Full wwPDB NMR Structure Validation Report (i)

Feb 17, 2022 – 11:42 AM EST

PDB ID	:	1P6Q
Title	:	NMR Structure of the Response regulator CheY2 from Sinorhizobium meliloti, complexed with Mg++
Authors	:	Riepl, H.; Scharf, B.; Maurer, T.; Schmitt, R.; Kalbitzer, H.R.; Structural Proteomics in Europe (SPINE)
Deposited on	:	2003-04-30

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:

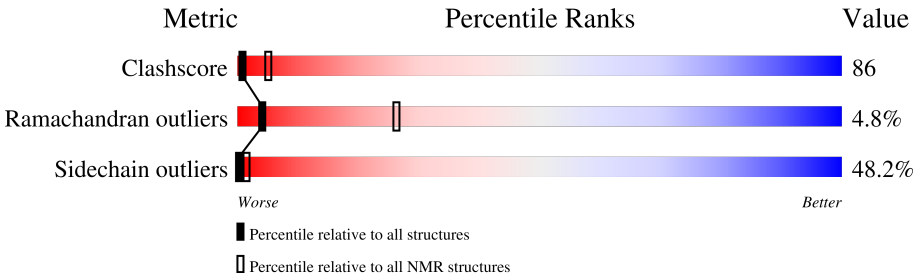
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	129	14% 43% 19% • 22%

2 Ensemble composition and analysis (i)

This entry contains 16 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:6-A:106 (101)	0.10	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 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1983 atoms, of which 1024 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CheY2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	129	1983	612	1024	168	173	6	0

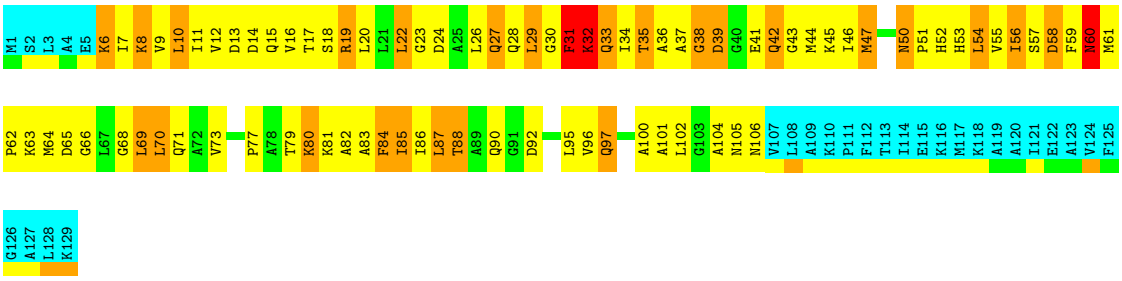
4 Residue-property plots (i)

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: CheY2

Chain A: 14% 43% 19% • 22%



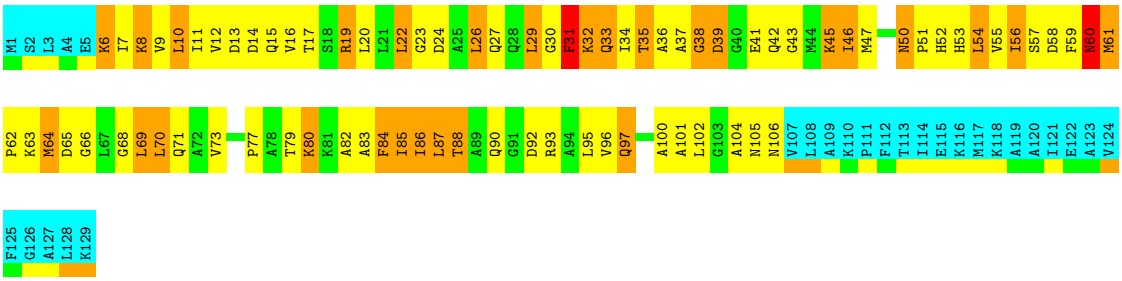
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: CheY2

Chain A: 16% 39% 22% • 22%



4.2.2 Score per residue for model 2

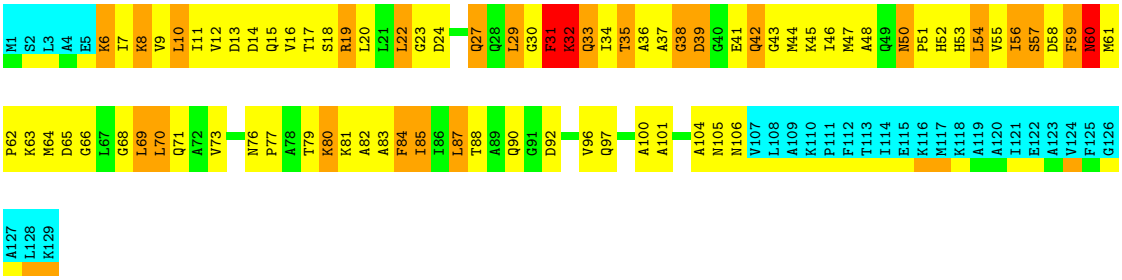
- Molecule 1: CheY2

Chain A: 17% 39% 20% • 22%

4.2.3 Score per residue for model 3

- Molecule 1: CheY2

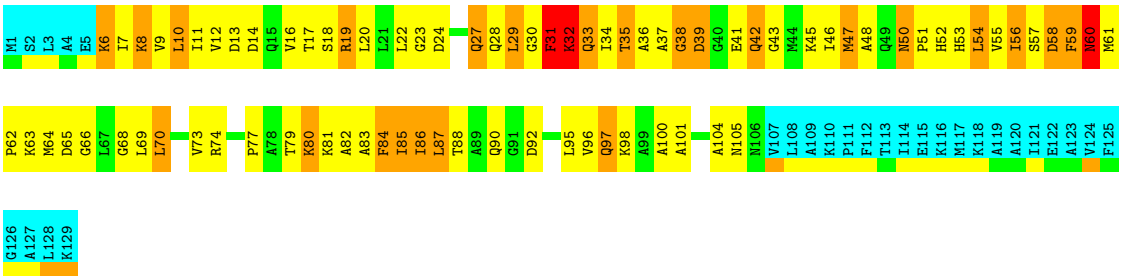
Chain A: 16% 42% 18% • 22%



4.2.4 Score per residue for model 4

- Molecule 1: CheY2

Chain A: 16% 41% 19% • 22%



4.2.5 Score per residue for model 5

- Molecule 1: CheY2

Chain A: 13% 43% 19% • 22%

M1 S2 L3 A4 E5 K6 I7 K8 V9 L10 I11 V12 D13 D14 Q15 V16 T17 S18 R19 L20 L21 L22 G23 D24 A25 L26 Q27 Q28 L29 G30 F31 K32 Q33 I34 T35 A36 A37 G38 D39 G40 E41 Q42 G43 M44 K45 I46 M47 A48 Q49 N50 P51 H52 H53 L54 V55 I56 S57 D58 F59 N60

