Full wwPDB NMR Structure Validation Report (i)

Mar 5, 2022 – 02:01 PM EST

PDB ID	:	2JS9
Title	:	Structure of caenopore-5 (81 Pro cis conformer)
Authors	:	Mysliwy, J.; Grotzinger, J.
Deposited on	:	2007-07-02

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

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

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

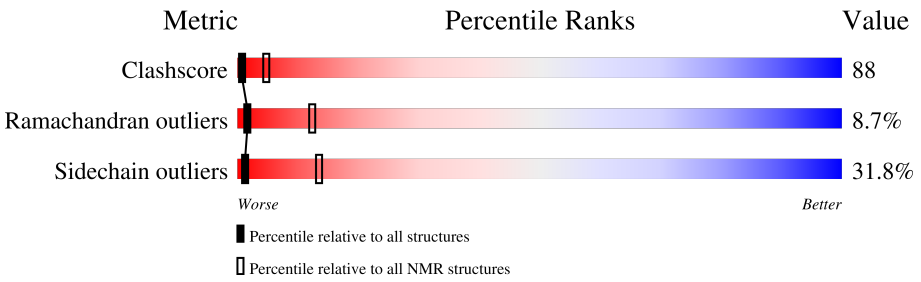
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	99	13% 47% 17% • 18%

2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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:5-A:81 (77)	0.36	12

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 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1264 atoms, of which 634 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Saposin-like protein family protein 5.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	81	1264	393	634	107	123	7	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP Q86FL8
A	-16	SER	-	expression tag	UNP Q86FL8
A	-15	GLY	-	expression tag	UNP Q86FL8
A	-14	SER	-	expression tag	UNP Q86FL8
A	-13	HIS	-	expression tag	UNP Q86FL8
A	-12	HIS	-	expression tag	UNP Q86FL8
A	-11	HIS	-	expression tag	UNP Q86FL8
A	-10	HIS	-	expression tag	UNP Q86FL8
A	-9	HIS	-	expression tag	UNP Q86FL8
A	-8	HIS	-	expression tag	UNP Q86FL8
A	-7	SER	-	expression tag	UNP Q86FL8
A	-6	SER	-	expression tag	UNP Q86FL8
A	-5	GLY	-	expression tag	UNP Q86FL8
A	-4	ILE	-	expression tag	UNP Q86FL8
A	-3	GLU	-	expression tag	UNP Q86FL8
A	-2	GLY	-	expression tag	UNP Q86FL8
A	-1	ARG	-	expression tag	UNP Q86FL8
A	0	GLY	-	expression tag	UNP Q86FL8

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: Saposin-like protein family protein 5

Chain A: 13% 47% 17% • 18%

MET SER GLY SER HIS HIS HIS HIS HIS HIS SER SER GLY ILE GLU GLY ARG GLY R1 S2 A3 L4 S5 C6 Q7 M8 C9 E10 L11 V12 V13 K14 K15 Y16 E17 G18 S19 A20 D21 K22 D23 A24 N25 V26 I27 K28 K29 D30 F31 D32 A33 E34 C35 K36 K37 L38 F39 H40 T41 I42

P43 F44 G45 E48 C49 Y52 V53 N54 S55 K56 V57 D58 P59 I60 I61 H62 E63 L64 T68 A69 P70 K71 D72 V73 C74 T75 K76 L77 N78 E79 C80 P81

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: Saposin-like protein family protein 5

Chain A: 15% 39% 22% • • 18%

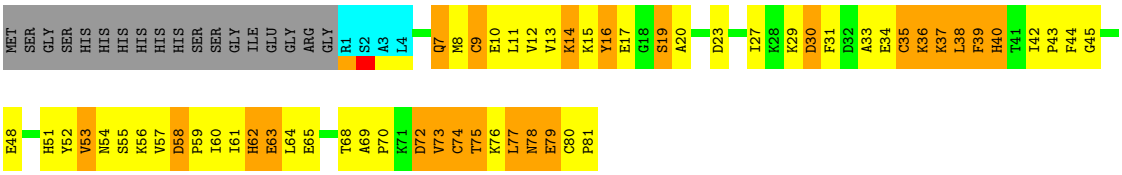
MET SER GLY SER HIS HIS HIS HIS HIS HIS SER SER GLY ILE GLU GLY ARG GLY R1 S2 A3 L4 S5 C6 Q7 M8 C9 E10 L11 V12 V13 K14 K15 Y16 E17 G18 S19 A20 D21 K22 D23 V26 I27 K28 K29 D30 F31 D32 A33 E34 C35 K36 K37 L38 F39 H40 T41 I42 P43

F44 G45 T46 R47 E48 C49 D50 H51 Y52 V53 N54 S55 K56 V57 D58 P59 I60 I61 H62 E63 L64 E65 A69 P70 K71 D72 V73 C74 T75 K76 L77 N78 E79 C80 P81

4.2.2 Score per residue for model 2

• Molecule 1: Saposin-like protein family protein 5

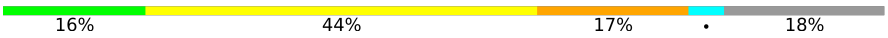
Chain A: 18% 36% 23% • 18%

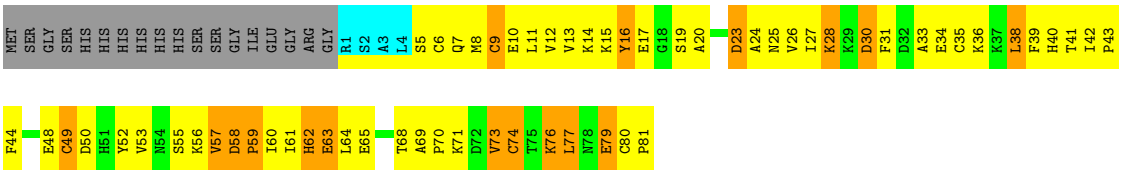


4.2.3 Score per residue for model 3

- Molecule 1: Saposin-like protein family protein 5

Chain A:

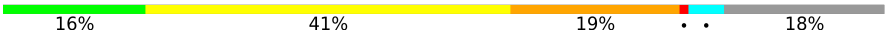




4.2.4 Score per residue for model 4

- Molecule 1: Saposin-like protein family protein 5

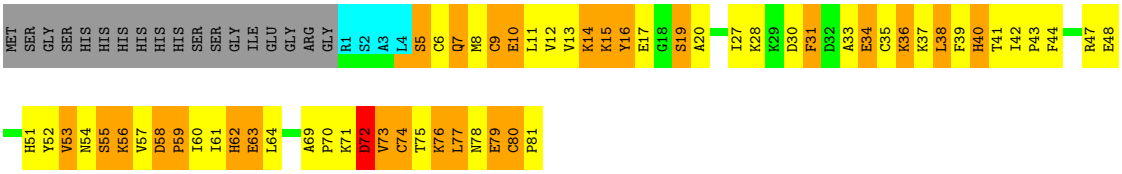
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Saposin-like protein family protein 5

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Saposin-like protein family protein 5

