Full wwPDB NMR Structure Validation Report (i)

Oct 16, 2021 – 07:34 PM EDT

PDB ID	:	1SW8
Title	:	Solution structure of the N-terminal domain of Human N60D calmodulin refined with paramagnetism based strategy
Authors	:	Bertini, I.; Del Bianco, C.; Gelis, I.; Katsaros, N.; Luchinat, C.; Parigi, G.; Peana, M.; Provenzani, A.; Zoroddu, M.A.; Structural Proteomics in Europe (SPINE)
Deposited on	:	2004-03-30

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:

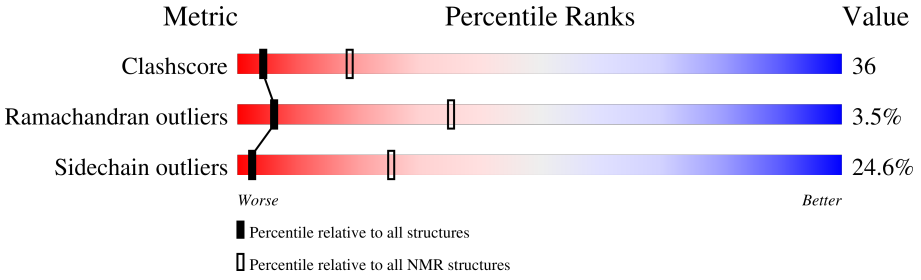
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	79	33% 58% 5% •

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:4-A:79 (76)	0.34	2

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 2 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1196 atoms, of which 582 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	79	1194	377	582	96	134	5	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	ASN	engineered mutation	UNP P62158

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	2	2	2

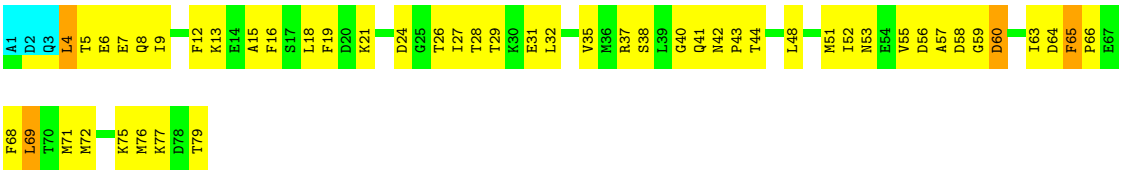
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Calmodulin

Chain A: 33% 58% 5%



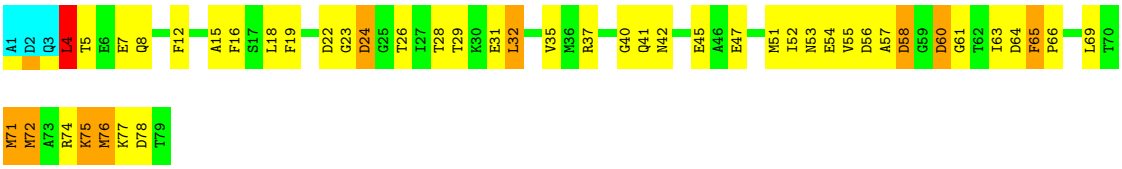
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Calmodulin

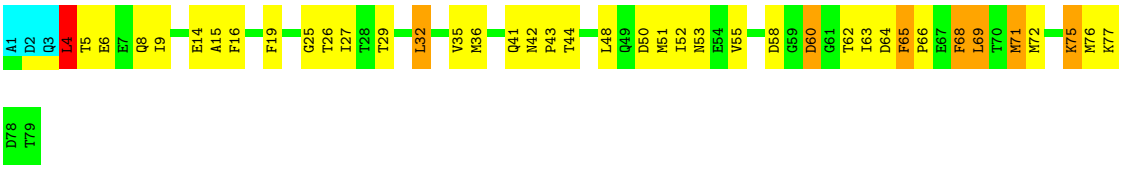
Chain A: 38% 46% 11%



4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Calmodulin

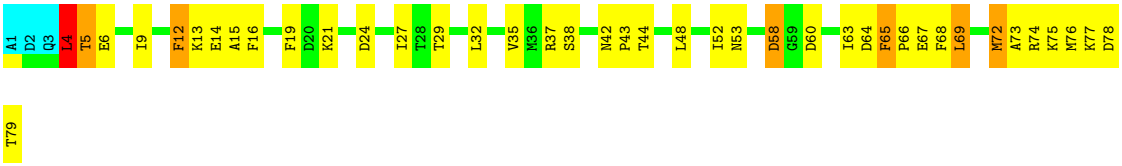
Chain A: 46% 41% 9%



4.2.3 Score per residue for model 3

- Molecule 1: Calmodulin

Chain A:



4.2.4 Score per residue for model 4

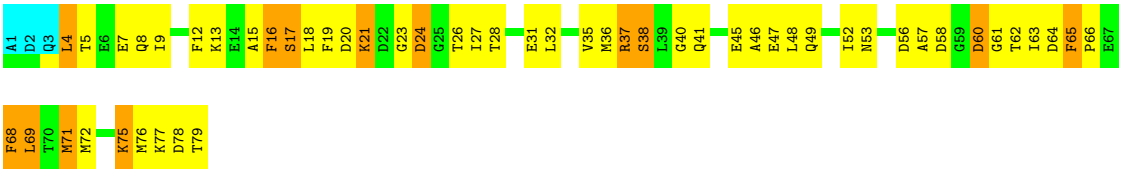
- Molecule 1: Calmodulin

Chain A:

4.2.5 Score per residue for model 5

- Molecule 1: Calmodulin

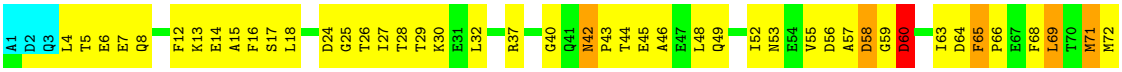
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Calmodulin

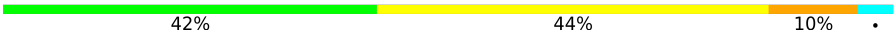
Chain A:

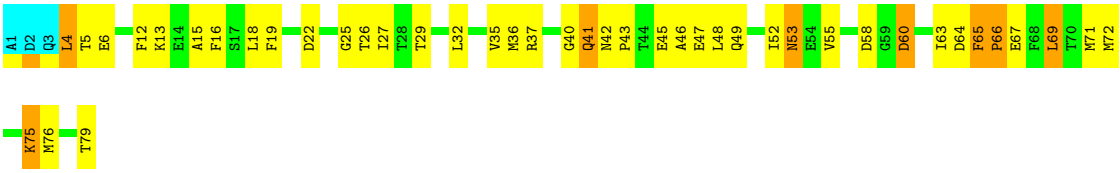


4.2.7 Score per residue for model 7

- Molecule 1: Calmodulin

Chain A:





4.2.8 Score per residue for model 8

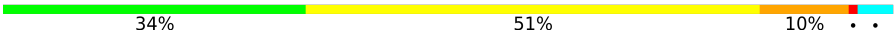
- Molecule 1: Calmodulin

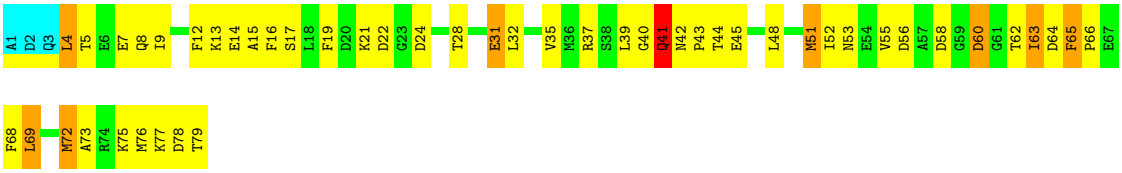
Chain A:

4.2.9 Score per residue for model 9

- Molecule 1: Calmodulin

Chain A:

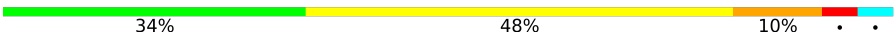


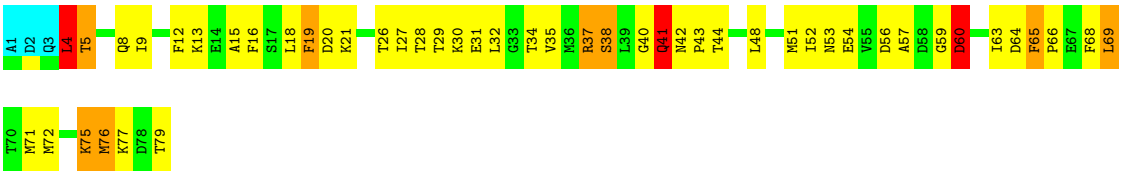


4.2.10 Score per residue for model 10

- Molecule 1: Calmodulin

Chain A:

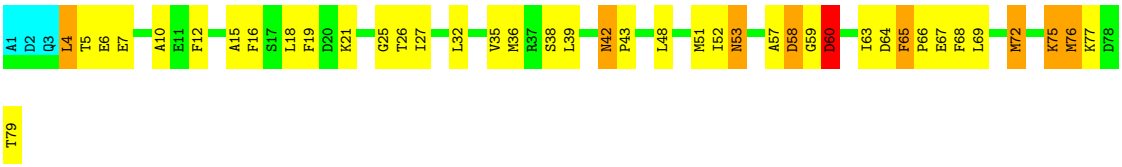




4.2.11 Score per residue for model 11

- Molecule 1: Calmodulin

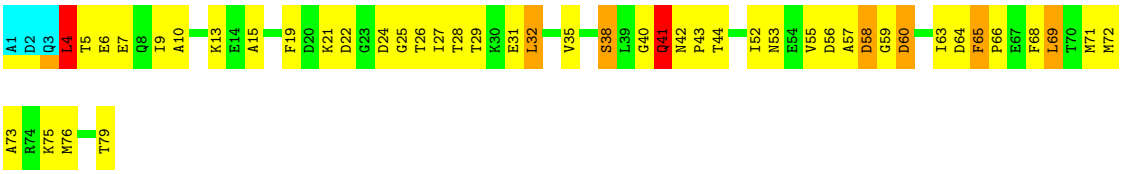
Chain A: 44% 41% 10%



4.2.12 Score per residue for model 12

- Molecule 1: Calmodulin

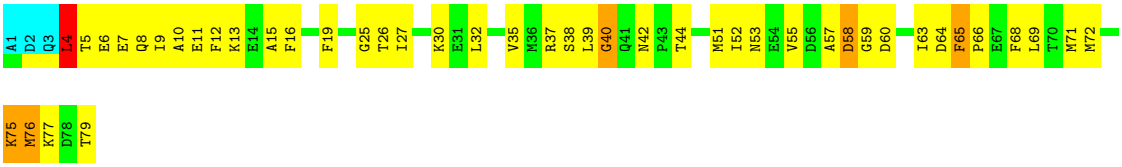
Chain A: 38% 48% 8%



4.2.13 Score per residue for model 13

- Molecule 1: Calmodulin

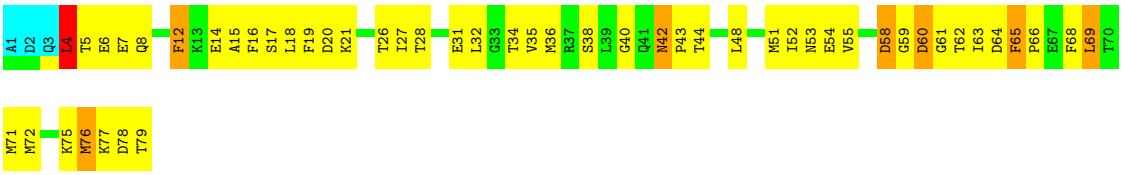
Chain A: 39% 49% 6%



4.2.14 Score per residue for model 14

- Molecule 1: Calmodulin

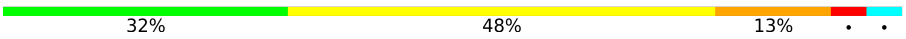
Chain A: 32% 54% 9%

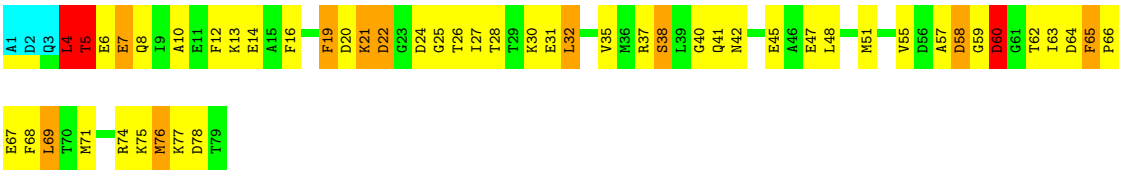


4.2.15 Score per residue for model 15

- Molecule 1: Calmodulin

Chain A:

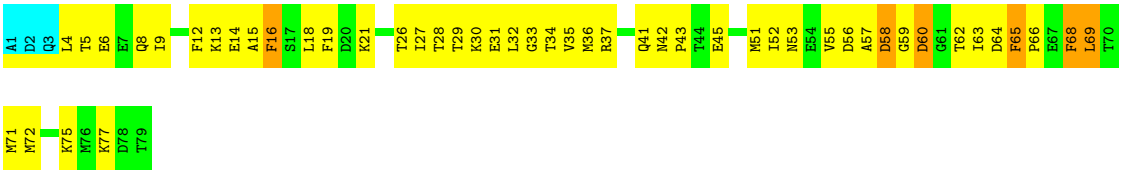




4.2.16 Score per residue for model 16

- Molecule 1: Calmodulin

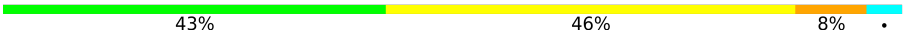
Chain A:

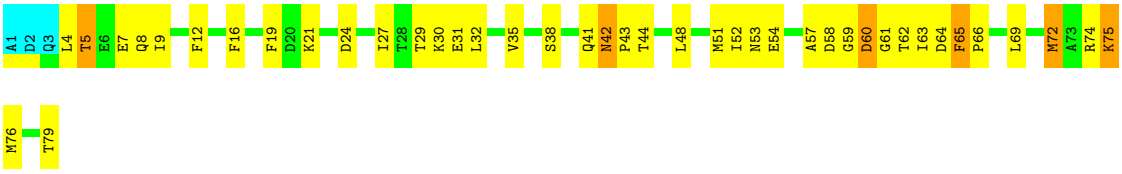


4.2.17 Score per residue for model 17

- Molecule 1: Calmodulin

Chain A:





4.2.18 Score per residue for model 18

- Molecule 1: Calmodulin

Chain A: 48% 39% 8%

A1 D2 Q3 L4 Q8 F12 K13 E14 A15 F16 S17 L18 F19 D20 K21 D22 G23 I27 K30 E31 L32 V35 G40 Q41 N42 P43 T44 L48 I52 N53 D56 A57 D58 G59 D60 I63 D64 F65 P66 L69 M72 A73 K74 K75 M76 K77 D78 T79

4.2.19 Score per residue for model 19

- Molecule 1: Calmodulin

Chain A: 37% 54%

A1 D2 Q3 L4 T5 Q8 I9 F12 A15 F16 S17 L18 F19 D20 K21 D22 G23 T26 I27 K30 E31 L32 G33 T34 V35 N36 R37 S38 N42 P43 A46 E47 L48 Q49 D50 M51 I52 N53 E54 V55 D56 A57 D58 G59 D60 G61 T62 I63 D64 F65 P66 E67 F68

L69 K75 M76 K77 D78 T79

4.2.20 Score per residue for model 20

- Molecule 1: Calmodulin

Chain A: 41% 49%

A1 D2 Q3 L4 T5 E6 E7 Q8 I9 A10 K13 F16 S17 L18 F19 D24 G25 T26 I27 T28 T29 K30 E31 L32 V35 S38 L39 G40 Q41 T44 E45 L48 M51 I52 N53 D56 A57 D58 G59 D60 G61 T62 I63 D64 F65 P66 L69 T70 M71 M72

K75 M76 K77 D78 T79

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry, simulated annealing, torsion angle dynamics.*

Of the 200 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
DYANA	structure solution	
DYANA	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

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	590	565	565	41±7
2	A	2	0	0	0±0
All	All	11840	11300	11300	828

