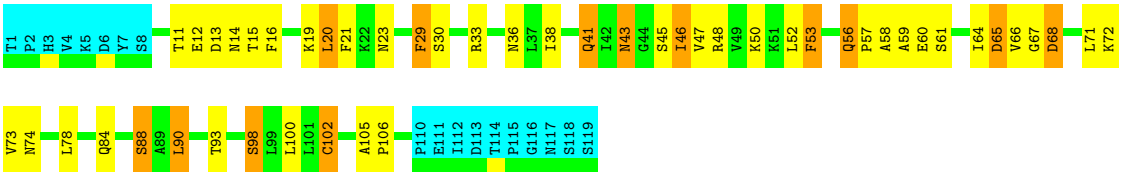
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: PDZ3

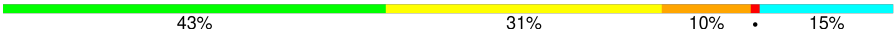
Chain A:

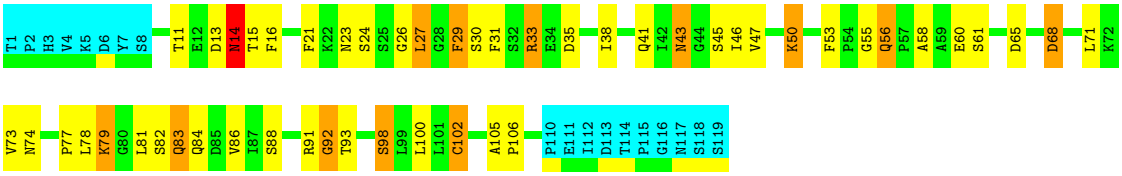


4.2.5 Score per residue for model 5

- Molecule 1: PDZ3

Chain A:





4.2.6 Score per residue for model 6

- Molecule 1: PDZ3

Chain A: 45% 30% 9% 15%

T1 P2 H3 V4 K5 D6 Y7 S8 T11 E12 D13 N14 T15 F16 E17 K22 N23 S24 S25 G26 L27 G28 F29 S30 F31 S32 R33 E34 D35 N36 L37 I38 N43 I46 V47 R48 V49 K50 K51 L52 F53 P54 G55 Q56 P57 A58 A59 E60 S61 I64 D65 V66 G67 D68 V69

N74 S82 Q83 Q84 S88 T93 S98 L99 L100 L101 C102 A105 P106 P110 E111 I112 D113 T114 P115 G116 N117 S118 S119

4.2.7 Score per residue for model 7

- Molecule 1: PDZ3

Chain A: 42% 32% 9% • 15%

T1 P2 H3 V4 K5 D6 Y7 S8 F9 V10 T11 E12 D13 N14 T15 F16 E17 S25 F29 S30 F31 S32 R33 E34 D35 N36 L37 I38 P39 E40 Q41 I42 N43 G44 S45 I46 V47 K50 K51 L52 F53 P54 G55 Q56 P57 A58 A59 E60 S61 G62 K63 I64 D65 D68 V73

N74 S82 Q83 Q84 D85 S88 T93 A94 P95 E96 V97 S98 L99 L100 A105 P106 P110 E111 I112 D113 T114 P115 G116 N117 S118 S119

4.2.8 Score per residue for model 8

- Molecule 1: PDZ3

Chain A: 43% 32% 9% • 15%

T1 P2 H3 V4 K5 D6 Y7 S8 F9 V10 T11 E12 D13 N14 T15 L20 F21 K22 N23 S24 S25 G26 F29 R33 E34 D35 N36 L37 I38 Q41 I42 N43 G44 S45 I46 V47 R48 K51 Q56 P57 A58 A59 E60 S61 I64 D65 V66 G67 D68 V73 N74

K79 S82 Q83 Q84 D85 S88 P95 E96 V97 S98 L99 L100 L101 C102 P110 E111 I112 D113 T114 P115 G116 N117 S118 S119

4.2.9 Score per residue for model 9

- Molecule 1: PDZ3

Chain A: 45% 31% 9% 15%

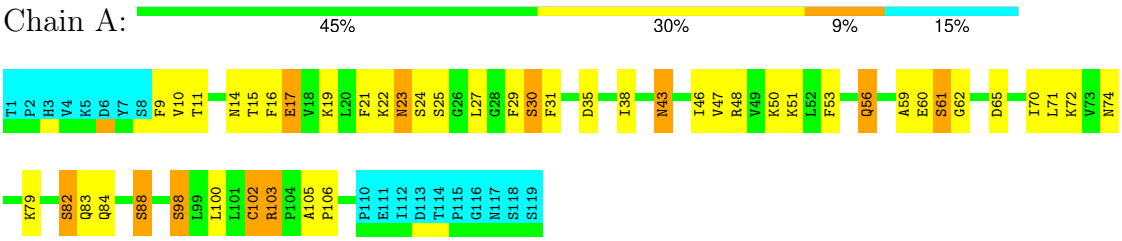
T1 P2 H3 V4 K5 D6 Y7 S8 F9 V10 T11 N14 T15 F16 F21 K22 N23 S24 S25 G26 L27 G28 F29 S30 F31 S32 D35 N36 E40 Q41 I42 N43 I46 V47 K50 K51 Q56 P57 A58 A59 E60 S61 G62 K63 I64 D65 V66 G67 D68 V69 V73 N74

Q84 D85 V86 I87 S88 T93 A94 S98 L99 L100 A105 P106 P110 E111 I112 D113 T114 P115 G116 N117 S118 S119

4.2.10 Score per residue for model 10

- Molecule 1: PDZ3

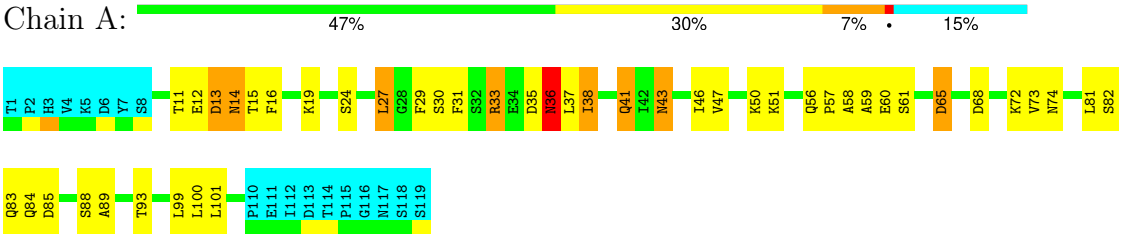
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: PDZ3