M61 P62 K63 M64 D65 G66 L67 G68 L69 L70 Q71 A72 V73 R74 A75 N76 P77 A78 T79 K80 K81 A82 A83 F84 I85 I86 L87 T88 A89 Q90 G91 D92 L95 V96 Q97 A100 A101 L102 G103 A104 N105 N106 V107 L108 A109 K110 P111 F112 T113 I114 E115 K116 M117 K118 A119 A120 I121 E122

A123 V124 F125 G126 A127 L128 K129

4.2.6 Score per residue for model 6

- Molecule 1: CheY2

Chain A: 15% 42% 19% • 22%

M1 S2 L3 A4 E5 K6 I7 K8 V9 L10 I11 V12 D13 D14 Q15 V16 T17 S18 R19 L20 L21 L22 G23 D24 Q27 Q28 L29 G30 F31 K32 Q33 I34 T35 A36 A37 G38 D39 G40 E41 Q42 G43 M44 K45 I46 M47 N50 P51 H52 H53 L54 V55 I56 S57 D58 F59 N60 M61 P62

K63 M64 D65 G66 L67 G68 L69 L70 Q71 A72 V73 R74 P77 A78 T79 K80 K81 A82 A83 F84 I85 I86 L87 T88 A89 Q90 G91 D92 R93 V96 Q97 K98 A99 A100 A101 L102 G103 A104 N105 N106 V107 L108 A109 K110 P111 F112 T113 I114 E115 K116 M117 K118 A119 A120 I121 E122 A123 V124

F125 G126 A127 L128 K129

4.2.7 Score per residue for model 7

- Molecule 1: CheY2

Chain A: 13% 43% 19% • 22%

M1 S2 L3 A4 E5 K6 I7 K8 V9 L10 I11 V12 D13 D14 Q15 V16 T17 S18 R19 L20 L21 L22 G23 D24 A25 L26 Q27 Q28 L29 G30 F31 K32 Q33 I34 T35 A36 A37 G38 D39 G40 E41 Q42 G43 M44 K45 I46 M47 A48 Q49 N50 P51 H52 H53 L54 V55 I56 S57 D58 F59 N60

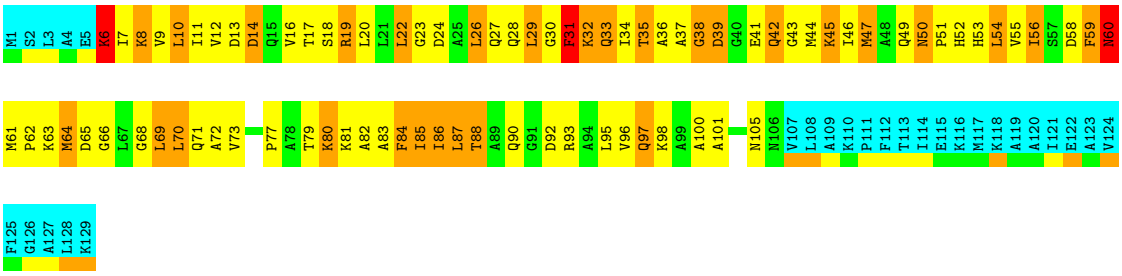
M61 P62 K63 M64 D65 G66 L67 G68 L69 L70 Q71 A72 V73 R74 P77 A78 T79 K80 K81 A82 A83 F84 I85 I86 L87 T88 A89 Q90 G91 D92 R93 V96 Q97 K98 A99 A100 A101 L102 G103 A104 N105 N106 V107 L108 A109 K110 P111 F112 T113 I114 E115 K116 M117 K118 A119 A120 I121 E122