Chain A: 17% 39% 20% • • 18%

MET SER GLY SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY ILE GLU GLY ARG GLY R1 S2 A3 L4 S5 C6 Q7 M8 C9 E10 L11 V12 V13 K14 K15 Y16 E17 G18 S19 A20 D21 K22 N25 V26 I27 D30 F31 D32 A33 E34 C35 K36 K37 L38 F39 H40 T41 I42 P43 F44

G45 T46 R47 E48 C49 Y52 V53 N54 S55 K56 V57 D58 P59 I60 I61 H62 E63 L64 T68 A69 P70 K71 D72 V73 C74 T75 K76 L77 N78 E79 C80 P81

4.2.7 Score per residue for model 7

- Molecule 1: Saposin-like protein family protein 5

Chain A: 22% 41% 13% • • 18%

MET SER GLY SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY ILE GLU GLY ARG GLY R1 S2 A3 L4 S5 C6 Q7 M8 C9 E10 L11 V12 V13 K14 K15 Y16 E17 G18 S19 A20 D21 K22 I27 K28 K29 D30 F31 D32 A33 E34 C35 K36 K37 L38 F39 I42 P43 F44 G45 T46

R47 E48 H51 Y52 V53 N54 S55 K56 V57 D58 P59 I60 I61 H62 E63 L64 T68 A69 P70 K71 D72 V73 C74 T75 K76 L77 N78 E79 C80 P81

4.2.8 Score per residue for model 8

- Molecule 1: Saposin-like protein family protein 5

Chain A: 19% 35% 23% • 18%

MET SER GLY SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY ILE GLU GLY ARG GLY R1 S2 A3 L4 S5 C6 Q7 M8 C9 E10 L11 V12 V13 K14 K15 Y16 E17 G18 S19 A20 D23 A24 N25 V26 I27 K28 F31 E34 C35 K36 K37 L38 F39 H40 T41 I42 P43 F44 G45

T46 R47 E48 C49 Y52 V53 N54 S55 K56 V57 D58 P59 I60 I61 H62 E63 L64 A69 P70 K71 D72 V73 C74 T75 K76 L77 N78 E79 C80 P81

4.2.9 Score per residue for model 9

- Molecule 1: Saposin-like protein family protein 5

Chain A: 16% 38% 21% • • 18%

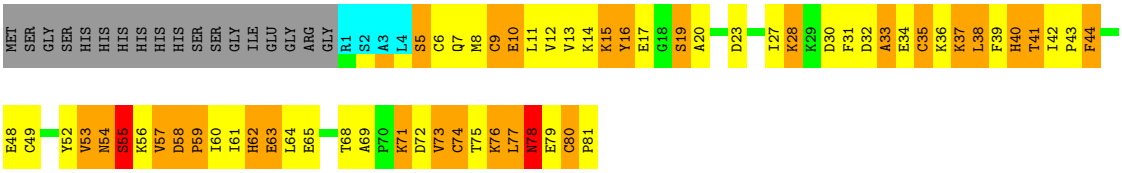
MET SER GLY SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY ILE GLU GLY ARG GLY R1 S2 A3 L4 S5 C6 Q7 M8 C9 E10 L11 V12 V13 K14 K15 Y16 E17 G18 S19 A20 D21 K22 D23 I27 K28 K29 D30 F31 D32 A33 E34 C35 K36 K37 L38 F39 H40 T41 I42 P43 F44

R47 E48 Y52 V53 N54 S55 K56 V57 D58 P59 I60 I61 H62 E63 L64 E65 G66 G67 T68 A69 P70 K71 D72 V73 C74 T75 K76 L77 N78 E79 C80 P81

4.2.10 Score per residue for model 10

- Molecule 1: Saposin-like protein family protein 5

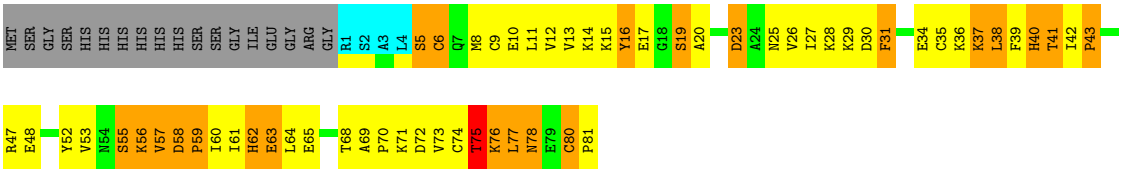
Chain A: 15% 33% 27% • • 18%



4.2.11 Score per residue for model 11

- Molecule 1: Saposin-like protein family protein 5

Chain A: 17% 37% 22% • • 18%



4.2.12 Score per residue for model 12 (medoid)

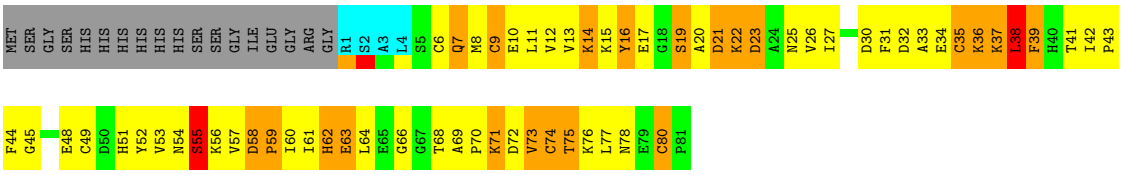
- Molecule 1: Saposin-like protein family protein 5

Chain A: 17% 39% 21% • 18%

4.2.13 Score per residue for model 13

- Molecule 1: Saposin-like protein family protein 5

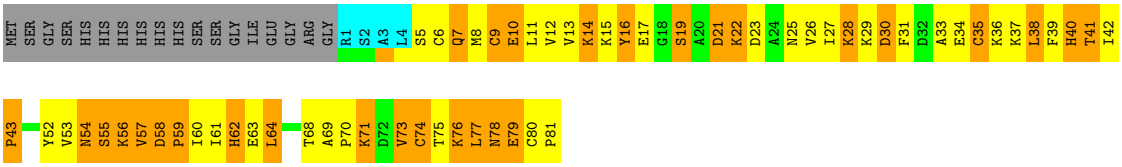
Chain A: 13% 41% 21% • • 18%



4.2.14 Score per residue for model 14

- Molecule 1: Saposin-like protein family protein 5

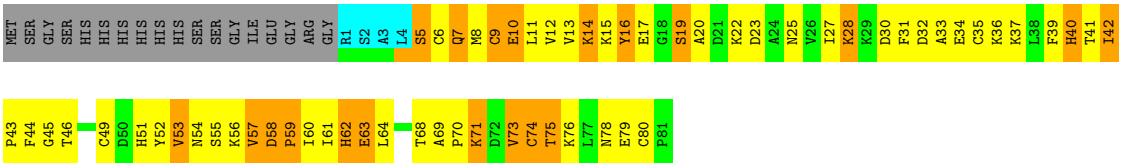
Chain A: 16% 31% 30% • 18%



4.2.15 Score per residue for model 15

- Molecule 1: Saposin-like protein family protein 5

Chain A: 15% 42% 20% • 18%



5 Refinement protocol and experimental data overview (i)

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

Of the 400 calculated structures, 15 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
DYANA 1.5	refinement	