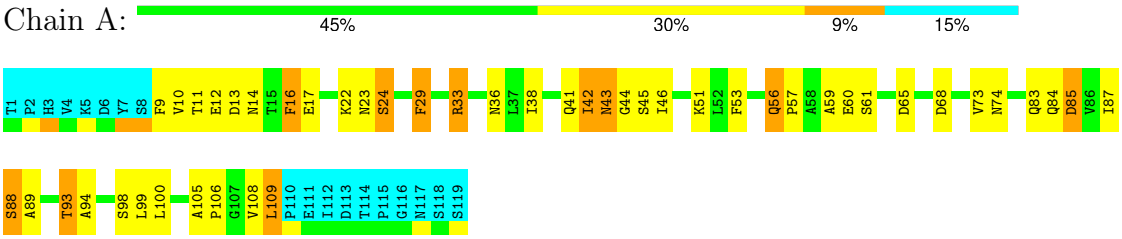
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: PDZ3

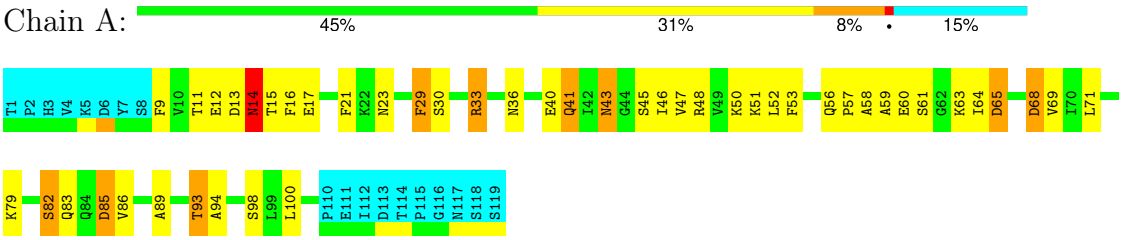
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: PDZ3

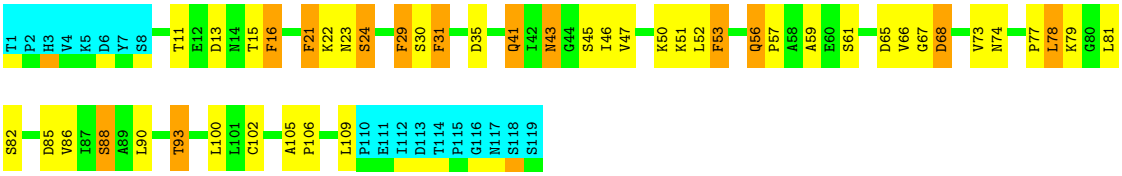
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: PDZ3