A123 V124 F125 G126 A127 L128 K129

4.2.8 Score per residue for model 8

- Molecule 1: CheY2

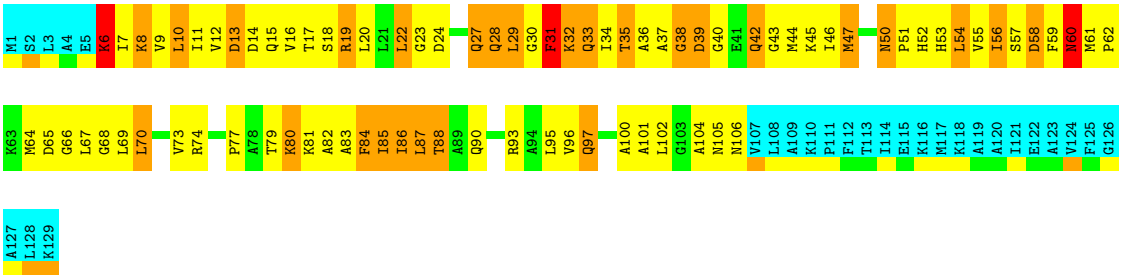
Chain A: 15% 39% 22% • 22%



4.2.9 Score per residue for model 9

- Molecule 1: CheY2

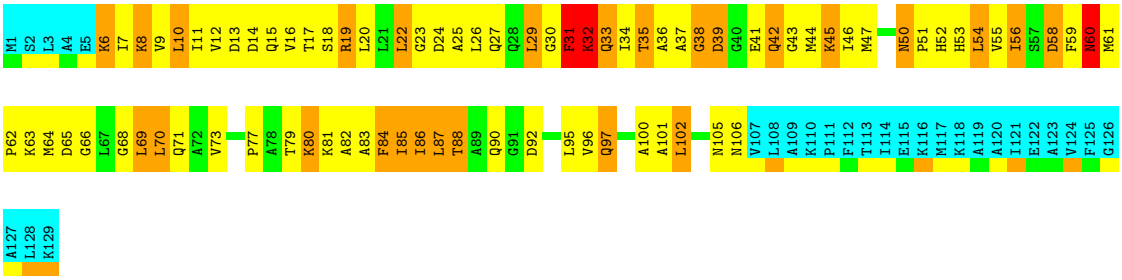
Chain A: 15% 40% 21% • 22%



4.2.10 Score per residue for model 10

- Molecule 1: CheY2

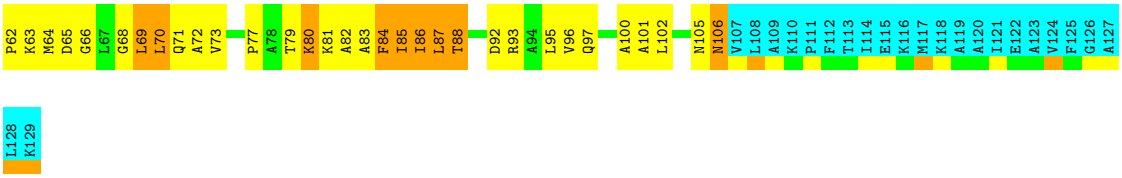
Chain A: 16% 40% 20% • 22%



4.2.11 Score per residue for model 11

- Molecule 1: CheY2

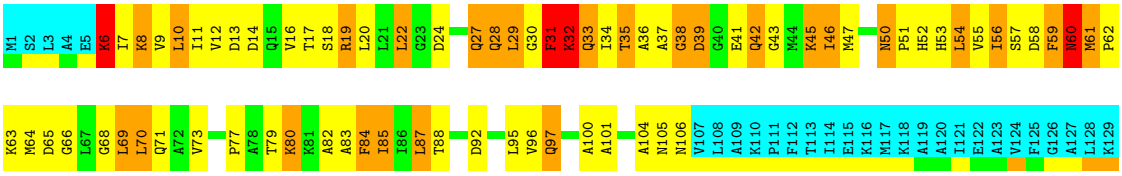
Chain A: 15% 39% 23% • 22%



4.2.12 Score per residue for model 12

- Molecule 1: CheY2

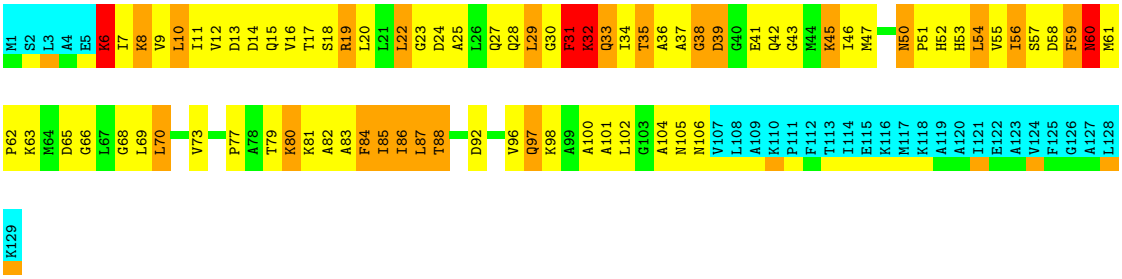
Chain A: 20% 35% 20% • 22%



4.2.13 Score per residue for model 13

- Molecule 1: CheY2

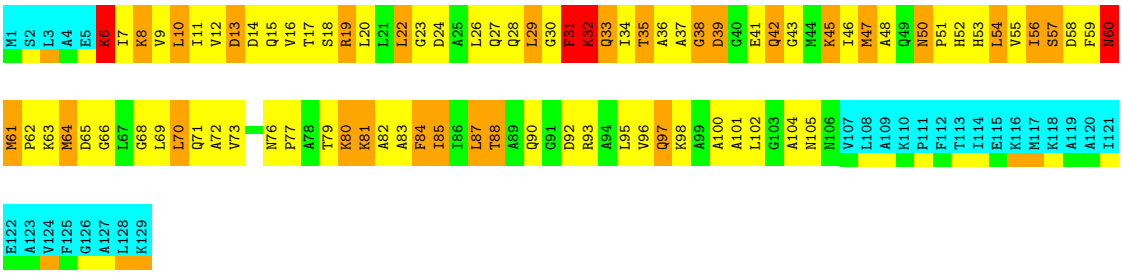
Chain A: 17% 41% 17% • 22%



4.2.14 Score per residue for model 14

- Molecule 1: CheY2

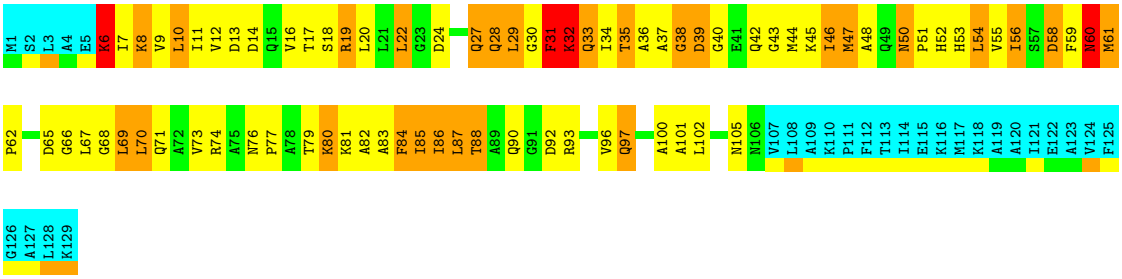
Chain A: 12% 42% 21% • 22%



4.2.15 Score per residue for model 15

- Molecule 1: CheY2

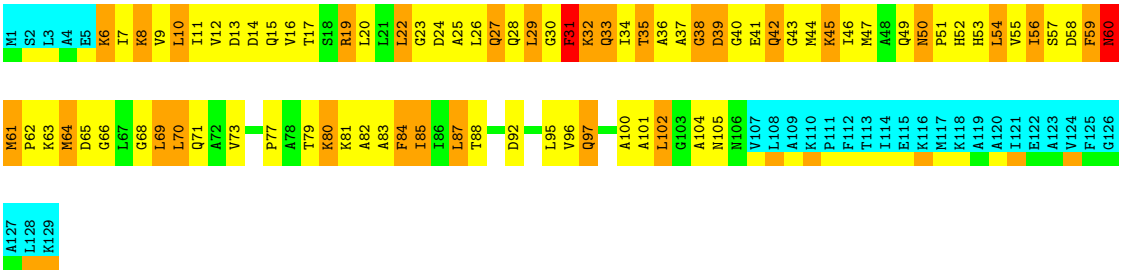
Chain A: 17% 37% 21% • 22%



4.2.16 Score per residue for model 16

- Molecule 1: CheY2

Chain A: 15% 40% 22% • 22%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 250 calculated structures, 16 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
DYANA	refinement	1.5

No chemical shift data was provided.