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ASP:HB2	2:A:80:CA:CA	1.03	0.87	12	1
1:A:9:ILE:HG22	1:A:69:LEU:HD11	1.00	1.33	16	2
1:A:32:LEU:HD12	1:A:63:ILE:HD11	0.94	1.39	3	11
1:A:52:ILE:HD12	1:A:53:ASN:N	0.90	1.81	7	16
1:A:19:PHE:CD1	1:A:35:VAL:HG21	0.89	2.03	15	5
1:A:19:PHE:CE1	1:A:35:VAL:HG11	0.86	2.05	15	3
1:A:22:ASP:CB	2:A:80:CA:CA	0.85	1.81	12	1
1:A:4:LEU:HD22	1:A:5:THR:N	0.84	1.86	3	1
1:A:4:LEU:HD13	1:A:5:THR:N	0.82	1.89	12	7
1:A:31:GLU:O	1:A:35:VAL:HG23	0.81	1.76	10	3
1:A:16:PHE:CD2	1:A:65:PHE:CE2	0.80	2.70	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:CE1	1:A:68:PHE:CE2	0.80	2.70	13	3
1:A:19:PHE:CZ	1:A:35:VAL:HG11	0.80	2.12	15	1
1:A:19:PHE:CZ	1:A:68:PHE:CD2	0.79	2.71	13	2
1:A:21:LYS:NZ	1:A:34:THR:HG21	0.79	1.93	10	1
1:A:32:LEU:HD12	1:A:63:ILE:CD1	0.78	2.08	3	10
1:A:16:PHE:CD1	1:A:65:PHE:CE2	0.76	2.73	3	5
1:A:19:PHE:CE1	1:A:68:PHE:CZ	0.75	2.74	13	1
1:A:19:PHE:CZ	1:A:68:PHE:CG	0.75	2.74	13	1
1:A:55:VAL:HG12	1:A:71:MET:SD	0.75	2.21	15	3
1:A:52:ILE:HD13	1:A:61:GLY:O	0.75	1.81	14	3
1:A:4:LEU:C	1:A:4:LEU:HD13	0.74	2.03	5	5
1:A:16:PHE:CG	1:A:65:PHE:CZ	0.74	2.76	5	10
1:A:52:ILE:HG22	1:A:63:ILE:HD11	0.73	1.60	1	6
1:A:66:PRO:HA	1:A:69:LEU:HD23	0.73	1.60	3	5
1:A:4:LEU:HD13	1:A:4:LEU:C	0.73	2.04	12	3
1:A:21:LYS:CE	1:A:35:VAL:HG23	0.72	2.14	11	3
1:A:15:ALA:HB1	1:A:19:PHE:CE2	0.72	2.19	12	6
1:A:32:LEU:C	1:A:32:LEU:HD23	0.72	2.04	8	8
1:A:25:GLY:O	1:A:26:THR:HG23	0.71	1.84	20	8
1:A:32:LEU:HD11	1:A:48:LEU:HD12	0.71	1.61	7	4
1:A:15:ALA:HB1	1:A:19:PHE:CZ	0.71	2.20	11	1
1:A:5:THR:O	1:A:9:ILE:HG23	0.71	1.86	16	7
1:A:28:THR:HA	1:A:62:THR:HG23	0.71	1.60	15	2
1:A:16:PHE:CG	1:A:65:PHE:CE2	0.70	2.78	5	10
1:A:8:GLN:OE1	1:A:69:LEU:HD22	0.69	1.88	13	1
1:A:4:LEU:HD12	1:A:4:LEU:O	0.69	1.87	1	3
1:A:44:THR:O	1:A:48:LEU:HD23	0.68	1.87	14	9
1:A:21:LYS:HZ3	1:A:34:THR:HG21	0.67	1.49	10	1
1:A:75:LYS:O	1:A:79:THR:HG23	0.66	1.89	17	1
1:A:32:LEU:HD13	1:A:63:ILE:HD12	0.66	1.66	17	1
1:A:21:LYS:HD3	1:A:34:THR:HG21	0.66	1.68	8	1
1:A:19:PHE:HA	1:A:35:VAL:HG21	0.64	1.68	10	13
1:A:20:ASP:HB2	1:A:27:ILE:HD11	0.64	1.67	10	1
1:A:32:LEU:HD21	1:A:48:LEU:HD12	0.64	1.69	11	4
1:A:21:LYS:NZ	1:A:35:VAL:HG23	0.64	2.08	11	1
1:A:21:LYS:CD	1:A:34:THR:HG21	0.63	2.23	8	1
1:A:36:MET:HA	1:A:39:LEU:HD12	0.63	1.68	11	1
1:A:32:LEU:HD23	1:A:32:LEU:O	0.63	1.92	14	7
1:A:32:LEU:HD23	1:A:32:LEU:C	0.63	2.14	14	2
1:A:4:LEU:HD12	1:A:8:GLN:HB2	0.62	1.71	18	2
1:A:27:ILE:HG22	1:A:27:ILE:O	0.62	1.93	2	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:HD12	1:A:8:GLN:HB3	0.62	1.72	13	1
1:A:32:LEU:CD2	1:A:48:LEU:HD12	0.62	2.25	11	3