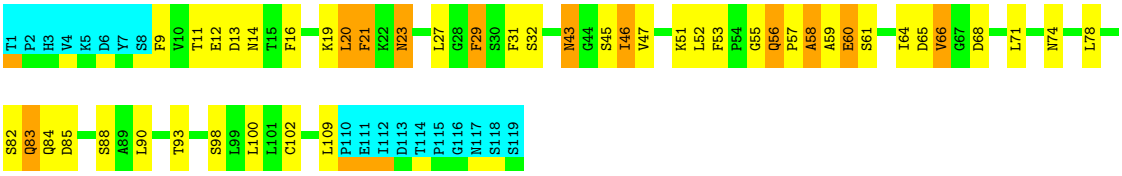
Chain A: 46% 28% 11% 15%



4.2.15 Score per residue for model 15

- Molecule 1: PDZ3

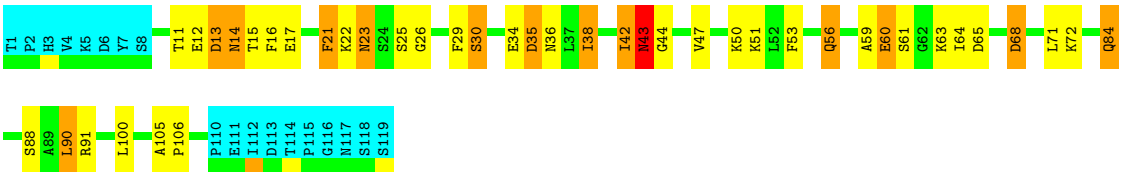
Chain A: 46% 29% 9% 15%



4.2.16 Score per residue for model 16

- Molecule 1: PDZ3

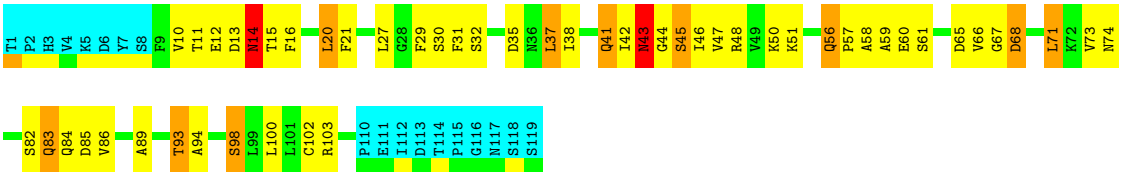
Chain A: 50% 24% 11% • 15%



4.2.17 Score per residue for model 17

- Molecule 1: PDZ3

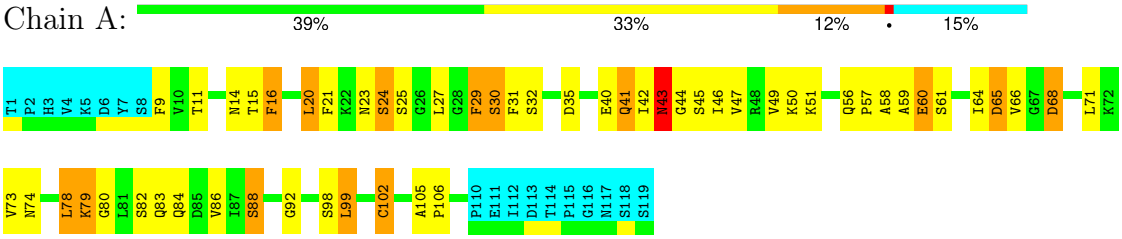
Chain A: 41% 34% 8% • 15%



4.2.18 Score per residue for model 18

- Molecule 1: PDZ3

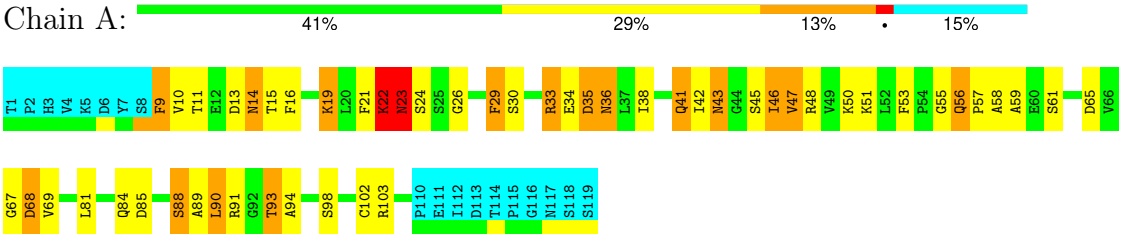
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: PDZ3

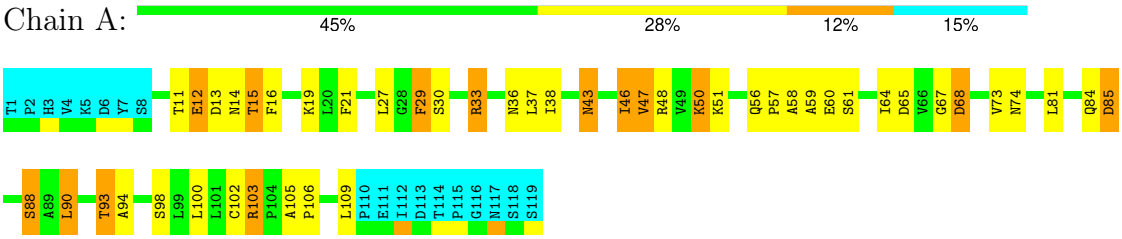
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: PDZ3

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure calculation	
Xplor-NIH	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1101
Number of shifts mapped to atoms	1101
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

6 Model quality (i)

6.1 Standard geometry (i)

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	757	783	783	41±7
All	All	15140	15660	15660	823