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	750	793	791	132±5
All	All	12000	12688	12656	2114

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 86.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:PHE:CE2	1:A:34:ILE:HG23	1.11	1.78	1	16
1:A:26:LEU:HD13	1:A:29:LEU:HD23	1.07	1.23	10	5
1:A:10:LEU:CD1	1:A:55:VAL:HG13	1.04	1.83	11	16
1:A:55:VAL:HG11	1:A:69:LEU:HD12	0.99	1.26	11	2
1:A:70:LEU:O	1:A:73:VAL:HG22	0.97	1.58	6	16
1:A:73:VAL:HG12	1:A:79:THR:HG23	0.94	1.39	5	14
1:A:70:LEU:HD22	1:A:70:LEU:O	0.94	1.63	2	2
1:A:87:LEU:O	1:A:87:LEU:HD13	0.93	1.62	16	16
1:A:10:LEU:C	1:A:10:LEU:HD22	0.92	1.83	4	16
1:A:69:LEU:O	1:A:73:VAL:HG13	0.92	1.65	10	16
1:A:55:VAL:HG11	1:A:69:LEU:HD22	0.92	1.40	4	8
1:A:70:LEU:O	1:A:70:LEU:HD22	0.92	1.63	11	9
1:A:22:LEU:HD13	1:A:56:ILE:HD11	0.90	1.43	5	15
1:A:55:VAL:CG1	1:A:69:LEU:HD22	0.88	1.98	9	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LEU:HD13	1:A:29:LEU:CD2	0.86	2.00	8	5
1:A:70:LEU:HD22	1:A:70:LEU:C	0.86	1.91	16	11
1:A:11:ILE:HD13	1:A:22:LEU:CD1	0.86	2.00	2	11
1:A:11:ILE:O	1:A:11:ILE:HD12	0.85	1.71	2	11
1:A:29:LEU:HD12	1:A:29:LEU:O	0.85	1.72	8	16
1:A:42:GLN:O	1:A:46:ILE:HD13	0.83	1.74	2	16
1:A:55:VAL:HG11	1:A:69:LEU:CD1	0.82	2.04	11	2
1:A:13:ASP:CG	1:A:22:LEU:HD21	0.81	1.96	7	16
1:A:55:VAL:HG11	1:A:69:LEU:HG	0.81	1.51	5	6
1:A:10:LEU:HD22	1:A:11:ILE:N	0.81	1.89	4	16
1:A:102:LEU:O	1:A:102:LEU:HD13	0.81	1.74	11	7
1:A:70:LEU:C	1:A:70:LEU:HD12	0.80	1.96	14	5
1:A:31:PHE:CD1	1:A:31:PHE:N	0.79	2.49	14	16
1:A:9:VAL:HG21	1:A:31:PHE:HB2	0.78	1.53	2	16
1:A:10:LEU:HD12	1:A:55:VAL:HG13	0.78	1.54	15	16
1:A:11:ILE:HD13	1:A:22:LEU:HD12	0.78	1.55	1	8
1:A:47:MET:SD	1:A:55:VAL:HG22	0.78	2.18	6	7
1:A:55:VAL:O	1:A:84:PHE:HA	0.77	1.79	4	16
1:A:66:GLY:HA2	1:A:69:LEU:HD12	0.77	1.54	6	6
1:A:31:PHE:CZ	1:A:34:ILE:HG23	0.75	2.16	2	1
1:A:7:ILE:HD12	1:A:53:HIS:CB	0.75	2.11	9	12
1:A:12:VAL:HG21	1:A:37:ALA:O	0.75	1.80	5	16
1:A:100:ALA:HA	1:A:104:ALA:HB3	0.73	1.60	5	5
1:A:22:LEU:CD1	1:A:56:ILE:HD11	0.73	2.13	5	13
1:A:87:LEU:HD22	1:A:87:LEU:C	0.73	2.04	1	16
1:A:55:VAL:HG11	1:A:69:LEU:CG	0.73	2.14	5	7
1:A:70:LEU:HD22	1:A:104:ALA:HB2	0.72	1.60	7	5
1:A:31:PHE:CE2	1:A:34:ILE:CG2	0.72	2.71	4	16
1:A:8:LYS:O	1:A:53:HIS:N	0.72	2.22	3	16
1:A:10:LEU:HD13	1:A:55:VAL:HA	0.71	1.60	8	16
1:A:10:LEU:C	1:A:10:LEU:CD2	0.71	2.58	4	16
1:A:55:VAL:HG11	1:A:69:LEU:CD2	0.70	2.16	8	4
1:A:55:VAL:HG12	1:A:69:LEU:HD13	0.70	1.64	6	8
1:A:73:VAL:CG1	1:A:79:THR:HG23	0.69	2.17	10	13
1:A:11:ILE:HD13	1:A:22:LEU:HD11	0.69	1.61	4	6
1:A:47:MET:SD	1:A:52:HIS:CD2	0.69	2.86	10	9
1:A:47:MET:CG	1:A:52:HIS:CG	0.69	2.76	9	16
1:A:13:ASP:OD1	1:A:22:LEU:HD21	0.68	1.88	13	15
1:A:22:LEU:HD13	1:A:56:ILE:CD1	0.68	2.17	5	7
1:A:73:VAL:HG12	1:A:79:THR:CG2	0.68	2.18	6	13
1:A:22:LEU:HD22	1:A:56:ILE:HD11	0.68	1.64	13	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ILE:HD12	1:A:22:LEU:HD12	0.68	1.64	12	4
1:A:31:PHE:N	1:A:31:PHE:HD1	0.67	1.85	14	15
1:A:11:ILE:O	1:A:36:ALA:HB2	0.67	1.89	5	16
1:A:7:ILE:HD12	1:A:53:HIS:HB3	0.67	1.66	12	11
1:A:55:VAL:O	1:A:84:PHE:CA	0.66	2.43	14	16
1:A:9:VAL:HG13	1:A:54:LEU:CB	0.66	2.20	5	16
1:A:56:ILE:C	1:A:56:ILE:HD12	0.66	2.10	5	8
1:A:10:LEU:HD11	1:A:55:VAL:HG13	0.65	1.66	8	16
1:A:82:ALA:O	1:A:84:PHE:CE1	0.65	2.50	14	16
1:A:50:ASN:CB	1:A:51:PRO:CD	0.65	2.75	14	16
1:A:61:MET:N	1:A:62:PRO:HD3	0.65	2.07	9	16
1:A:55:VAL:CG1	1:A:69:LEU:HD12	0.65	2.14	11	1
1:A:47:MET:HG2	1:A:52:HIS:CG	0.65	2.26	14	16
1:A:73:VAL:HG11	1:A:84:PHE:CE1	0.65	2.27	14	13
1:A:70:LEU:HD13	1:A:71:GLN:N	0.64	2.07	8	11