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	600	600	583	105±10
All	All	9000	9000	8745	1570

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 88.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:CYS:SG	1:A:80:CYS:SG	1.28	2.29	1	10
1:A:13:VAL:HG12	1:A:64:LEU:HD11	1.09	1.25	1	15
1:A:16:TYR:CE2	1:A:61:ILE:HG23	1.05	1.84	7	14
1:A:11:LEU:HD23	1:A:31:PHE:CD2	0.96	1.95	7	15
1:A:38:LEU:HD22	1:A:38:LEU:O	0.94	1.62	13	1
1:A:69:ALA:O	1:A:73:VAL:HG23	0.93	1.63	9	15
1:A:13:VAL:CG1	1:A:64:LEU:HD11	0.92	1.95	13	11
1:A:77:LEU:N	1:A:77:LEU:HD13	0.89	1.82	10	1
1:A:73:VAL:HG13	1:A:77:LEU:HD23	0.89	1.43	11	1
1:A:11:LEU:HD11	1:A:34:GLU:HG3	0.88	1.45	10	3
1:A:12:VAL:CG2	1:A:60:ILE:HG21	0.87	1.99	6	15
1:A:63:GLU:HB3	1:A:73:VAL:HG22	0.87	1.46	9	15
1:A:13:VAL:HG12	1:A:64:LEU:CD1	0.85	1.98	8	5
1:A:9:CYS:O	1:A:13:VAL:HG13	0.85	1.72	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:LEU:HG	1:A:73:VAL:HG21	0.84	1.49	8	7
1:A:11:LEU:HD23	1:A:31:PHE:CE2	0.83	2.08	7	15
1:A:9:CYS:SG	1:A:80:CYS:SG	0.82	2.78	8	4
1:A:31:PHE:CD1	1:A:53:VAL:CG1	0.80	2.64	6	14
1:A:60:ILE:HG23	1:A:73:VAL:HG11	0.80	1.54	2	12
1:A:30:ASP:O	1:A:33:ALA:HB3	0.80	1.76	6	12
1:A:53:VAL:O	1:A:53:VAL:HG23	0.78	1.77	9	10
1:A:69:ALA:HB1	1:A:70:PRO:HD2	0.78	1.53	13	10
1:A:63:GLU:OE1	1:A:77:LEU:HD21	0.78	1.78	1	1
1:A:11:LEU:HD11	1:A:34:GLU:HB3	0.77	1.56	13	8
1:A:59:PRO:O	1:A:62:HIS:CD2	0.77	2.37	7	15
1:A:31:PHE:CD1	1:A:53:VAL:HG12	0.77	2.15	13	6
1:A:63:GLU:CB	1:A:73:VAL:HG22	0.76	2.10	8	11
1:A:11:LEU:HD21	1:A:31:PHE:O	0.76	1.81	5	15
1:A:63:GLU:OE1	1:A:77:LEU:HD11	0.74	1.81	9	5
1:A:35:CYS:HA	1:A:38:LEU:HD23	0.74	1.59	8	3
1:A:23:ASP:HB3	1:A:26:VAL:HG23	0.73	1.59	13	5
1:A:56:LYS:O	1:A:60:ILE:HD12	0.73	1.83	14	10
1:A:69:ALA:HB1	1:A:70:PRO:CD	0.73	2.13	13	8
1:A:38:LEU:HD22	1:A:38:LEU:C	0.72	2.04	13	1
1:A:31:PHE:CE2	1:A:52:TYR:CD2	0.71	2.79	8	6
1:A:31:PHE:CZ	1:A:52:TYR:CD2	0.71	2.78	8	5
1:A:11:LEU:CD2	1:A:31:PHE:CD2	0.71	2.73	7	13
1:A:38:LEU:HD13	1:A:39:PHE:N	0.70	2.01	13	1
1:A:59:PRO:HB2	1:A:77:LEU:HD13	0.70	1.60	3	4
1:A:58:ASP:N	1:A:59:PRO:CD	0.68	2.56	12	15
1:A:43:PRO:O	1:A:44:PHE:CG	0.67	2.47	15	4
1:A:16:TYR:CD2	1:A:61:ILE:HG23	0.67	2.24	5	14
1:A:16:TYR:HB2	1:A:27:ILE:HG21	0.67	1.67	14	13
1:A:12:VAL:HG21	1:A:60:ILE:HG21	0.67	1.66	12	7
1:A:63:GLU:CG	1:A:77:LEU:HD22	0.67	2.20	11	1
1:A:63:GLU:OE2	1:A:77:LEU:HD21	0.66	1.90	8	1
1:A:42:ILE:HG22	1:A:45:GLY:HA3	0.66	1.67	15	2
1:A:64:LEU:CD2	1:A:73:VAL:HG21	0.66	2.21	10	5
1:A:12:VAL:HG23	1:A:60:ILE:HG21	0.65	1.68	5	6
1:A:73:VAL:HG12	1:A:74:CYS:N	0.65	2.05	6	11
1:A:9:CYS:O	1:A:13:VAL:HG22	0.65	1.90	1	12
1:A:11:LEU:HD11	1:A:34:GLU:CG	0.65	2.22	6	3
1:A:12:VAL:CG1	1:A:31:PHE:CD2	0.64	2.81	6	15
1:A:62:HIS:NE2	1:A:77:LEU:HD21	0.64	2.07	3	2
1:A:34:GLU:O	1:A:38:LEU:N	0.64	2.31	5	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LEU:HD13	1:A:39:PHE:CZ	0.64	2.27	2	1
1:A:42:ILE:HG23	1:A:43:PRO:HD2	0.64	1.70	9	9
1:A:19:SER:O	1:A:20:ALA:HB3	0.64	1.93	6	13
1:A:16:TYR:HA	1:A:27:ILE:HD12	0.63	1.70	13	1
1:A:31:PHE:CD1	1:A:53:VAL:HG11	0.63	2.28	6	9
1:A:31:PHE:CZ	1:A:35:CYS:SG	0.63	2.92	4	2
1:A:12:VAL:HG11	1:A:57:VAL:HG23	0.63	1.71	1	2
1:A:62:HIS:CD2	1:A:63:GLU:OE1	0.62	2.51	1	4
1:A:63:GLU:OE2	1:A:68:THR:HG21	0.62	1.93	12	2
1:A:17:GLU:HG2	1:A:64:LEU:HD13	0.62	1.72	1	4
1:A:40:HIS:CD2	1:A:41:THR:HG23	0.62	2.28	15	3
1:A:62:HIS:CD2	1:A:62:HIS:C	0.62	2.73	2	15
1:A:53:VAL:O	1:A:53:VAL:CG2	0.61	2.48	9	10
1:A:31:PHE:CE1	1:A:35:CYS:SG	0.61	2.93	15	4
1:A:8:MET:CE	1:A:39:PHE:CE2	0.61	2.84	6	2
1:A:38:LEU:CD2	1:A:39:PHE:CE2	0.60	2.85	12	1
1:A:38:LEU:HD11	1:A:39:PHE:CE1	0.60	2.32	5	3
1:A:75:THR:HG22	1:A:76:LYS:N	0.60	2.12	11	1
1:A:62:HIS:CD2	1:A:63:GLU:N	0.60	2.70	6	15
1:A:43:PRO:O	1:A:44:PHE:CD2	0.60	2.54	15	4
1:A:38:LEU:CD2	1:A:39:PHE:CZ	0.59	2.85	12	1
1:A:13:VAL:HG23	1:A:14:LYS:N	0.59	2.12	6	15
1:A:21:ASP:OD2	1:A:26:VAL:HG21	0.59	1.97	1	1
1:A:59:PRO:O	1:A:62:HIS:CG	0.59	2.55	11	11
1:A:64:LEU:HD21	1:A:73:VAL:HG21	0.59	1.75	14	2