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ILE:H	1:A:46:ILE:HD12	0.86	1.27	4	5
1:A:19:LYS:C	1:A:20:LEU:HD23	0.78	1.99	15	1
1:A:20:LEU:H	1:A:20:LEU:HD12	0.76	1.41	17	4
1:A:46:ILE:HD12	1:A:46:ILE:N	0.75	1.96	15	6
1:A:99:LEU:N	1:A:99:LEU:HD23	0.74	1.97	8	2
1:A:71:LEU:HD13	1:A:102:CYS:SG	0.74	2.22	17	2
1:A:38:ILE:O	1:A:38:ILE:HG23	0.73	1.84	20	13
1:A:71:LEU:HD11	1:A:102:CYS:SG	0.73	2.24	5	3
1:A:20:LEU:HD12	1:A:20:LEU:N	0.72	1.98	17	4
1:A:10:VAL:HG13	1:A:10:VAL:O	0.72	1.83	19	5
1:A:27:LEU:HD23	1:A:29:PHE:CE2	0.72	2.20	15	3
1:A:11:THR:HG23	1:A:13:ASP:H	0.71	1.46	11	5
1:A:98:SER:C	1:A:99:LEU:HD23	0.71	2.07	8	2
1:A:33:ARG:NE	1:A:33:ARG:H	0.71	1.84	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD22	1:A:48:ARG:NH1	0.71	2.01	8	1
1:A:52:LEU:C	1:A:52:LEU:HD13	0.70	2.06	4	2
1:A:33:ARG:NH1	1:A:83:GLN:NE2	0.69	2.41	2	3
1:A:23:ASN:ND2	1:A:24:SER:N	0.67	2.43	1	2
1:A:20:LEU:HD23	1:A:20:LEU:N	0.66	2.06	15	1
1:A:93:THR:HG23	1:A:94:ALA:H	0.66	1.51	20	3
1:A:66:VAL:O	1:A:66:VAL:HG13	0.65	1.90	9	6
1:A:29:PHE:N	1:A:29:PHE:CD1	0.65	2.64	13	8
1:A:43:ASN:HD22	1:A:43:ASN:N	0.65	1.87	14	19
1:A:56:GLN:NE2	1:A:56:GLN:N	0.65	2.45	5	9
1:A:63:LYS:O	1:A:64:ILE:HD13	0.65	1.91	9	3
1:A:29:PHE:CD2	1:A:29:PHE:N	0.64	2.65	12	11
1:A:46:ILE:HD12	1:A:46:ILE:H	0.64	1.51	9	1
1:A:11:THR:N	1:A:14:ASN:ND2	0.64	2.46	12	3
1:A:23:ASN:N	1:A:23:ASN:HD22	0.64	1.91	16	2
1:A:52:LEU:HD23	1:A:53:PHE:N	0.63	2.07	6	2
1:A:23:ASN:HD22	1:A:24:SER:N	0.63	1.92	1	1
1:A:33:ARG:HE	1:A:33:ARG:H	0.63	1.37	12	2
1:A:23:ASN:ND2	1:A:23:ASN:H	0.63	1.89	15	1
1:A:78:LEU:HD21	1:A:85:ASP:OD1	0.63	1.93	15	1
1:A:73:VAL:HG13	1:A:73:VAL:O	0.62	1.94	17	5
1:A:21:PHE:O	1:A:21:PHE:CG	0.62	2.53	10	7
1:A:27:LEU:HD23	1:A:27:LEU:H	0.62	1.55	6	1
1:A:27:LEU:HD23	1:A:27:LEU:N	0.62	2.08	6	2
1:A:43:ASN:N	1:A:43:ASN:ND2	0.61	2.44	14	15
1:A:33:ARG:NE	1:A:33:ARG:N	0.61	2.47	8	3
1:A:46:ILE:N	1:A:46:ILE:CD1	0.61	2.61	8	6
1:A:33:ARG:CZ	1:A:83:GLN:NE2	0.61	2.64	5	1
1:A:29:PHE:CE1	1:A:58:ALA:HB2	0.61	2.30	18	2
1:A:33:ARG:H	1:A:33:ARG:NE	0.61	1.93	12	3
1:A:49:VAL:HG21	1:A:68:ASP:OD2	0.60	1.95	18	1
1:A:100:LEU:N	1:A:100:LEU:HD12	0.60	2.10	20	13
1:A:74:ASN:N	1:A:98:SER:O	0.60	2.35	17	9
1:A:100:LEU:N	1:A:100:LEU:CD2	0.60	2.65	10	5
1:A:20:LEU:N	1:A:20:LEU:CD1	0.59	2.65	18	4
1:A:23:ASN:HD22	1:A:23:ASN:H	0.59	1.39	16	1
1:A:56:GLN:O	1:A:60:GLU:N	0.59	2.35	16	6
1:A:21:PHE:CD2	1:A:21:PHE:O	0.59	2.56	13	2
1:A:35:ASP:O	1:A:36:ASN:ND2	0.59	2.36	7	2
1:A:11:THR:O	1:A:14:ASN:ND2	0.59	2.36	7	16
1:A:21:PHE:O	1:A:21:PHE:CD2	0.58	2.56	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:PHE:CZ	1:A:22:LYS:O	0.58	2.56	14	2
1:A:27:LEU:H	1:A:27:LEU:CD2	0.58	2.07	6	1
1:A:82:SER:O	1:A:84:GLN:N	0.58	2.36	17	8
1:A:56:GLN:H	1:A:56:GLN:CD	0.58	2.02	14	1
1:A:21:PHE:CD2	1:A:22:LYS:N	0.58	2.71	16	1
1:A:58:ALA:O	1:A:64:ILE:HG21	0.58	1.98	2	5
1:A:11:THR:O	1:A:14:ASN:N	0.58	2.37	12	4
1:A:84:GLN:N	1:A:84:GLN:OE1	0.57	2.38	12	2
1:A:33:ARG:HE	1:A:33:ARG:N	0.57	1.98	12	2
1:A:33:ARG:H	1:A:33:ARG:CD	0.57	2.13	5	1
1:A:52:LEU:HD13	1:A:53:PHE:N	0.57	2.15	14	2
1:A:46:ILE:O	1:A:46:ILE:HD12	0.57	2.00	3	9
1:A:33:ARG:NE	1:A:33:ARG:O	0.57	2.37	8	1
1:A:33:ARG:H	1:A:33:ARG:CZ	0.56	2.13	8	1
1:A:57:PRO:O	1:A:60:GLU:N	0.56	2.37	15	11
1:A:23:ASN:N	1:A:23:ASN:ND2	0.56	2.53	16	1
1:A:31:PHE:CD2	1:A:31:PHE:C	0.56	2.79	18	5
1:A:29:PHE:CE2	1:A:58:ALA:HB2	0.56	2.35	8	5
1:A:23:ASN:ND2	1:A:23:ASN:N	0.56	2.52	15	1
1:A:56:GLN:N	1:A:56:GLN:CD	0.56	2.59	5	1
1:A:16:PHE:CD2	1:A:16:PHE:C	0.56	2.79	14	7
1:A:33:ARG:NH2	1:A:81:LEU:O	0.56	2.39	20	1
1:A:69:VAL:HG13	1:A:69:VAL:O	0.56	2.01	9	1
1:A:16:PHE:C	1:A:16:PHE:CD1	0.55	2.80	12	10
1:A:48:ARG:HH21	1:A:67:GLY:CA	0.55	2.14	4	3
1:A:31:PHE:C	1:A:31:PHE:CD1	0.55	2.80	15	4
1:A:81:LEU:HD13	1:A:85:ASP:OD1	0.55	2.02	1	1
1:A:30:SER:O	1:A:50:LYS:CB	0.55	2.55	6	16
1:A:33:ARG:CD	1:A:33:ARG:N	0.54	2.69	5	1
1:A:105:ALA:HB3	1:A:108:VAL:CG2	0.54	2.32	12	1
1:A:90:LEU:O	1:A:90:LEU:HD13	0.54	2.03	16	4
1:A:11:THR:OG1	1:A:12:GLU:N	0.54	2.40	17	8
1:A:33:ARG:NH1	1:A:83:GLN:OE1	0.54	2.39	12	1
1:A:21:PHE:CE1	1:A:22:LYS:O	0.54	2.60	16	1
1:A:11:THR:O	1:A:13:ASP:N	0.54	2.40	12	2
1:A:56:GLN:CD	1:A:56:GLN:N	0.54	2.59	3	9
1:A:27:LEU:N	1:A:27:LEU:HD12	0.54	2.16	10	1
1:A:27:LEU:N	1:A:27:LEU:CD1	0.54	2.71	10	1
1:A:29:PHE:CB	1:A:51:LYS:O	0.54	2.56	16	18
1:A:71:LEU:CD1	1:A:102:CYS:SG	0.54	2.95	5	2
1:A:16:PHE:CD1	1:A:16:PHE:O	0.53	2.61	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:VAL:HG12	1:A:99:LEU:CD2	0.53	2.33	8	1