1:A:9:VAL:O	1:A:33:GLN:O	0.64	2.15	13	16
1:A:10:LEU:HD23	1:A:35:THR:O	0.63	1.94	4	16
1:A:30:GLY:O	1:A:31:PHE:O	0.63	2.17	11	16
1:A:47:MET:SD	1:A:52:HIS:CE1	0.63	2.92	4	7
1:A:31:PHE:CD2	1:A:34:ILE:HG23	0.62	2.29	11	11
1:A:70:LEU:C	1:A:70:LEU:CD2	0.62	2.67	16	11
1:A:11:ILE:CD1	1:A:34:ILE:HG22	0.62	2.25	14	2
1:A:55:VAL:O	1:A:85:ILE:N	0.61	2.31	1	16
1:A:11:ILE:CG2	1:A:56:ILE:CD1	0.60	2.79	1	2
1:A:37:ALA:O	1:A:39:ASP:N	0.60	2.35	12	16
1:A:30:GLY:O	1:A:31:PHE:C	0.59	2.41	10	16
1:A:96:VAL:O	1:A:100:ALA:CB	0.59	2.51	13	16
1:A:11:ILE:HG22	1:A:56:ILE:HG12	0.59	1.73	4	3
1:A:11:ILE:O	1:A:11:ILE:CD1	0.58	2.48	2	11
1:A:11:ILE:HB	1:A:22:LEU:HD13	0.58	1.74	8	10
1:A:37:ALA:HB3	1:A:43:GLY:HA2	0.58	1.73	2	15
1:A:26:LEU:HB3	1:A:31:PHE:CD1	0.58	2.33	2	1
1:A:55:VAL:HG11	1:A:69:LEU:HD23	0.58	1.75	8	2
1:A:13:ASP:OD2	1:A:22:LEU:HD21	0.58	1.97	16	15
1:A:11:ILE:HD11	1:A:34:ILE:HG22	0.58	1.75	8	2
1:A:7:ILE:HG23	1:A:32:LYS:HG2	0.58	1.74	6	10
1:A:83:ALA:HB1	1:A:106:ASN:HB3	0.58	1.75	2	4
1:A:65:ASP:OD1	1:A:86:ILE:HD13	0.57	1.99	2	2
1:A:50:ASN:CB	1:A:51:PRO:HD2	0.57	2.30	13	16
1:A:47:MET:O	1:A:50:ASN:O	0.57	2.21	2	16
1:A:97:GLN:O	1:A:101:ALA:CB	0.57	2.53	6	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:ILE:HD12	1:A:53:HIS:CG	0.56	2.34	14	8
1:A:10:LEU:HD12	1:A:47:MET:SD	0.56	2.40	1	7
1:A:9:VAL:HB	1:A:33:GLN:O	0.56	2.00	14	16
1:A:52:HIS:NE2	1:A:79:THR:CB	0.56	2.68	3	7
1:A:61:MET:N	1:A:62:PRO:CD	0.56	2.68	9	16
1:A:52:HIS:NE2	1:A:82:ALA:CB	0.56	2.68	7	6
1:A:10:LEU:CD1	1:A:55:VAL:CG1	0.56	2.75	11	16
1:A:52:HIS:HE2	1:A:79:THR:CB	0.56	2.13	14	1
1:A:14:ASP:CB	1:A:60:ASN:CB	0.56	2.84	4	16
1:A:66:GLY:CA	1:A:69:LEU:HD12	0.56	2.29	12	4
1:A:11:ILE:HG22	1:A:56:ILE:CG1	0.55	2.31	2	6
1:A:22:LEU:HD22	1:A:56:ILE:CD1	0.55	2.32	13	10
1:A:70:LEU:C	1:A:70:LEU:CD1	0.55	2.71	14	5
1:A:52:HIS:CD2	1:A:82:ALA:CB	0.55	2.89	9	8
1:A:16:VAL:HG13	1:A:19:ARG:NH1	0.54	2.16	1	1
1:A:69:LEU:O	1:A:69:LEU:HD13	0.54	2.02	8	2
1:A:31:PHE:CZ	1:A:34:ILE:CG2	0.54	2.89	2	1
1:A:11:ILE:HG22	1:A:56:ILE:CD1	0.54	2.31	1	1
1:A:11:ILE:CG2	1:A:56:ILE:HD13	0.54	2.33	1	1
1:A:55:VAL:CG1	1:A:69:LEU:CD1	0.54	2.83	11	1
1:A:87:LEU:HD22	1:A:88:THR:N	0.54	2.18	8	16
1:A:47:MET:HG3	1:A:52:HIS:CD2	0.54	2.38	2	7
1:A:47:MET:CE	1:A:52:HIS:CE1	0.53	2.91	9	2
1:A:47:MET:HE3	1:A:52:HIS:CE1	0.53	2.38	9	2
1:A:23:GLY:O	1:A:27:GLN:CG	0.53	2.57	10	8
1:A:74:ARG:NH2	1:A:102:LEU:HD21	0.53	2.18	9	1
1:A:42:GLN:O	1:A:46:ILE:CD1	0.53	2.56	9	12
1:A:19:ARG:HA	1:A:22:LEU:HD21	0.53	1.80	4	11
1:A:47:MET:CG	1:A:52:HIS:CD2	0.52	2.93	14	8
1:A:27:GLN:CG	1:A:28:GLN:N	0.52	2.73	11	8
1:A:11:ILE:HG22	1:A:56:ILE:HD13	0.52	1.80	1	1
1:A:13:ASP:OD2	1:A:22:LEU:CD2	0.52	2.58	7	16
1:A:43:GLY:O	1:A:47:MET:CB	0.52	2.57	10	7
1:A:65:ASP:O	1:A:68:GLY:N	0.52	2.43	7	16
1:A:7:ILE:CD1	1:A:53:HIS:CG	0.52	2.93	14	5
1:A:19:ARG:HA	1:A:22:LEU:HD11	0.52	1.82	2	10
1:A:8:LYS:CB	1:A:51:PRO:O	0.52	2.58	10	16
1:A:22:LEU:CD2	1:A:56:ILE:HD11	0.51	2.34	13	4
1:A:18:SER:O	1:A:22:LEU:CD2	0.51	2.58	15	8
1:A:87:LEU:C	1:A:87:LEU:CD2	0.51	2.79	4	11
1:A:70:LEU:HD21	1:A:102:LEU:HD23	0.51	1.81	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:ARG:CD	1:A:19:ARG:C	0.51	2.78	4	10
1:A:87:LEU:O	1:A:87:LEU:CD1	0.51	2.51	16	14
1:A:97:GLN:O	1:A:101:ALA:HB3	0.51	2.06	12	16
1:A:60:ASN:C	1:A:61:MET:CG	0.51	2.79	8	8
1:A:73:VAL:HA	1:A:79:THR:HG23	0.51	1.82	3	2
1:A:77:PRO:O	1:A:80:LYS:CG	0.51	2.59	9	15
1:A:22:LEU:HB2	1:A:56:ILE:HD11	0.50	1.82	4	1
1:A:27:GLN:HA	1:A:31:PHE:CE1	0.50	2.41	3	14
1:A:47:MET:SD	1:A:52:HIS:NE2	0.50	2.85	8	5