1:A:19:PHE:CE1	1:A:35:VAL:CG1	0.62	2.82	15	1
1:A:4:LEU:HD13	1:A:4:LEU:N	0.61	2.10	4	2
1:A:16:PHE:CB	1:A:65:PHE:CZ	0.61	2.84	5	8
1:A:19:PHE:CE2	1:A:68:PHE:CD2	0.61	2.89	3	3
1:A:4:LEU:HD22	1:A:4:LEU:C	0.61	2.15	3	3
1:A:26:THR:HB	1:A:62:THR:HG21	0.60	1.73	19	1
1:A:4:LEU:HD12	1:A:8:GLN:CD	0.60	2.16	2	1
1:A:69:LEU:HD12	1:A:69:LEU:O	0.60	1.96	7	3
1:A:21:LYS:HE2	1:A:35:VAL:HG23	0.60	1.74	17	2
1:A:68:PHE:CE1	1:A:71:MET:SD	0.60	2.95	5	1
1:A:55:VAL:HG11	1:A:71:MET:HG3	0.60	1.73	8	4
1:A:69:LEU:HD12	1:A:69:LEU:C	0.60	2.17	7	1
1:A:29:THR:HG22	1:A:52:ILE:HG12	0.60	1.74	12	3
1:A:76:MET:HA	1:A:79:THR:HG22	0.59	1.74	7	9
1:A:52:ILE:HG22	1:A:63:ILE:CD1	0.59	2.27	1	2
1:A:32:LEU:C	1:A:32:LEU:HD13	0.59	2.18	5	4
1:A:65:PHE:N	1:A:66:PRO:CD	0.58	2.65	19	20
1:A:75:LYS:O	1:A:79:THR:HG22	0.58	1.97	10	2
1:A:52:ILE:HG22	1:A:63:ILE:HG13	0.58	1.76	20	2
1:A:4:LEU:HD22	1:A:4:LEU:O	0.58	1.99	11	3
1:A:32:LEU:HD13	1:A:63:ILE:CD1	0.58	2.28	17	1
1:A:27:ILE:N	1:A:27:ILE:HD12	0.57	2.14	20	6
1:A:19:PHE:CE2	1:A:68:PHE:CE2	0.57	2.93	10	2
1:A:21:LYS:HE2	1:A:35:VAL:HG22	0.57	1.77	4	2
1:A:7:GLU:O	1:A:10:ALA:HB3	0.57	2.00	15	5
1:A:8:GLN:CG	1:A:12:PHE:CE2	0.55	2.89	6	2
1:A:16:PHE:CZ	1:A:20:ASP:OD2	0.55	2.60	5	2
1:A:19:PHE:HD1	1:A:35:VAL:HG21	0.55	1.62	19	2
1:A:48:LEU:HD13	1:A:51:MET:SD	0.55	2.42	9	1
1:A:42:ASN:N	1:A:43:PRO:HD3	0.55	2.17	14	14
1:A:18:LEU:O	1:A:21:LYS:CE	0.55	2.54	11	4
1:A:32:LEU:C	1:A:32:LEU:CD2	0.54	2.76	8	10
1:A:21:LYS:CE	1:A:35:VAL:HG22	0.54	2.31	4	3
1:A:9:ILE:HD11	1:A:69:LEU:HD11	0.54	1.80	13	1
1:A:16:PHE:O	1:A:20:ASP:CB	0.53	2.56	10	3
1:A:16:PHE:CE1	1:A:20:ASP:OD2	0.53	2.61	15	2
1:A:5:THR:O	1:A:9:ILE:CG1	0.53	2.57	19	11
1:A:68:PHE:CD1	1:A:68:PHE:C	0.53	2.81	15	2
1:A:16:PHE:HB2	1:A:65:PHE:CZ	0.53	2.38	8	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:CD2	1:A:68:PHE:CE2	0.52	2.97	16	1
1:A:8:GLN:HG3	1:A:12:PHE:CZ	0.52	2.39	15	2
1:A:29:THR:HA	1:A:52:ILE:HG21	0.52	1.82	7	6
1:A:8:GLN:HG3	1:A:12:PHE:CE2	0.52	2.40	6	2
1:A:32:LEU:HD22	1:A:63:ILE:HD11	0.52	1.81	17	3
1:A:32:LEU:HD11	1:A:48:LEU:CD1	0.52	2.34	7	2
1:A:63:ILE:HG22	1:A:64:ASP:H	0.51	1.65	10	8
1:A:19:PHE:CD2	1:A:27:ILE:HG12	0.51	2.41	13	2
1:A:19:PHE:CZ	1:A:68:PHE:CE2	0.51	2.98	13	1
1:A:28:THR:O	1:A:31:GLU:N	0.51	2.43	9	10
1:A:25:GLY:O	1:A:26:THR:CG2	0.51	2.58	20	5
1:A:63:ILE:HG22	1:A:64:ASP:N	0.51	2.20	7	13
1:A:8:GLN:CG	1:A:12:PHE:CZ	0.51	2.93	15	1
1:A:65:PHE:CB	1:A:66:PRO:HD3	0.51	2.36	3	18
1:A:4:LEU:C	1:A:4:LEU:HD12	0.51	2.26	9	1
1:A:52:ILE:HG22	1:A:63:ILE:CG1	0.51	2.34	1	4
1:A:4:LEU:O	1:A:4:LEU:CD2	0.51	2.59	4	1
1:A:4:LEU:O	1:A:8:GLN:CB	0.51	2.59	18	1