1:A:73:VAL:O	1:A:77:LEU:HD22	0.59	1.97	10	1
1:A:23:ASP:O	1:A:27:ILE:HG12	0.59	1.98	13	1
1:A:43:PRO:C	1:A:44:PHE:CG	0.58	2.75	10	7
1:A:35:CYS:O	1:A:39:PHE:N	0.58	2.37	10	5
1:A:40:HIS:CG	1:A:41:THR:N	0.58	2.72	10	4
1:A:40:HIS:C	1:A:40:HIS:CD2	0.58	2.77	11	1
1:A:73:VAL:CG1	1:A:77:LEU:HD23	0.58	2.26	11	1
1:A:8:MET:HB3	1:A:52:TYR:CE2	0.58	2.33	11	13
1:A:59:PRO:O	1:A:62:HIS:N	0.57	2.37	14	15
1:A:38:LEU:HD22	1:A:39:PHE:CD1	0.57	2.34	4	1
1:A:40:HIS:CD2	1:A:41:THR:N	0.57	2.71	14	2
1:A:8:MET:CB	1:A:52:TYR:CE2	0.57	2.87	10	11
1:A:12:VAL:HG13	1:A:31:PHE:CD2	0.57	2.34	6	11
1:A:16:TYR:CE2	1:A:61:ILE:CG2	0.57	2.78	2	9
1:A:28:LYS:CB	1:A:57:VAL:HG11	0.57	2.29	12	2
1:A:73:VAL:O	1:A:76:LYS:N	0.57	2.37	2	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:PRO:HB2	1:A:77:LEU:HD22	0.57	1.75	14	1
1:A:11:LEU:CG	1:A:31:PHE:CD2	0.56	2.88	12	12
1:A:63:GLU:OE2	1:A:77:LEU:CD2	0.56	2.53	8	1
1:A:72:ASP:O	1:A:73:VAL:C	0.56	2.43	12	8
1:A:38:LEU:HD13	1:A:39:PHE:HB2	0.56	1.76	13	1
1:A:16:TYR:CD2	1:A:64:LEU:HD12	0.56	2.35	14	7
1:A:56:LYS:O	1:A:60:ILE:CD1	0.56	2.54	14	3
1:A:74:CYS:C	1:A:75:THR:OG1	0.56	2.45	7	1
1:A:49:CYS:O	1:A:53:VAL:HG13	0.56	2.01	13	1
1:A:15:LYS:O	1:A:19:SER:CB	0.56	2.54	6	13
1:A:9:CYS:HB2	1:A:60:ILE:HD11	0.55	1.77	15	6
1:A:38:LEU:CD1	1:A:39:PHE:CD1	0.55	2.89	11	3
1:A:43:PRO:O	1:A:44:PHE:HB3	0.55	2.00	9	1
1:A:38:LEU:HD21	1:A:39:PHE:CZ	0.55	2.37	12	1
1:A:13:VAL:CG2	1:A:14:LYS:N	0.55	2.70	6	15
1:A:73:VAL:O	1:A:74:CYS:C	0.55	2.44	1	13
1:A:31:PHE:CD1	1:A:31:PHE:C	0.55	2.79	12	9
1:A:47:ARG:O	1:A:51:HIS:CG	0.55	2.60	1	1
1:A:8:MET:HB3	1:A:52:TYR:CD2	0.55	2.37	13	12
1:A:59:PRO:O	1:A:62:HIS:CB	0.55	2.55	13	10
1:A:64:LEU:HD21	1:A:70:PRO:HA	0.55	1.78	3	2
1:A:52:TYR:CD1	1:A:56:LYS:HB2	0.55	2.37	15	2
1:A:31:PHE:C	1:A:31:PHE:CD1	0.54	2.80	8	1
1:A:30:ASP:O	1:A:33:ALA:CB	0.54	2.54	9	9
1:A:62:HIS:HD2	1:A:63:GLU:N	0.54	2.00	7	9
1:A:8:MET:CB	1:A:52:TYR:CZ	0.54	2.90	8	2
1:A:69:ALA:CB	1:A:70:PRO:CD	0.54	2.84	13	2
1:A:11:LEU:HG	1:A:31:PHE:CD2	0.54	2.38	12	5
1:A:77:LEU:HD23	1:A:77:LEU:N	0.54	2.17	5	1
1:A:11:LEU:HD23	1:A:31:PHE:CG	0.54	2.38	13	3
1:A:43:PRO:O	1:A:44:PHE:CB	0.54	2.56	10	6
1:A:77:LEU:N	1:A:77:LEU:CD1	0.54	2.56	10	1
1:A:64:LEU:CG	1:A:73:VAL:HG21	0.54	2.30	8	2
1:A:44:PHE:CD1	1:A:44:PHE:O	0.54	2.61	9	1
1:A:63:GLU:OE2	1:A:68:THR:OG1	0.54	2.26	14	3
1:A:63:GLU:OE2	1:A:76:LYS:CG	0.54	2.56	14	3
1:A:58:ASP:N	1:A:59:PRO:HD2	0.53	2.16	12	15
1:A:56:LYS:O	1:A:60:ILE:CG1	0.53	2.57	6	12
1:A:42:ILE:HG22	1:A:45:GLY:N	0.53	2.17	12	2
1:A:38:LEU:C	1:A:38:LEU:HD23	0.53	2.23	4	2
1:A:57:VAL:C	1:A:59:PRO:HD2	0.53	2.23	8	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:TYR:OH	1:A:60:ILE:HD11	0.53	2.04	6	2
1:A:63:GLU:CD	1:A:68:THR:CB	0.53	2.77	7	4
1:A:28:LYS:O	1:A:53:VAL:CG1	0.53	2.57	11	2
1:A:73:VAL:O	1:A:77:LEU:CB	0.53	2.57	11	1
1:A:63:GLU:CA	1:A:63:GLU:OE1	0.53	2.57	13	1
1:A:28:LYS:HB3	1:A:57:VAL:HG11	0.53	1.79	12	1
1:A:63:GLU:OE2	1:A:76:LYS:CD	0.53	2.56	12	3
1:A:12:VAL:CG2	1:A:60:ILE:CG2	0.53	2.82	6	2
1:A:52:TYR:CE1	1:A:56:LYS:HB2	0.53	2.39	11	3
1:A:77:LEU:O	1:A:78:ASN:CB	0.53	2.55	5	1
1:A:39:PHE:CG	1:A:42:ILE:HG13	0.53	2.39	13	4
1:A:12:VAL:HG12	1:A:31:PHE:CD2	0.52	2.38	10	8
1:A:74:CYS:O	1:A:75:THR:OG1	0.52	2.23	11	2
1:A:11:LEU:HB3	1:A:31:PHE:CD2	0.52	2.40	12	6
1:A:38:LEU:HG	1:A:39:PHE:CE2	0.52	2.39	12	1
1:A:52:TYR:CE1	1:A:56:LYS:CB	0.52	2.92	10	2
1:A:16:TYR:C	1:A:16:TYR:CD1	0.52	2.82	14	10
1:A:38:LEU:CD2	1:A:38:LEU:C	0.52	2.78	9	1
1:A:63:GLU:OE2	1:A:73:VAL:O	0.52	2.28	1	5
1:A:12:VAL:O	1:A:27:ILE:CG2	0.52	2.57	13	1
1:A:13:VAL:O	1:A:17:GLU:N	0.51	2.44	14	15
1:A:63:GLU:HG2	1:A:77:LEU:HD22	0.51	1.82	11	1
1:A:36:LYS:O	1:A:40:HIS:N	0.51	2.43	8	4
1:A:75:THR:O	1:A:78:ASN:N	0.51	2.43	12	12
1:A:74:CYS:O	1:A:80:CYS:CB	0.51	2.58	7	1
1:A:37:LYS:O	1:A:37:LYS:CD	0.51	2.58	13	1
1:A:74:CYS:CB	1:A:79:GLU:HB3	0.51	2.35	14	9
1:A:42:ILE:HG22	1:A:45:GLY:H	0.51	1.65	7	2
1:A:19:SER:O	1:A:20:ALA:CB	0.51	2.59	6	9
1:A:16:TYR:HA	1:A:27:ILE:HD13	0.51	1.82	3	1