1:A:9:VAL:HG13	1:A:54:LEU:HB3	0.50	1.83	5	11
1:A:52:HIS:NE2	1:A:79:THR:OG1	0.50	2.45	5	12
1:A:40:GLY:O	1:A:44:MET:CB	0.50	2.60	9	6
1:A:53:HIS:CG	1:A:53:HIS:O	0.50	2.64	4	8
1:A:55:VAL:CG1	1:A:69:LEU:HD23	0.50	2.37	5	1
1:A:56:ILE:HG22	1:A:85:ILE:HB	0.50	1.84	7	7
1:A:18:SER:CB	1:A:58:ASP:OD2	0.50	2.60	4	8
1:A:47:MET:HG3	1:A:52:HIS:CG	0.50	2.41	8	11
1:A:44:MET:SD	1:A:72:ALA:CB	0.50	3.00	11	2
1:A:11:ILE:O	1:A:11:ILE:HG13	0.50	2.07	9	3
1:A:55:VAL:CG1	1:A:69:LEU:CD2	0.49	2.84	13	6
1:A:14:ASP:CB	1:A:60:ASN:CG	0.49	2.81	5	2
1:A:64:MET:CE	1:A:72:ALA:HB2	0.49	2.37	14	2
1:A:8:LYS:O	1:A:52:HIS:HA	0.49	2.08	15	16
1:A:16:VAL:O	1:A:20:LEU:CB	0.49	2.60	16	16
1:A:54:LEU:HA	1:A:83:ALA:O	0.49	2.08	10	16
1:A:11:ILE:HG22	1:A:56:ILE:HG13	0.49	1.84	5	2
1:A:44:MET:CE	1:A:72:ALA:HB1	0.49	2.38	6	1
1:A:70:LEU:O	1:A:70:LEU:HD12	0.48	2.08	14	5
1:A:64:MET:HE3	1:A:72:ALA:HB2	0.48	1.85	8	1
1:A:80:LYS:O	1:A:80:LYS:NZ	0.48	2.46	2	2
1:A:102:LEU:O	1:A:102:LEU:HD23	0.48	2.09	9	1
1:A:70:LEU:HD23	1:A:104:ALA:HA	0.48	1.85	3	4
1:A:37:ALA:O	1:A:38:GLY:C	0.48	2.52	13	16
1:A:64:MET:CE	1:A:72:ALA:CB	0.48	2.92	8	1
1:A:13:ASP:HB2	1:A:19:ARG:CB	0.48	2.39	7	9
1:A:22:LEU:HD12	1:A:23:GLY:N	0.48	2.24	4	1
1:A:74:ARG:NH2	1:A:102:LEU:HD22	0.48	2.23	5	1
1:A:73:VAL:HG11	1:A:84:PHE:CZ	0.48	2.44	14	2
1:A:86:ILE:CG2	1:A:86:ILE:O	0.48	2.62	13	5
1:A:16:VAL:O	1:A:20:LEU:N	0.47	2.43	4	16
1:A:59:PHE:CD1	1:A:59:PHE:N	0.47	2.81	12	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:VAL:HA	1:A:19:ARG:CG	0.47	2.39	5	6
1:A:46:ILE:O	1:A:50:ASN:ND2	0.47	2.47	6	9
1:A:50:ASN:N	1:A:50:ASN:OD1	0.47	2.47	3	5
1:A:79:THR:OG1	1:A:82:ALA:HB3	0.47	2.09	6	1
1:A:47:MET:HG3	1:A:52:HIS:CB	0.47	2.40	13	7
1:A:11:ILE:HB	1:A:22:LEU:CD1	0.47	2.39	13	8
1:A:9:VAL:HG13	1:A:54:LEU:HB2	0.47	1.84	15	2
1:A:11:ILE:HD12	1:A:11:ILE:C	0.47	2.29	2	3
1:A:31:PHE:H	1:A:31:PHE:HD1	0.47	1.51	2	1
1:A:102:LEU:O	1:A:102:LEU:CD1	0.47	2.59	10	2
1:A:31:PHE:CE2	1:A:34:ILE:HG12	0.47	2.43	2	11
1:A:31:PHE:HD1	1:A:31:PHE:H	0.47	1.51	14	14
1:A:31:PHE:HE2	1:A:34:ILE:N	0.47	2.07	8	6
1:A:55:VAL:HG12	1:A:69:LEU:HD23	0.47	1.86	3	2
1:A:47:MET:SD	1:A:48:ALA:N	0.47	2.87	2	6
1:A:20:LEU:O	1:A:24:ASP:N	0.47	2.49	7	16
1:A:23:GLY:O	1:A:27:GLN:CB	0.46	2.63	8	8
1:A:18:SER:O	1:A:22:LEU:HG	0.46	2.09	12	10
1:A:77:PRO:O	1:A:80:LYS:HG2	0.46	2.10	10	3
1:A:10:LEU:CD1	1:A:55:VAL:HA	0.46	2.40	3	11
1:A:64:MET:O	1:A:69:LEU:CD2	0.46	2.63	11	1
1:A:65:ASP:O	1:A:66:GLY:C	0.46	2.52	6	16
1:A:29:LEU:O	1:A:29:LEU:CD1	0.46	2.59	16	6
1:A:55:VAL:CG1	1:A:69:LEU:HD13	0.46	2.39	6	2
1:A:80:LYS:CE	1:A:80:LYS:O	0.46	2.64	9	1
1:A:14:ASP:CB	1:A:60:ASN:HB3	0.46	2.41	11	10
1:A:46:ILE:N	1:A:46:ILE:CD1	0.46	2.79	12	3
1:A:13:ASP:OD2	1:A:58:ASP:CB	0.46	2.64	9	1
1:A:47:MET:SD	1:A:55:VAL:CG2	0.46	3.03	3	4
1:A:60:ASN:H	1:A:60:ASN:ND2	0.46	2.08	15	1
1:A:10:LEU:CD2	1:A:11:ILE:N	0.45	2.72	5	16
1:A:86:ILE:O	1:A:86:ILE:HG23	0.45	2.11	13	6
1:A:20:LEU:O	1:A:24:ASP:HB2	0.45	2.12	6	5
1:A:52:HIS:CE1	1:A:79:THR:OG1	0.45	2.70	15	4
1:A:55:VAL:HG12	1:A:69:LEU:CD1	0.45	2.40	6	2
1:A:53:HIS:O	1:A:53:HIS:CD2	0.45	2.69	1	1
1:A:73:VAL:HA	1:A:79:THR:CG2	0.45	2.42	6	13
1:A:8:LYS:HB2	1:A:51:PRO:O	0.45	2.11	2	14
1:A:76:ASN:HB3	1:A:79:THR:HG22	0.45	1.88	14	2
1:A:31:PHE:CG	1:A:32:LYS:N	0.45	2.85	15	15
1:A:41:GLU:CG	1:A:63:LYS:HB2	0.45	2.42	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:SER:O	1:A:22:LEU:HD23	0.45	2.11	15	1
1:A:77:PRO:HA	1:A:80:LYS:HB3	0.45	1.89	6	2
1:A:31:PHE:CZ	1:A:34:ILE:HG12	0.45	2.48	2	1
1:A:6:LYS:HA	1:A:51:PRO:CB	0.44	2.42	8	2
1:A:86:ILE:O	1:A:86:ILE:CG2	0.44	2.66	6	1