1:A:4:LEU:N	1:A:4:LEU:CD1	0.51	2.73	4	1
1:A:19:PHE:CD1	1:A:68:PHE:CE2	0.51	2.98	3	2
1:A:28:THR:HG21	1:A:30:LYS:HE3	0.51	1.83	6	1
1:A:27:ILE:CD1	1:A:31:GLU:OE2	0.51	2.59	17	1
1:A:52:ILE:HD12	1:A:52:ILE:C	0.50	2.27	2	2
1:A:32:LEU:CD1	1:A:63:ILE:HD11	0.50	2.31	4	2
1:A:35:VAL:CG1	1:A:36:MET:N	0.50	2.75	14	3
1:A:63:ILE:HG21	1:A:68:PHE:CD1	0.50	2.41	9	5
1:A:4:LEU:HD11	1:A:8:GLN:HG2	0.50	1.82	17	1
1:A:55:VAL:HG11	1:A:71:MET:CG	0.50	2.37	7	2
1:A:69:LEU:C	1:A:69:LEU:HD12	0.50	2.27	15	3
1:A:16:PHE:CD2	1:A:65:PHE:CZ	0.50	3.00	5	2
1:A:4:LEU:C	1:A:4:LEU:CD1	0.50	2.78	10	4
1:A:21:LYS:HG3	1:A:34:THR:HG21	0.50	1.83	14	2
1:A:52:ILE:CD1	1:A:53:ASN:N	0.50	2.70	17	4
1:A:19:PHE:CE1	1:A:68:PHE:CD2	0.49	3.00	3	1
1:A:16:PHE:HB2	1:A:65:PHE:CE1	0.49	2.43	5	3
1:A:19:PHE:CZ	1:A:27:ILE:HG21	0.49	2.42	3	2
1:A:72:MET:O	1:A:75:LYS:CB	0.49	2.61	13	4
1:A:19:PHE:CD2	1:A:35:VAL:HG11	0.49	2.43	16	1
1:A:20:ASP:OD2	1:A:25:GLY:CA	0.49	2.60	8	1
1:A:8:GLN:O	1:A:12:PHE:CD2	0.48	2.66	5	1
1:A:33:GLY:O	1:A:37:ARG:CG	0.48	2.61	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:THR:CG2	1:A:62:THR:CG2	0.48	2.91	16	1
1:A:27:ILE:HD13	1:A:31:GLU:OE2	0.48	2.08	17	1
1:A:4:LEU:HD13	1:A:7:GLU:OE2	0.48	2.07	1	1
1:A:63:ILE:C	1:A:64:ASP:OD1	0.48	2.52	15	3
1:A:15:ALA:HB1	1:A:19:PHE:CD2	0.48	2.43	4	1
1:A:16:PHE:CZ	1:A:27:ILE:HD13	0.48	2.42	16	1
1:A:64:ASP:CB	1:A:66:PRO:HD2	0.48	2.39	19	4
1:A:19:PHE:CD1	1:A:35:VAL:HG11	0.48	2.43	15	3
1:A:22:ASP:OD1	1:A:23:GLY:N	0.48	2.47	19	3
1:A:35:VAL:HG13	1:A:36:MET:N	0.48	2.24	16	3
1:A:55:VAL:CG1	1:A:71:MET:SD	0.48	3.01	14	2
1:A:4:LEU:O	1:A:7:GLU:N	0.47	2.48	13	2
1:A:4:LEU:O	1:A:5:THR:C	0.47	2.53	13	4
1:A:19:PHE:CZ	1:A:68:PHE:CD1	0.47	3.02	13	1
1:A:26:THR:HG22	1:A:62:THR:CG2	0.47	2.39	4	1
1:A:32:LEU:CD1	1:A:48:LEU:HD12	0.47	2.36	7	1
1:A:19:PHE:CZ	1:A:35:VAL:CG1	0.47	2.94	15	1
1:A:15:ALA:CB	1:A:19:PHE:CE2	0.47	2.94	12	2
1:A:4:LEU:O	1:A:6:GLU:N	0.47	2.48	15	4
1:A:5:THR:O	1:A:9:ILE:CG2	0.47	2.61	2	4
1:A:60:ASP:OD1	1:A:62:THR:N	0.47	2.48	9	3
1:A:12:PHE:CE2	1:A:69:LEU:HA	0.47	2.44	5	1
1:A:65:PHE:N	1:A:66:PRO:HD2	0.47	2.24	19	7
1:A:8:GLN:HB3	1:A:12:PHE:CE2	0.47	2.45	10	1
1:A:57:ALA:O	1:A:58:ASP:C	0.47	2.54	13	7
1:A:26:THR:HG23	1:A:64:ASP:OD1	0.47	2.10	1	1
1:A:8:GLN:HG3	1:A:12:PHE:CE1	0.47	2.45	16	1
1:A:63:ILE:CG2	1:A:64:ASP:N	0.47	2.78	11	4
1:A:26:THR:CG2	1:A:62:THR:HG21	0.46	2.40	8	2
1:A:12:PHE:HA	1:A:15:ALA:HB3	0.46	1.85	16	2
1:A:30:LYS:O	1:A:34:THR:N	0.46	2.47	16	1
1:A:12:PHE:CZ	1:A:69:LEU:HA	0.46	2.45	3	1
1:A:26:THR:C	1:A:27:ILE:HD12	0.46	2.31	16	3
1:A:65:PHE:HB3	1:A:66:PRO:HD3	0.46	1.87	19	3