1:A:31:PHE:CD1	1:A:32:ASP:N	0.51	2.79	9	6
1:A:63:GLU:HB2	1:A:73:VAL:HG13	0.51	1.82	12	9
1:A:44:PHE:CD2	1:A:47:ARG:HD3	0.51	2.40	9	1
1:A:30:ASP:O	1:A:33:ALA:N	0.51	2.43	13	8
1:A:31:PHE:CZ	1:A:49:CYS:SG	0.51	3.04	3	1
1:A:77:LEU:O	1:A:78:ASN:CG	0.51	2.49	4	1
1:A:23:ASP:O	1:A:26:VAL:N	0.51	2.41	13	2
1:A:38:LEU:C	1:A:38:LEU:CD2	0.51	2.79	4	2
1:A:35:CYS:HA	1:A:38:LEU:HD12	0.51	1.82	13	1
1:A:36:LYS:O	1:A:40:HIS:CB	0.50	2.59	2	6
1:A:9:CYS:CA	1:A:52:TYR:OH	0.50	2.59	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LYS:O	1:A:40:HIS:CA	0.50	2.59	1	2
1:A:38:LEU:HD23	1:A:38:LEU:O	0.50	2.07	9	2
1:A:77:LEU:O	1:A:78:ASN:C	0.50	2.50	14	4
1:A:38:LEU:CD1	1:A:39:PHE:CE1	0.50	2.95	5	2
1:A:63:GLU:OE2	1:A:77:LEU:CG	0.50	2.60	8	1
1:A:24:ALA:O	1:A:28:LYS:CD	0.50	2.59	3	1
1:A:16:TYR:CE2	1:A:64:LEU:HB2	0.50	2.41	3	4
1:A:38:LEU:HD23	1:A:39:PHE:CE2	0.50	2.41	12	1
1:A:40:HIS:NE2	1:A:41:THR:HG23	0.50	2.22	5	1
1:A:54:ASN:O	1:A:55:SER:CB	0.50	2.60	6	4
1:A:44:PHE:CD1	1:A:44:PHE:N	0.50	2.79	10	1
1:A:6:CYS:O	1:A:9:CYS:N	0.50	2.44	5	11
1:A:9:CYS:O	1:A:13:VAL:CG1	0.50	2.56	14	2
1:A:74:CYS:O	1:A:77:LEU:N	0.49	2.45	13	2
1:A:63:GLU:OE1	1:A:63:GLU:HA	0.49	2.07	13	3
1:A:39:PHE:O	1:A:42:ILE:N	0.49	2.45	13	3
1:A:74:CYS:SG	1:A:80:CYS:CB	0.49	3.00	3	3
1:A:38:LEU:HD12	1:A:38:LEU:O	0.49	2.07	12	2
1:A:77:LEU:O	1:A:79:GLU:N	0.49	2.46	14	8
1:A:24:ALA:HA	1:A:27:ILE:HD12	0.49	1.84	3	1
1:A:78:ASN:O	1:A:78:ASN:ND2	0.49	2.45	4	1
1:A:43:PRO:C	1:A:44:PHE:CD2	0.49	2.85	15	1
1:A:7:GLN:O	1:A:10:GLU:N	0.49	2.46	12	13
1:A:62:HIS:NE2	1:A:63:GLU:OE1	0.49	2.46	14	1
1:A:55:SER:O	1:A:59:PRO:CD	0.49	2.60	15	1
1:A:15:LYS:O	1:A:19:SER:CA	0.49	2.61	3	4
1:A:68:THR:HG22	1:A:69:ALA:N	0.49	2.23	6	2
1:A:62:HIS:CD2	1:A:63:GLU:CD	0.49	2.85	8	1
1:A:16:TYR:CD1	1:A:27:ILE:HD13	0.49	2.43	3	2
1:A:34:GLU:O	1:A:35:CYS:C	0.49	2.51	8	5
1:A:63:GLU:OE1	1:A:68:THR:CB	0.49	2.61	11	3
1:A:38:LEU:HD13	1:A:39:PHE:CB	0.49	2.37	13	1
1:A:52:TYR:CD1	1:A:56:LYS:CD	0.48	2.95	5	1
1:A:63:GLU:HB2	1:A:77:LEU:CD2	0.48	2.38	11	1
1:A:8:MET:HB2	1:A:52:TYR:CZ	0.48	2.43	15	8
1:A:13:VAL:HG23	1:A:14:LYS:H	0.48	1.67	13	12
1:A:63:GLU:OE2	1:A:68:THR:CG2	0.48	2.61	12	2
1:A:23:ASP:OD1	1:A:25:ASN:CB	0.48	2.61	14	1
1:A:63:GLU:OE2	1:A:68:THR:CB	0.48	2.61	14	1
1:A:16:TYR:HD2	1:A:64:LEU:HD12	0.48	1.69	12	7
1:A:27:ILE:O	1:A:30:ASP:N	0.48	2.47	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LYS:NZ	1:A:46:THR:O	0.48	2.47	8	1
1:A:74:CYS:CB	1:A:79:GLU:HB2	0.48	2.39	5	1
1:A:11:LEU:CD2	1:A:35:CYS:SG	0.48	3.02	13	1
1:A:57:VAL:O	1:A:61:ILE:HD12	0.48	2.08	14	3
1:A:39:PHE:CD1	1:A:39:PHE:N	0.48	2.82	2	1
1:A:15:LYS:CG	1:A:34:GLU:OE2	0.48	2.62	10	1
1:A:16:TYR:CA	1:A:27:ILE:HD12	0.48	2.36	13	1
1:A:23:ASP:CG	1:A:26:VAL:HG23	0.48	2.29	14	1
1:A:63:GLU:CD	1:A:68:THR:OG1	0.48	2.51	10	6
1:A:34:GLU:O	1:A:38:LEU:CB	0.48	2.62	9	2
1:A:55:SER:O	1:A:59:PRO:CG	0.48	2.62	15	1
1:A:35:CYS:SG	1:A:39:PHE:CE2	0.48	3.07	15	1
1:A:16:TYR:HA	1:A:27:ILE:CD1	0.48	2.39	5	12
1:A:57:VAL:O	1:A:61:ILE:HG13	0.48	2.08	12	15
1:A:72:ASP:O	1:A:75:THR:N	0.48	2.47	12	4
1:A:63:GLU:HA	1:A:63:GLU:OE1	0.48	2.08	4	3
1:A:11:LEU:HD23	1:A:31:PHE:CZ	0.48	2.44	13	1
1:A:72:ASP:O	1:A:75:THR:CB	0.47	2.62	2	2
1:A:23:ASP:CB	1:A:26:VAL:HG23	0.47	2.35	13	1
1:A:77:LEU:C	1:A:79:GLU:N	0.47	2.66	4	10
1:A:42:ILE:HG22	1:A:44:PHE:CD1	0.47	2.44	1	2
1:A:42:ILE:HG22	1:A:45:GLY:CA	0.47	2.37	15	2
1:A:11:LEU:HB3	1:A:31:PHE:CE2	0.47	2.44	13	4
1:A:45:GLY:O	1:A:48:GLU:N	0.47	2.47	6	2
1:A:63:GLU:OE1	1:A:63:GLU:CA	0.47	2.62	11	2
1:A:9:CYS:HA	1:A:60:ILE:HD13	0.47	1.86	6	1
1:A:57:VAL:O	1:A:61:ILE:CG1	0.47	2.62	9	4
1:A:53:VAL:HA	1:A:57:VAL:CG2	0.47	2.39	3	4
1:A:17:GLU:CD	1:A:64:LEU:HD22	0.47	2.30	4	1
1:A:64:LEU:HD23	1:A:73:VAL:HG21	0.47	1.85	10	1
1:A:9:CYS:N	1:A:52:TYR:OH	0.47	2.48	15	3
1:A:42:ILE:CG2	1:A:43:PRO:HD2	0.47	2.39	14	5
1:A:74:CYS:O	1:A:79:GLU:N	0.47	2.43	6	6
1:A:57:VAL:N	1:A:59:PRO:HD2	0.47	2.25	8	9
1:A:74:CYS:O	1:A:75:THR:CB	0.47	2.63	11	1
1:A:31:PHE:CE2	1:A:52:TYR:CE2	0.47	3.03	12	1