1:A:38:ILE:O	1:A:38:ILE:CG2	0.53	2.56	12	9
1:A:99:LEU:N	1:A:99:LEU:CD2	0.53	2.63	8	2
1:A:23:ASN:ND2	1:A:25:SER:OG	0.53	2.42	1	1
1:A:16:PHE:CZ	1:A:64:ILE:HD12	0.53	2.39	9	3
1:A:84:GLN:N	1:A:84:GLN:CD	0.53	2.61	12	2
1:A:11:THR:H	1:A:14:ASN:ND2	0.53	2.02	2	4
1:A:41:GLN:HE22	1:A:46:ILE:HG23	0.53	1.62	17	1
1:A:81:LEU:N	1:A:81:LEU:HD22	0.52	2.18	19	1
1:A:81:LEU:N	1:A:81:LEU:CD2	0.52	2.73	19	1
1:A:11:THR:C	1:A:13:ASP:N	0.52	2.63	12	5
1:A:24:SER:O	1:A:26:GLY:N	0.52	2.42	9	2
1:A:37:LEU:CD2	1:A:48:ARG:NH1	0.52	2.73	17	1
1:A:82:SER:OG	1:A:83:GLN:N	0.52	2.42	2	1
1:A:56:GLN:HE21	1:A:56:GLN:CA	0.52	2.17	5	2
1:A:9:PHE:N	1:A:9:PHE:CD2	0.52	2.77	10	1
1:A:82:SER:C	1:A:84:GLN:N	0.52	2.63	5	6
1:A:100:LEU:N	1:A:100:LEU:HD22	0.52	2.20	3	5
1:A:81:LEU:HD23	1:A:85:ASP:HB2	0.52	1.82	14	1
1:A:56:GLN:O	1:A:59:ALA:N	0.51	2.41	10	11
1:A:47:VAL:O	1:A:69:VAL:HG23	0.51	2.04	9	1
1:A:93:THR:HG23	1:A:94:ALA:N	0.51	2.20	20	3
1:A:85:ASP:O	1:A:89:ALA:HB2	0.51	2.04	11	3
1:A:21:PHE:O	1:A:21:PHE:CD1	0.51	2.63	10	2
1:A:93:THR:HG22	1:A:94:ALA:N	0.51	2.20	9	1
1:A:43:ASN:HD22	1:A:43:ASN:H	0.51	1.47	18	5
1:A:16:PHE:CZ	1:A:64:ILE:CD1	0.51	2.94	15	2
1:A:30:SER:O	1:A:50:LYS:N	0.50	2.43	9	10
1:A:78:LEU:O	1:A:79:LYS:O	0.50	2.28	5	1
1:A:25:SER:OG	1:A:26:GLY:N	0.50	2.42	6	2
1:A:74:ASN:HD21	1:A:97:VAL:HG13	0.50	1.66	8	1
1:A:105:ALA:HB1	1:A:106:PRO:HD2	0.50	1.83	5	13
1:A:31:PHE:CZ	1:A:86:VAL:HG12	0.50	2.41	18	4
1:A:26:GLY:O	1:A:27:LEU:O	0.50	2.29	9	2
1:A:73:VAL:O	1:A:74:ASN:CB	0.50	2.60	17	10
1:A:14:ASN:O	1:A:102:CYS:SG	0.50	2.64	6	1
1:A:73:VAL:HG11	1:A:89:ALA:O	0.50	2.06	3	1
1:A:40:GLU:O	1:A:41:GLN:O	0.50	2.30	13	4
1:A:84:GLN:O	1:A:88:SER:OG	0.50	2.30	6	13
1:A:83:GLN:O	1:A:86:VAL:N	0.50	2.45	13	2
1:A:81:LEU:HD13	1:A:85:ASP:OD2	0.50	2.07	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:GLY:C	1:A:56:GLN:NE2	0.49	2.65	6	6
1:A:57:PRO:C	1:A:59:ALA:N	0.49	2.66	20	15
1:A:37:LEU:HD22	1:A:48:ARG:HH12	0.49	1.65	8	1
1:A:10:VAL:O	1:A:10:VAL:CG1	0.49	2.59	2	5
1:A:57:PRO:O	1:A:59:ALA:N	0.49	2.45	15	13
1:A:84:GLN:H	1:A:84:GLN:CD	0.49	2.11	3	1
1:A:91:ARG:O	1:A:92:GLY:O	0.49	2.31	5	2
1:A:9:PHE:O	1:A:11:THR:HG22	0.49	2.07	9	2
1:A:33:ARG:NH1	1:A:83:GLN:N	0.49	2.61	13	1
1:A:65:ASP:O	1:A:68:ASP:OD2	0.49	2.30	4	5
1:A:31:PHE:CE1	1:A:90:LEU:HD22	0.49	2.43	14	1
1:A:47:VAL:O	1:A:69:VAL:HG13	0.49	2.07	19	1
1:A:54:PRO:O	1:A:56:GLN:OE1	0.49	2.31	3	2
1:A:14:ASN:O	1:A:15:THR:HG23	0.49	2.08	8	3
1:A:27:LEU:CD1	1:A:90:LEU:HD21	0.48	2.37	1	1
1:A:42:ILE:O	1:A:44:GLY:N	0.48	2.46	8	6
1:A:65:ASP:O	1:A:68:ASP:OD1	0.48	2.32	2	5
1:A:71:LEU:CD1	1:A:71:LEU:N	0.48	2.77	15	1
1:A:33:ARG:HH11	1:A:83:GLN:CD	0.48	2.12	12	2
1:A:38:ILE:O	1:A:41:GLN:OE1	0.48	2.31	11	1
1:A:33:ARG:NH1	1:A:83:GLN:CD	0.48	2.67	12	2
1:A:57:PRO:C	1:A:59:ALA:H	0.48	2.12	2	13
1:A:21:PHE:O	1:A:22:LYS:O	0.48	2.30	9	1
1:A:33:ARG:NH2	1:A:46:ILE:N	0.48	2.61	19	1
1:A:84:GLN:CD	1:A:84:GLN:H	0.48	2.12	12	1
1:A:43:ASN:ND2	1:A:43:ASN:H	0.48	2.07	17	1
1:A:41:GLN:HE22	1:A:46:ILE:HD11	0.47	1.68	19	1
1:A:27:LEU:HD12	1:A:29:PHE:CZ	0.47	2.44	5	1
1:A:93:THR:OG1	1:A:94:ALA:N	0.47	2.46	7	5
1:A:52:LEU:C	1:A:52:LEU:CD1	0.47	2.79	4	2
1:A:88:SER:C	1:A:90:LEU:N	0.47	2.67	3	2
1:A:53:PHE:O	1:A:56:GLN:OE1	0.47	2.33	6	1
1:A:66:VAL:O	1:A:66:VAL:CG1	0.47	2.61	8	2
1:A:46:ILE:C	1:A:46:ILE:HD12	0.47	2.30	1	1
1:A:14:ASN:CB	1:A:103:ARG:O	0.47	2.62	10	1
1:A:27:LEU:HD23	1:A:29:PHE:CZ	0.47	2.45	10	1
1:A:99:LEU:O	1:A:101:LEU:HD12	0.47	2.10	11	1
1:A:85:ASP:OD1	1:A:85:ASP:O	0.47	2.32	15	1
1:A:27:LEU:HD22	1:A:27:LEU:N	0.47	2.25	17	1
1:A:27:LEU:N	1:A:27:LEU:CD2	0.47	2.77	17	1
1:A:100:LEU:N	1:A:100:LEU:CD1	0.47	2.77	20	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:LEU:HD11	1:A:86:VAL:HG23	0.47	1.87	14	1
1:A:71:LEU:N	1:A:71:LEU:HD12	0.47	2.25	15	1
1:A:35:ASP:O	1:A:36:ASN:CB	0.47	2.62	6	2
1:A:56:GLN:NE2	1:A:56:GLN:CA	0.46	2.77	5	4
1:A:16:PHE:CD1	1:A:16:PHE:C	0.46	2.88	10	2
1:A:20:LEU:N	1:A:20:LEU:CD2	0.46	2.69	15	1
1:A:31:PHE:CZ	1:A:86:VAL:CG1	0.46	2.98	9	1
1:A:29:PHE:CE1	1:A:58:ALA:CB	0.46	2.99	15	1
1:A:13:ASP:O	1:A:15:THR:OG1	0.46	2.33	20	1
1:A:21:PHE:O	1:A:22:LYS:C	0.46	2.54	16	3
1:A:74:ASN:ND2	1:A:98:SER:H	0.46	2.07	15	1
1:A:79:LYS:C	1:A:81:LEU:H	0.46	2.14	5	1
1:A:52:LEU:HD21	1:A:59:ALA:HB2	0.46	1.88	4	3
1:A:11:THR:C	1:A:13:ASP:H	0.46	2.14	19	4
1:A:88:SER:O	1:A:90:LEU:N	0.46	2.49	3	1
1:A:16:PHE:O	1:A:16:PHE:CG	0.46	2.68	5	1
1:A:85:ASP:O	1:A:89:ALA:HB3	0.46	2.10	13	1
1:A:78:LEU:HD11	1:A:86:VAL:CG2	0.46	2.41	3	2