1:A:11:ILE:CD1	1:A:23:GLY:HA2	0.44	2.42	9	1
1:A:87:LEU:C	1:A:88:THR:CG2	0.44	2.85	16	1
1:A:80:LYS:O	1:A:105:ASN:OD1	0.44	2.36	13	14
1:A:19:ARG:CD	1:A:20:LEU:N	0.44	2.80	8	10
1:A:84:PHE:CD1	1:A:84:PHE:N	0.44	2.85	13	5
1:A:14:ASP:HB3	1:A:60:ASN:CB	0.44	2.42	11	10
1:A:19:ARG:HA	1:A:22:LEU:CG	0.44	2.43	5	6
1:A:41:GLU:HG3	1:A:63:LYS:CB	0.44	2.42	2	12
1:A:16:VAL:HA	1:A:19:ARG:HG3	0.44	1.89	12	6
1:A:60:ASN:ND2	1:A:60:ASN:H	0.44	2.09	5	1
1:A:14:ASP:HB2	1:A:60:ASN:CB	0.44	2.43	8	14
1:A:26:LEU:O	1:A:30:GLY:N	0.44	2.51	2	1
1:A:56:ILE:CD1	1:A:56:ILE:C	0.44	2.80	5	1
1:A:45:LYS:HG3	1:A:46:ILE:CD1	0.44	2.42	12	3
1:A:13:ASP:CG	1:A:22:LEU:CD2	0.44	2.83	8	1
1:A:13:ASP:HB2	1:A:19:ARG:HB3	0.43	1.90	15	2
1:A:19:ARG:HA	1:A:22:LEU:CD2	0.43	2.43	4	1
1:A:50:ASN:OD1	1:A:50:ASN:N	0.43	2.50	7	6
1:A:26:LEU:O	1:A:31:PHE:HD1	0.43	1.95	2	1
1:A:44:MET:HG2	1:A:64:MET:CE	0.43	2.43	8	1
1:A:11:ILE:O	1:A:11:ILE:CG1	0.43	2.67	6	5
1:A:42:GLN:O	1:A:45:LYS:HG2	0.43	2.13	8	2
1:A:43:GLY:O	1:A:47:MET:HB3	0.43	2.14	5	11
1:A:73:VAL:CB	1:A:79:THR:HG23	0.43	2.43	9	3
1:A:31:PHE:HE2	1:A:34:ILE:HG23	0.43	1.58	14	1
1:A:56:ILE:HD12	1:A:57:SER:N	0.43	2.28	5	4
1:A:65:ASP:OD1	1:A:86:ILE:CG1	0.43	2.67	4	1
1:A:20:LEU:O	1:A:24:ASP:CB	0.43	2.67	6	1
1:A:27:GLN:HG2	1:A:28:GLN:N	0.43	2.28	7	8
1:A:64:MET:O	1:A:69:LEU:HD23	0.43	2.14	11	1
1:A:11:ILE:CD1	1:A:22:LEU:CD1	0.43	2.90	1	1
1:A:45:LYS:HG3	1:A:46:ILE:HD12	0.43	1.89	13	3
1:A:69:LEU:O	1:A:69:LEU:CD1	0.42	2.67	8	1
1:A:59:PHE:CE2	1:A:87:LEU:HD21	0.42	2.50	4	1
1:A:100:ALA:CA	1:A:104:ALA:HB3	0.42	2.39	5	1
1:A:74:ARG:CZ	1:A:102:LEU:O	0.42	2.67	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ILE:CD1	1:A:23:GLY:CA	0.42	2.97	9	1
1:A:102:LEU:HD13	1:A:102:LEU:C	0.42	2.32	7	1
1:A:16:VAL:O	1:A:20:LEU:HB3	0.42	2.14	11	8
1:A:52:HIS:CE1	1:A:79:THR:HB	0.42	2.50	3	1
1:A:50:ASN:HB3	1:A:51:PRO:CD	0.42	2.45	10	4
1:A:69:LEU:CD1	1:A:73:VAL:CG1	0.42	2.98	8	1
1:A:80:LYS:O	1:A:80:LYS:CE	0.42	2.68	10	1
1:A:56:ILE:HB	1:A:85:ILE:CG2	0.42	2.45	14	3
1:A:64:MET:CG	1:A:69:LEU:HD13	0.42	2.44	1	1
1:A:69:LEU:HD12	1:A:73:VAL:CG1	0.42	2.45	8	1
1:A:41:GLU:CG	1:A:63:LYS:CB	0.42	2.98	14	1
1:A:41:GLU:OE2	1:A:64:MET:SD	0.42	2.78	14	1
1:A:8:LYS:CB	1:A:52:HIS:HA	0.41	2.45	7	1
1:A:69:LEU:CD1	1:A:69:LEU:C	0.41	2.89	8	1
1:A:88:THR:HG1	1:A:90:GLN:CD	0.41	2.18	14	1
1:A:96:VAL:O	1:A:100:ALA:HB3	0.41	2.16	5	3
1:A:7:ILE:CD1	1:A:53:HIS:CB	0.41	2.95	14	1
1:A:102:LEU:HD23	1:A:102:LEU:O	0.41	2.15	5	1
1:A:80:LYS:O	1:A:105:ASN:CG	0.41	2.59	9	1
1:A:11:ILE:CD1	1:A:19:ARG:HG2	0.41	2.46	7	1
1:A:45:LYS:CG	1:A:46:ILE:HD13	0.41	2.45	12	1
1:A:44:MET:HE3	1:A:48:ALA:HB2	0.41	1.92	3	1
1:A:53:HIS:O	1:A:53:HIS:CG	0.41	2.73	3	1
1:A:83:ALA:CB	1:A:106:ASN:HB2	0.41	2.46	3	1
1:A:49:GLN:C	1:A:50:ASN:OD1	0.41	2.60	8	4
1:A:11:ILE:CG2	1:A:56:ILE:CG1	0.41	2.99	8	1
1:A:10:LEU:HD12	1:A:55:VAL:HG22	0.40	1.93	2	1
1:A:11:ILE:CB	1:A:56:ILE:HG13	0.40	2.46	5	1
1:A:19:ARG:HA	1:A:22:LEU:CD1	0.40	2.46	8	1
1:A:64:MET:HE3	1:A:72:ALA:CB	0.40	2.45	8	1
1:A:42:GLN:O	1:A:45:LYS:HG3	0.40	2.16	10	1
1:A:81:LYS:CD	1:A:81:LYS:O	0.40	2.69	14	1
1:A:44:MET:SD	1:A:69:LEU:HD11	0.40	2.56	5	1
1:A:64:MET:HB3	1:A:69:LEU:CD2	0.40	2.46	16	1
1:A:67:LEU:N	1:A:67:LEU:HD23	0.40	2.31	9	1
1:A:13:ASP:OD2	1:A:58:ASP:OD1	0.40	2.40	10	1
1:A:66:GLY:HA3	1:A:86:ILE:HG23	0.40	1.94	10	1
1:A:67:LEU:HD23	1:A:67:LEU:N	0.40	2.31	15	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	101/129 (78%)	84±1 (84±1%)	12±1 (12±1%)	5±0 (5±0%)	4 26
All	All	1616/2064 (78%)	1350 (84%)	188 (12%)	78 (5%)	4 26