1:A:8:MET:HB2	1:A:52:TYR:CE2	0.47	2.45	13	1
1:A:11:LEU:HD22	1:A:35:CYS:SG	0.47	2.50	13	1
1:A:13:VAL:O	1:A:16:TYR:N	0.47	2.48	1	13
1:A:10:GLU:O	1:A:14:LYS:CE	0.47	2.63	14	1
1:A:47:ARG:O	1:A:51:HIS:CD2	0.47	2.69	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:HIS:CD2	1:A:63:GLU:HG3	0.47	2.45	5	1
1:A:37:LYS:O	1:A:38:LEU:CB	0.47	2.63	13	1
1:A:35:CYS:SG	1:A:39:PHE:CD2	0.46	3.08	15	1
1:A:57:VAL:HG12	1:A:58:ASP:N	0.46	2.26	8	1
1:A:79:GLU:C	1:A:81:PRO:C	0.46	2.74	10	2
1:A:64:LEU:HD21	1:A:70:PRO:CA	0.46	2.40	3	1
1:A:39:PHE:CD1	1:A:42:ILE:HD12	0.46	2.46	15	2
1:A:48:GLU:O	1:A:52:TYR:CB	0.46	2.63	12	1
1:A:34:GLU:O	1:A:37:LYS:N	0.46	2.48	5	2
1:A:12:VAL:HG11	1:A:57:VAL:HG22	0.46	1.86	12	1
1:A:63:GLU:HG3	1:A:77:LEU:CD2	0.46	2.41	13	1
1:A:38:LEU:C	1:A:38:LEU:HD12	0.46	2.30	1	1
1:A:38:LEU:HB3	1:A:39:PHE:CE1	0.46	2.46	2	1
1:A:10:GLU:HA	1:A:13:VAL:CG2	0.46	2.41	2	12
1:A:63:GLU:CD	1:A:68:THR:HG1	0.46	2.14	13	1
1:A:40:HIS:CD2	1:A:41:THR:CG2	0.46	2.99	15	1
1:A:23:ASP:C	1:A:25:ASN:N	0.46	2.68	13	3
1:A:46:THR:O	1:A:49:CYS:N	0.46	2.48	15	2
1:A:42:ILE:CG2	1:A:44:PHE:CE1	0.46	2.98	7	1
1:A:52:TYR:C	1:A:54:ASN:N	0.46	2.69	8	1
1:A:62:HIS:NE2	1:A:63:GLU:OE2	0.46	2.48	8	1
1:A:40:HIS:ND1	1:A:40:HIS:C	0.46	2.69	9	1
1:A:12:VAL:CG1	1:A:57:VAL:HG22	0.46	2.41	12	1
1:A:60:ILE:HA	1:A:73:VAL:CG1	0.46	2.41	7	5
1:A:8:MET:HE3	1:A:39:PHE:CE2	0.46	2.46	6	1
1:A:38:LEU:HG	1:A:39:PHE:N	0.45	2.26	10	2
1:A:6:CYS:O	1:A:7:GLN:C	0.45	2.53	13	7
1:A:13:VAL:CG2	1:A:14:LYS:H	0.45	2.24	6	8
1:A:34:GLU:O	1:A:36:LYS:N	0.45	2.49	3	2
1:A:62:HIS:CD2	1:A:63:GLU:HG2	0.45	2.46	12	2
1:A:74:CYS:O	1:A:75:THR:C	0.45	2.54	13	3
1:A:43:PRO:HG2	1:A:44:PHE:CE2	0.45	2.47	4	3
1:A:63:GLU:OE1	1:A:68:THR:OG1	0.45	2.33	11	2
1:A:37:LYS:O	1:A:40:HIS:N	0.45	2.50	12	1
1:A:34:GLU:C	1:A:36:LYS:N	0.45	2.69	3	2
1:A:37:LYS:O	1:A:38:LEU:C	0.45	2.54	12	2
1:A:39:PHE:CD1	1:A:42:ILE:HG13	0.45	2.46	8	2
1:A:37:LYS:O	1:A:39:PHE:N	0.45	2.49	12	1
1:A:56:LYS:C	1:A:59:PRO:HD2	0.45	2.32	12	7
1:A:35:CYS:C	1:A:37:LYS:N	0.45	2.69	2	3
1:A:35:CYS:O	1:A:37:LYS:N	0.45	2.49	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:SER:O	1:A:6:CYS:C	0.45	2.55	1	3
1:A:28:LYS:O	1:A:53:VAL:HG11	0.45	2.11	11	1
1:A:16:TYR:OH	1:A:65:GLU:CG	0.45	2.65	3	3
1:A:63:GLU:OE1	1:A:77:LEU:CD2	0.45	2.58	1	1
1:A:19:SER:OG	1:A:20:ALA:N	0.45	2.50	3	1
1:A:8:MET:HE2	1:A:39:PHE:CE2	0.45	2.47	15	1
1:A:74:CYS:CB	1:A:80:CYS:SG	0.44	3.03	1	2
1:A:40:HIS:ND1	1:A:40:HIS:O	0.44	2.50	4	1
1:A:59:PRO:HB2	1:A:77:LEU:CD1	0.44	2.42	8	3
1:A:37:LYS:O	1:A:37:LYS:CE	0.44	2.65	13	1
1:A:52:TYR:O	1:A:54:ASN:N	0.44	2.50	8	1
1:A:26:VAL:O	1:A:30:ASP:CG	0.44	2.56	13	1
1:A:10:GLU:HA	1:A:13:VAL:HG22	0.44	1.89	15	6
1:A:59:PRO:O	1:A:62:HIS:HB3	0.44	2.13	13	2
1:A:8:MET:HB3	1:A:52:TYR:CZ	0.44	2.48	8	1
1:A:31:PHE:CE1	1:A:52:TYR:HB3	0.44	2.48	8	1
1:A:80:CYS:SG	1:A:81:PRO:HA	0.44	2.53	11	1
1:A:28:LYS:HG3	1:A:29:LYS:N	0.44	2.27	14	1
1:A:15:LYS:CD	1:A:30:ASP:HB3	0.44	2.43	13	3
1:A:12:VAL:HG11	1:A:57:VAL:CG2	0.44	2.42	12	1
1:A:45:GLY:O	1:A:46:THR:C	0.44	2.55	4	2
1:A:63:GLU:OE1	1:A:73:VAL:HG13	0.44	2.13	8	1
1:A:17:GLU:CD	1:A:17:GLU:C	0.44	2.77	15	4
1:A:15:LYS:CE	1:A:34:GLU:OE2	0.44	2.64	6	1
1:A:76:LYS:C	1:A:77:LEU:HD13	0.44	2.30	10	1
1:A:63:GLU:CD	1:A:77:LEU:HD21	0.44	2.33	5	1
1:A:75:THR:CG2	1:A:76:LYS:N	0.44	2.80	11	1
1:A:34:GLU:OE2	1:A:38:LEU:N	0.44	2.48	12	1
1:A:56:LYS:O	1:A:60:ILE:HB	0.44	2.13	15	1
1:A:12:VAL:CG1	1:A:57:VAL:HG23	0.43	2.41	1	1
1:A:8:MET:C	1:A:52:TYR:CE2	0.43	2.92	4	1
1:A:65:GLU:CD	1:A:65:GLU:C	0.43	2.77	9	2
1:A:57:VAL:O	1:A:61:ILE:CD1	0.43	2.66	14	2
1:A:80:CYS:N	1:A:81:PRO:C	0.43	2.72	8	1
1:A:11:LEU:CD2	1:A:31:PHE:O	0.43	2.62	10	1
1:A:43:PRO:C	1:A:45:GLY:N	0.43	2.72	15	1
1:A:35:CYS:O	1:A:36:LYS:C	0.43	2.57	2	2
1:A:38:LEU:HB3	1:A:39:PHE:CD1	0.43	2.49	2	1
1:A:13:VAL:CB	1:A:64:LEU:HD11	0.43	2.44	13	1
1:A:39:PHE:CG	1:A:42:ILE:CG1	0.43	3.02	13	1
1:A:45:GLY:O	1:A:49:CYS:SG	0.43	2.77	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:CYS:HA	1:A:81:PRO:C	0.43	2.34	11	7