1:A:60:GLU:C	1:A:62:GLY:N	0.46	2.70	10	1
1:A:45:SER:OG	1:A:46:ILE:N	0.46	2.48	17	1
1:A:63:LYS:C	1:A:64:ILE:HD13	0.45	2.30	9	1
1:A:33:ARG:NH2	1:A:46:ILE:O	0.45	2.49	19	1
1:A:36:ASN:OD1	1:A:36:ASN:N	0.45	2.49	20	1
1:A:13:ASP:O	1:A:14:ASN:C	0.45	2.55	17	6
1:A:52:LEU:HD11	1:A:58:ALA:O	0.45	2.12	6	1
1:A:13:ASP:O	1:A:15:THR:N	0.45	2.50	17	2
1:A:46:ILE:HD12	1:A:46:ILE:C	0.45	2.32	11	3
1:A:48:ARG:HG2	1:A:69:VAL:HG22	0.45	1.87	13	2
1:A:60:GLU:O	1:A:62:GLY:N	0.45	2.50	10	1
1:A:35:ASP:O	1:A:35:ASP:OD2	0.45	2.35	11	1
1:A:13:ASP:OD1	1:A:13:ASP:N	0.45	2.49	16	1
1:A:24:SER:O	1:A:25:SER:OG	0.45	2.33	18	1
1:A:41:GLN:NE2	1:A:46:ILE:HD11	0.45	2.27	19	1
1:A:78:LEU:HD23	1:A:81:LEU:HD12	0.45	1.89	5	1
1:A:70:ILE:C	1:A:71:LEU:HD12	0.45	2.32	10	1
1:A:11:THR:O	1:A:14:ASN:CG	0.45	2.55	13	2
1:A:73:VAL:O	1:A:73:VAL:HG13	0.44	2.11	4	1
1:A:82:SER:O	1:A:83:GLN:C	0.44	2.55	13	6
1:A:79:LYS:O	1:A:81:LEU:N	0.44	2.47	5	1
1:A:14:ASN:CG	1:A:103:ARG:O	0.44	2.56	20	1
1:A:48:ARG:NH2	1:A:67:GLY:CA	0.44	2.80	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:PHE:CD1	1:A:21:PHE:O	0.44	2.70	14	2
1:A:64:ILE:O	1:A:65:ASP:CG	0.44	2.56	15	1
1:A:22:LYS:C	1:A:23:ASN:OD1	0.44	2.56	6	1
1:A:31:PHE:CD1	1:A:32:SER:N	0.44	2.85	1	1
1:A:95:PRO:O	1:A:97:VAL:HG23	0.44	2.12	8	1
1:A:35:ASP:O	1:A:35:ASP:CG	0.44	2.55	19	1
1:A:31:PHE:CE1	1:A:90:LEU:HD13	0.44	2.48	3	1
1:A:64:ILE:O	1:A:65:ASP:OD1	0.44	2.36	13	2
1:A:88:SER:C	1:A:90:LEU:H	0.44	2.16	3	1
1:A:52:LEU:HD23	1:A:53:PHE:H	0.44	1.72	6	1
1:A:67:GLY:O	1:A:68:ASP:C	0.44	2.56	14	4
1:A:21:PHE:CD1	1:A:21:PHE:N	0.43	2.85	4	1
1:A:93:THR:CG2	1:A:94:ALA:H	0.43	2.26	12	2
1:A:29:PHE:CE2	1:A:58:ALA:CB	0.43	3.01	8	1
1:A:48:ARG:NE	1:A:67:GLY:O	0.43	2.51	19	1
1:A:19:LYS:CG	1:A:19:LYS:O	0.43	2.66	19	2
1:A:47:VAL:CG1	1:A:48:ARG:N	0.43	2.82	10	1
1:A:46:ILE:C	1:A:46:ILE:CD1	0.43	2.86	1	1
1:A:85:ASP:O	1:A:89:ALA:CB	0.43	2.67	17	5
1:A:56:GLN:N	1:A:56:GLN:NE2	0.43	2.67	1	3
1:A:74:ASN:ND2	1:A:97:VAL:HG13	0.43	2.28	8	1
1:A:83:GLN:HE21	1:A:87:ILE:HD11	0.43	1.73	12	1
1:A:69:VAL:O	1:A:69:VAL:CG1	0.43	2.67	9	1
1:A:68:ASP:OD2	1:A:68:ASP:N	0.43	2.46	4	1
1:A:109:LEU:CD1	1:A:109:LEU:H	0.43	2.27	12	1
1:A:23:ASN:O	1:A:23:ASN:CG	0.43	2.56	19	1
1:A:33:ARG:HB3	1:A:47:VAL:HG12	0.43	1.91	5	2
1:A:27:LEU:HD12	1:A:29:PHE:O	0.43	2.14	11	1
1:A:53:PHE:O	1:A:59:ALA:CB	0.43	2.67	14	1
1:A:13:ASP:O	1:A:13:ASP:CG	0.43	2.57	17	1
1:A:17:GLU:HB3	1:A:100:LEU:HD13	0.42	1.89	12	2
1:A:42:ILE:C	1:A:44:GLY:N	0.42	2.71	16	1
1:A:35:ASP:OD2	1:A:35:ASP:N	0.42	2.50	8	1
1:A:36:ASN:C	1:A:37:LEU:HD22	0.42	2.34	11	1
1:A:42:ILE:HD12	1:A:43:ASN:ND2	0.42	2.29	19	1
1:A:73:VAL:O	1:A:73:VAL:CG1	0.42	2.66	17	1
1:A:21:PHE:CD2	1:A:21:PHE:C	0.42	2.91	20	1
1:A:64:ILE:HG22	1:A:65:ASP:N	0.42	2.29	15	4
1:A:46:ILE:HD12	1:A:46:ILE:O	0.42	2.14	1	1
1:A:33:ARG:N	1:A:33:ARG:NE	0.42	2.67	2	1
1:A:47:VAL:HG12	1:A:48:ARG:N	0.42	2.29	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ARG:O	1:A:33:ARG:CD	0.42	2.68	7	2
1:A:78:LEU:O	1:A:79:LYS:C	0.42	2.58	18	1
1:A:85:ASP:N	1:A:85:ASP:OD1	0.42	2.53	20	1
1:A:35:ASP:OD1	1:A:35:ASP:C	0.41	2.58	16	1
1:A:21:PHE:CE2	1:A:22:LYS:O	0.41	2.73	14	1
1:A:23:ASN:ND2	1:A:23:ASN:C	0.41	2.73	1	1
1:A:19:LYS:O	1:A:19:LYS:CG	0.41	2.68	20	1
1:A:78:LEU:O	1:A:80:GLY:N	0.41	2.53	18	1
1:A:48:ARG:NH2	1:A:67:GLY:O	0.41	2.50	19	1
1:A:56:GLN:CA	1:A:56:GLN:HE21	0.41	2.29	19	1
1:A:54:PRO:C	1:A:56:GLN:OE1	0.41	2.59	3	1
1:A:73:VAL:O	1:A:73:VAL:HG22	0.41	2.16	4	1
1:A:21:PHE:CD2	1:A:21:PHE:N	0.41	2.89	1	2
1:A:71:LEU:HD12	1:A:71:LEU:N	0.41	2.30	2	1
1:A:74:ASN:HD21	1:A:97:VAL:CG1	0.41	2.28	8	1
1:A:33:ARG:HH22	1:A:45:SER:CB	0.41	2.29	19	1
1:A:33:ARG:O	1:A:33:ARG:CG	0.41	2.68	7	1
1:A:109:LEU:H	1:A:109:LEU:HD12	0.41	1.76	12	1
1:A:20:LEU:HD23	1:A:57:PRO:HB2	0.41	1.92	4	1
1:A:72:LYS:HG3	1:A:100:LEU:HD22	0.41	1.93	16	1
1:A:42:ILE:O	1:A:43:ASN:C	0.40	2.59	16	1
1:A:56:GLN:N	1:A:56:GLN:HE21	0.40	2.12	19	1
1:A:82:SER:C	1:A:84:GLN:H	0.40	2.20	5	1
1:A:24:SER:O	1:A:24:SER:OG	0.40	2.39	12	1
1:A:71:LEU:N	1:A:71:LEU:CD1	0.40	2.84	2	1
1:A:11:THR:N	1:A:14:ASN:HD21	0.40	2.10	12	1
1:A:41:GLN:O	1:A:42:ILE:C	0.40	2.60	12	1
1:A:73:VAL:HG13	1:A:76:ALA:HB3	0.40	1.92	1	1
1:A:101:LEU:C	1:A:102:CYS:SG	0.40	3.00	3	1
1:A:12:GLU:O	1:A:12:GLU:CG	0.40	2.69	4	1
1:A:105:ALA:O	1:A:108:VAL:HG23	0.40	2.17	12	1
1:A:93:THR:CG2	1:A:94:ALA:N	0.40	2.84	20	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	101/119 (85%)	79±4 (78±4%)	18±4 (18±4%)	4±2 (4±2%)	5 32
All	All	2020/2380 (85%)	1576 (78%)	366 (18%)	78 (4%)	5 32