All 5 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	6	LYS	16
1	A	31	PHE	16
1	A	38	GLY	16
1	A	60	ASN	16
1	A	32	LYS	14

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	77/98 (79%)	40±2 (52±2%)	37±2 (48±2%)	0 1
All	All	1232/1568 (79%)	638 (52%)	594 (48%)	0 1

All 54 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	6	LYS	16
1	A	8	LYS	16
1	A	10	LEU	16
1	A	17	THR	16
1	A	19	ARG	16

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Mol	Chain	Res	Type	Models (Total)
1	A	29	LEU	16
1	A	31	PHE	16
1	A	35	THR	16
1	A	39	ASP	16
1	A	50	ASN	16
1	A	54	LEU	16
1	A	56	ILE	16
1	A	58	ASP	16
1	A	59	PHE	16
1	A	60	ASN	16
1	A	70	LEU	16
1	A	80	LYS	16
1	A	84	PHE	16
1	A	85	ILE	16
1	A	87	LEU	16
1	A	33	GLN	15
1	A	92	ASP	15
1	A	45	LYS	14
1	A	81	LYS	14
1	A	22	LEU	13
1	A	97	GLN	13
1	A	42	GLN	13
1	A	64	MET	12
1	A	32	LYS	12
1	A	28	GLN	12
1	A	86	ILE	11
1	A	95	LEU	11
1	A	27	GLN	11
1	A	15	GLN	10
1	A	69	LEU	10
1	A	88	THR	10
1	A	90	GLN	10
1	A	57	SER	9
1	A	93	ARG	8
1	A	47	MET	8
1	A	61	MET	7
1	A	98	LYS	6
1	A	106	ASN	5
1	A	44	MET	4
1	A	46	ILE	3
1	A	74	ARG	3
1	A	102	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	26	LEU	2
1	A	18	SER	2
1	A	34	ILE	2
1	A	76	ASN	2
1	A	13	ASP	2
1	A	14	ASP	1
1	A	71	GLN	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)

No chemical shift data were provided