1:A:60:ILE:HA	1:A:77:LEU:HD11	0.43	1.91	7	1
1:A:16:TYR:HD2	1:A:64:LEU:HD13	0.43	1.74	8	1
1:A:8:MET:O	1:A:11:LEU:N	0.43	2.46	13	1
1:A:9:CYS:CB	1:A:52:TYR:OH	0.43	2.67	15	1
1:A:35:CYS:HA	1:A:39:PHE:CD1	0.43	2.49	2	1
1:A:68:THR:CG2	1:A:69:ALA:N	0.43	2.82	14	2
1:A:23:ASP:OD2	1:A:26:VAL:HG23	0.43	2.14	14	1
1:A:40:HIS:O	1:A:40:HIS:CG	0.42	2.72	4	1
1:A:31:PHE:O	1:A:35:CYS:CB	0.42	2.67	12	1
1:A:63:GLU:CG	1:A:77:LEU:HD21	0.42	2.44	13	1
1:A:52:TYR:CD1	1:A:56:LYS:CB	0.42	3.02	15	1
1:A:27:ILE:O	1:A:28:LYS:C	0.42	2.58	9	5
1:A:21:ASP:O	1:A:22:LYS:C	0.42	2.57	13	2
1:A:71:LYS:CG	1:A:71:LYS:O	0.42	2.67	13	1
1:A:73:VAL:O	1:A:77:LEU:HB2	0.42	2.14	11	2
1:A:12:VAL:CG2	1:A:13:VAL:N	0.42	2.82	13	1
1:A:72:ASP:O	1:A:73:VAL:O	0.42	2.38	4	2
1:A:42:ILE:CG2	1:A:45:GLY:HA3	0.42	2.45	6	1
1:A:16:TYR:O	1:A:17:GLU:C	0.42	2.58	14	1
1:A:53:VAL:HA	1:A:57:VAL:HG21	0.42	1.92	14	1
1:A:54:ASN:O	1:A:55:SER:OG	0.42	2.38	14	1
1:A:77:LEU:O	1:A:78:ASN:OD1	0.42	2.37	4	1
1:A:73:VAL:C	1:A:75:THR:H	0.42	2.16	7	1
1:A:16:TYR:CB	1:A:27:ILE:HD13	0.42	2.44	1	2
1:A:31:PHE:CD1	1:A:53:VAL:HG13	0.42	2.49	5	1
1:A:23:ASP:O	1:A:25:ASN:N	0.42	2.52	3	1
1:A:31:PHE:CE1	1:A:49:CYS:SG	0.42	3.12	3	1
1:A:32:ASP:O	1:A:36:LYS:CG	0.42	2.68	13	1
1:A:63:GLU:OE2	1:A:73:VAL:C	0.42	2.58	1	1
1:A:49:CYS:O	1:A:52:TYR:N	0.42	2.47	10	2
1:A:72:ASP:OD1	1:A:72:ASP:O	0.42	2.37	10	1
1:A:6:CYS:O	1:A:9:CYS:SG	0.42	2.78	5	3
1:A:6:CYS:SG	1:A:81:PRO:HA	0.42	2.55	5	2
1:A:73:VAL:CG1	1:A:74:CYS:N	0.42	2.81	8	3
1:A:63:GLU:OE1	1:A:77:LEU:CD1	0.42	2.63	9	1
1:A:45:GLY:O	1:A:47:ARG:N	0.42	2.53	4	1
1:A:63:GLU:O	1:A:68:THR:O	0.42	2.37	6	2
1:A:72:ASP:O	1:A:76:LYS:N	0.41	2.51	5	1
1:A:12:VAL:HG12	1:A:31:PHE:CG	0.41	2.50	6	1
1:A:37:LYS:CD	1:A:38:LEU:N	0.41	2.83	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LYS:HG2	1:A:29:LYS:N	0.41	2.31	11	1
1:A:23:ASP:O	1:A:27:ILE:CG1	0.41	2.68	10	1
1:A:34:GLU:OE2	1:A:37:LYS:O	0.41	2.38	13	1
1:A:38:LEU:C	1:A:38:LEU:HD13	0.41	2.35	13	1
1:A:9:CYS:HB2	1:A:60:ILE:CD1	0.41	2.46	9	1
1:A:12:VAL:HG23	1:A:13:VAL:N	0.41	2.30	13	1
1:A:63:GLU:OE2	1:A:77:LEU:HG	0.41	2.14	2	2
1:A:28:LYS:HG2	1:A:57:VAL:CG1	0.41	2.46	3	1
1:A:62:HIS:CD2	1:A:77:LEU:HD21	0.41	2.51	11	1
1:A:40:HIS:C	1:A:42:ILE:N	0.41	2.72	14	1
1:A:11:LEU:CD2	1:A:35:CYS:HB2	0.41	2.46	6	1
1:A:75:THR:N	1:A:80:CYS:HB2	0.41	2.31	6	1
1:A:28:LYS:CE	1:A:57:VAL:HG11	0.41	2.46	3	1
1:A:6:CYS:O	1:A:9:CYS:HB3	0.41	2.16	11	1
1:A:39:PHE:C	1:A:41:THR:N	0.41	2.73	13	1
1:A:38:LEU:HD11	1:A:39:PHE:CD1	0.41	2.50	11	1
1:A:34:GLU:O	1:A:34:GLU:OE2	0.41	2.38	12	1
1:A:38:LEU:HG	1:A:39:PHE:CZ	0.41	2.50	12	1
1:A:12:VAL:O	1:A:27:ILE:HG23	0.41	2.15	13	1
1:A:9:CYS:SG	1:A:10:GLU:OE1	0.41	2.79	14	1
1:A:42:ILE:CG2	1:A:44:PHE:CD1	0.41	3.04	7	1
1:A:78:ASN:O	1:A:81:PRO:O	0.41	2.38	10	1
1:A:16:TYR:CD1	1:A:16:TYR:C	0.40	2.94	3	1
1:A:41:THR:O	1:A:42:ILE:C	0.40	2.59	3	1
1:A:75:THR:C	1:A:77:LEU:N	0.40	2.74	4	1
1:A:74:CYS:HA	1:A:79:GLU:HB2	0.40	1.94	7	1
1:A:52:TYR:CD1	1:A:56:LYS:HG3	0.40	2.51	10	1
1:A:11:LEU:CB	1:A:31:PHE:CD2	0.40	3.04	15	2
1:A:38:LEU:HG	1:A:39:PHE:CD2	0.40	2.51	12	1
1:A:34:GLU:O	1:A:34:GLU:CG	0.40	2.69	15	1
1:A:40:HIS:NE2	1:A:41:THR:CG2	0.40	2.84	5	1
1:A:30:ASP:O	1:A:34:GLU:OE2	0.40	2.40	6	1
1:A:37:LYS:C	1:A:39:PHE:N	0.40	2.71	12	1
1:A:43:PRO:HG2	1:A:44:PHE:CD2	0.40	2.52	12	1
1:A:5:SER:O	1:A:8:MET:HB2	0.40	2.16	15	1
1:A:78:ASN:O	1:A:81:PRO:C	0.40	2.59	8	1
1:A:77:LEU:HD22	1:A:77:LEU:H	0.40	1.76	10	1
1:A:16:TYR:O	1:A:19:SER:N	0.40	2.52	12	1
1:A:34:GLU:O	1:A:38:LEU:HB3	0.40	2.17	1	2
1:A:48:GLU:O	1:A:48:GLU:OE1	0.40	2.39	9	1
1:A:74:CYS:O	1:A:80:CYS:HB3	0.40	2.16	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:GLU:OE1	1:A:48:GLU:O	0.40	2.39	8	1
1:A:52:TYR:O	1:A:53:VAL:C	0.40	2.59	8	1
1:A:38:LEU:CG	1:A:39:PHE:CE2	0.40	3.04	12	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	76/99 (77%)	51±2 (67±3%)	19±2 (25±3%)	7±1 (9±2%)	1	12
All	All	1140/1485 (77%)	760 (67%)	281 (25%)	99 (9%)	1	12