All 23 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	41	GLN	12
1	A	83	GLN	7
1	A	58	ALA	6
1	A	93	THR	6
1	A	43	ASN	5
1	A	14	ASN	4
1	A	36	ASN	4
1	A	9	PHE	3
1	A	77	PRO	3
1	A	92	GLY	3
1	A	27	LEU	3
1	A	23	ASN	3
1	A	66	VAL	3
1	A	73	VAL	2
1	A	79	LYS	2
1	A	10	VAL	2
1	A	22	LYS	2
1	A	25	SER	2
1	A	12	GLU	2
1	A	28	GLY	1
1	A	61	SER	1
1	A	42	ILE	1
1	A	26	GLY	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	85/102 (83%)	65±4 (76±4%)	20±4 (24±4%)	3 27
All	All	1700/2040 (83%)	1299 (76%)	401 (24%)	3 27

All 63 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	61	SER	20
1	A	43	ASN	19
1	A	68	ASP	17
1	A	88	SER	16
1	A	29	PHE	15
1	A	47	VAL	15
1	A	65	ASP	15
1	A	35	ASP	12
1	A	53	PHE	12
1	A	98	SER	12
1	A	23	ASN	11
1	A	45	SER	11
1	A	33	ARG	11
1	A	56	GLN	11
1	A	24	SER	10
1	A	36	ASN	10
1	A	15	THR	9
1	A	102	CYS	9
1	A	93	THR	9
1	A	30	SER	7
1	A	82	SER	7
1	A	46	ILE	7
1	A	14	ASN	6
1	A	32	SER	6
1	A	19	LYS	5
1	A	9	PHE	5
1	A	16	PHE	5
1	A	78	LEU	5
1	A	103	ARG	5
1	A	20	LEU	5
1	A	90	LEU	5
1	A	17	GLU	5
1	A	85	ASP	5
1	A	37	LEU	4
1	A	38	ILE	4
1	A	34	GLU	4
1	A	72	LYS	4
1	A	60	GLU	4
1	A	79	LYS	4
1	A	109	LEU	4
1	A	25	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	A	63	LYS	3
1	A	12	GLU	3
1	A	91	ARG	3
1	A	13	ASP	3
1	A	50	LYS	3
1	A	74	ASN	3
1	A	99	LEU	3
1	A	22	LYS	3
1	A	71	LEU	3
1	A	21	PHE	3
1	A	31	PHE	2
1	A	52	LEU	2
1	A	101	LEU	2
1	A	41	GLN	2
1	A	27	LEU	2
1	A	42	ILE	2
1	A	51	LYS	1
1	A	11	THR	1
1	A	96	GLU	1
1	A	73	VAL	1
1	A	84	GLN	1
1	A	48	ARG	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)

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 (i)

The completeness of assignment taking into account all chemical shift lists is 76% for the well-defined parts and 71% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1101
Number of shifts mapped to atoms	1101
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	111	0.24 ± 0.18	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	96	0.59 ± 0.13	Should be applied
$^{13}C'$	95	0.38 ± 0.16	None needed (< 0.5 ppm)
^{15}N	96	-0.37 ± 0.48	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 76%, i.e. 1019 atoms were assigned a chemical shift out of a possible 1348. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	478/501 (95%)	199/205 (97%)	189/202 (94%)	90/94 (96%)
Sidechain	534/787 (68%)	366/514 (71%)	164/245 (67%)	4/28 (14%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	7/60 (12%)	7/30 (23%)	0/30 (0%)	0/0 (—%)
Overall	1019/1348 (76%)	572/749 (76%)	353/477 (74%)	94/122 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 71%, i.e. 1101 atoms were assigned a chemical shift out of a possible 1561. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	518/586 (88%)	216/239 (90%)	206/238 (87%)	96/109 (88%)
Sidechain	575/899 (64%)	393/586 (67%)	178/283 (63%)	4/30 (13%)
Aromatic	8/76 (11%)	8/38 (21%)	0/37 (0%)	0/1 (0%)
Overall	1101/1561 (71%)	617/863 (71%)	384/558 (69%)	100/140 (71%)

7.1.4 Statistically unusual chemical shifts (i)

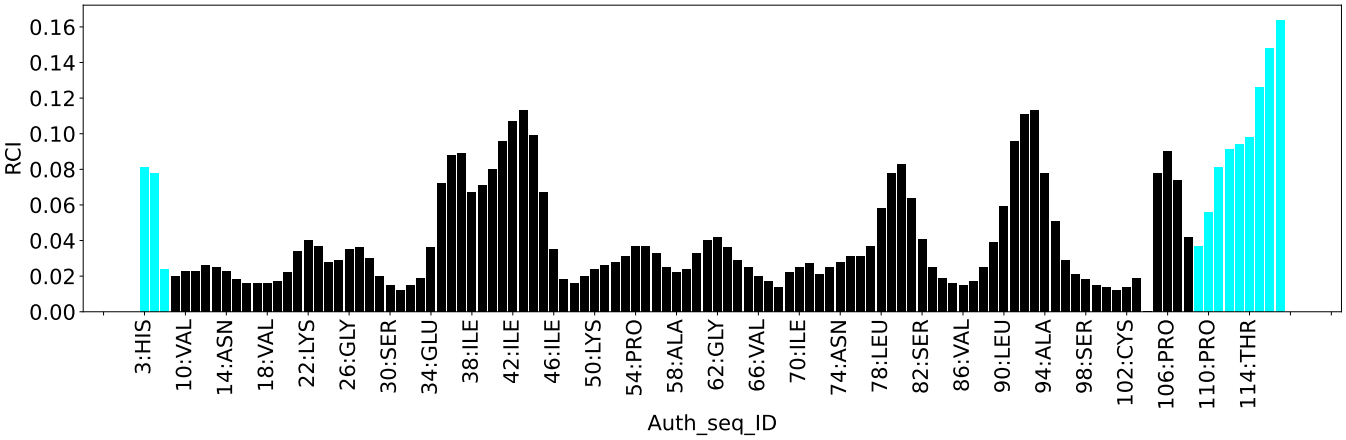
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	68	ASP	CA	67.17	44.71 – 64.67	6.2

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
3:HIS
10:VAL
14:ASN
18:VAL
22:LYS
26:GLY
30:SER
34:GLU
38:ILE
42:ILE
46:ILE
50:LYS
54:PRO
58:ALA
62:GLY
66:VAL
70:ILE
74:ASN
78:LEU
82:SER
86:VAL
90:LEU
94:ALA
98:SER
102:CYS
106:PRO
110:PRO
114:THR
Auth_seq_ID