All 21 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	55	SER	14
1	A	73	VAL	13
1	A	59	PRO	12
1	A	53	VAL	10
1	A	54	ASN	10
1	A	72	ASP	6
1	A	5	SER	5
1	A	71	LYS	5
1	A	75	THR	5
1	A	78	ASN	4
1	A	43	PRO	3
1	A	44	PHE	2
1	A	33	ALA	2
1	A	68	THR	1
1	A	49	CYS	1
1	A	45	GLY	1
1	A	36	LYS	1
1	A	6	CYS	1
1	A	67	GLY	1

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Mol	Chain	Res	Type	Models (Total)
1	A	38	LEU	1
1	A	66	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	69/86 (80%)	47±4 (68±6%)	22±4 (32±6%)	1 13
All	All	1035/1290 (80%)	706 (68%)	329 (32%)	1 13

All 50 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	58	ASP	15
1	A	62	HIS	15
1	A	16	TYR	14
1	A	9	CYS	13
1	A	63	GLU	13
1	A	74	CYS	13
1	A	19	SER	12
1	A	37	LYS	11
1	A	76	LYS	11
1	A	77	LEU	11
1	A	38	LEU	10
1	A	40	HIS	10
1	A	48	GLU	10
1	A	71	LYS	10
1	A	30	ASP	9
1	A	55	SER	9
1	A	57	VAL	9
1	A	80	CYS	9
1	A	14	LYS	8
1	A	23	ASP	8
1	A	7	GLN	8
1	A	79	GLU	7
1	A	36	LYS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	28	LYS	7
1	A	56	LYS	6
1	A	5	SER	6
1	A	10	GLU	6
1	A	22	LYS	6
1	A	35	CYS	5
1	A	51	HIS	5
1	A	75	THR	4
1	A	25	ASN	4
1	A	31	PHE	4
1	A	47	ARG	4
1	A	44	PHE	3
1	A	78	ASN	3
1	A	21	ASP	3
1	A	41	THR	3
1	A	39	PHE	2
1	A	50	ASP	2
1	A	15	LYS	2
1	A	34	GLU	2
1	A	72	ASP	2
1	A	65	GLU	2
1	A	29	LYS	1
1	A	49	CYS	1
1	A	6	CYS	1
1	A	54	ASN	1
1	A	64	LEU	1
1	A	42	ILE	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