1:A:15:ALA:O	1:A:18:LEU:N	0.46	2.48	19	9
1:A:43:PRO:HB2	1:A:48:LEU:HD21	0.46	1.87	10	3
1:A:60:ASP:OD1	1:A:61:GLY:N	0.46	2.49	17	2
1:A:32:LEU:HD22	1:A:52:ILE:CG2	0.46	2.41	19	1
1:A:37:ARG:O	1:A:40:GLY:N	0.46	2.49	13	6
1:A:28:THR:N	1:A:31:GLU:OE1	0.46	2.49	5	1
1:A:27:ILE:O	1:A:27:ILE:CG2	0.46	2.64	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ALA:O	1:A:49:GLN:CB	0.46	2.64	7	4
1:A:29:THR:HG22	1:A:52:ILE:CG1	0.46	2.41	12	1
1:A:57:ALA:O	1:A:59:GLY:N	0.46	2.49	13	4
1:A:15:ALA:O	1:A:17:SER:N	0.46	2.49	5	1
1:A:68:PHE:O	1:A:71:MET:N	0.46	2.49	14	5
1:A:52:ILE:O	1:A:56:ASP:CB	0.46	2.64	10	1
1:A:52:ILE:CD1	1:A:61:GLY:O	0.46	2.58	14	1
1:A:4:LEU:C	1:A:6:GLU:N	0.45	2.69	15	7
1:A:15:ALA:O	1:A:16:PHE:C	0.45	2.54	13	12
1:A:69:LEU:O	1:A:72:MET:CE	0.45	2.64	3	1
1:A:42:ASN:N	1:A:43:PRO:CD	0.45	2.78	14	4
1:A:21:LYS:CE	1:A:34:THR:HG21	0.45	2.41	10	1
1:A:6:GLU:CG	1:A:7:GLU:N	0.45	2.79	14	1
1:A:55:VAL:CG2	1:A:56:ASP:N	0.45	2.79	9	3
1:A:72:MET:SD	1:A:73:ALA:N	0.45	2.89	3	1
1:A:20:ASP:O	1:A:23:GLY:N	0.45	2.50	5	1
1:A:5:THR:HG23	1:A:9:ILE:HG23	0.45	1.89	12	1
1:A:8:GLN:NE2	1:A:72:MET:SD	0.45	2.90	9	2
1:A:66:PRO:O	1:A:67:GLU:C	0.44	2.54	7	1
1:A:57:ALA:N	1:A:67:GLU:OE2	0.44	2.49	15	1
1:A:60:ASP:CG	1:A:61:GLY:N	0.44	2.70	19	1
1:A:21:LYS:CD	1:A:34:THR:CG2	0.44	2.95	8	1
1:A:41:GLN:O	1:A:42:ASN:ND2	0.44	2.50	12	1
1:A:48:LEU:O	1:A:51:MET:N	0.44	2.50	15	2
1:A:55:VAL:HG23	1:A:56:ASP:N	0.44	2.28	12	3
1:A:19:PHE:CD2	1:A:68:PHE:CD2	0.44	3.06	10	1
1:A:30:LYS:CG	1:A:31:GLU:N	0.44	2.81	10	1
1:A:4:LEU:CD1	1:A:5:THR:N	0.44	2.74	12	1
1:A:56:ASP:OD1	1:A:59:GLY:N	0.44	2.49	12	2
1:A:8:GLN:OE1	1:A:12:PHE:CG	0.44	2.71	8	1
1:A:21:LYS:NZ	1:A:35:VAL:HG22	0.44	2.28	8	1
1:A:5:THR:HG23	1:A:9:ILE:CG2	0.44	2.42	12	1
1:A:55:VAL:HG11	1:A:71:MET:SD	0.44	2.53	13	1
1:A:64:ASP:OD1	1:A:65:PHE:N	0.44	2.49	5	2
1:A:35:VAL:O	1:A:36:MET:C	0.44	2.56	8	2
1:A:76:MET:O	1:A:79:THR:HG22	0.44	2.13	9	1
1:A:4:LEU:C	1:A:4:LEU:CD2	0.44	2.86	3	1
1:A:29:THR:HG22	1:A:52:ILE:HG21	0.44	1.90	8	1
1:A:72:MET:O	1:A:75:LYS:N	0.44	2.50	2	3
1:A:73:ALA:O	1:A:76:MET:CG	0.44	2.66	4	4
1:A:64:ASP:O	1:A:68:PHE:CB	0.44	2.65	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:CE1	1:A:27:ILE:HG21	0.44	2.48	13	1
1:A:18:LEU:O	1:A:21:LYS:NZ	0.44	2.51	18	3
1:A:19:PHE:O	1:A:31:GLU:OE2	0.44	2.36	17	1
1:A:37:ARG:C	1:A:39:LEU:N	0.43	2.70	8	3
1:A:58:ASP:OD1	1:A:60:ASP:OD2	0.43	2.36	20	2
1:A:8:GLN:OE1	1:A:69:LEU:CD2	0.43	2.63	13	1
1:A:57:ALA:C	1:A:59:GLY:N	0.43	2.70	15	8
1:A:12:PHE:O	1:A:16:PHE:CB	0.43	2.66	5	1
1:A:37:ARG:O	1:A:39:LEU:N	0.43	2.52	8	3
1:A:25:GLY:C	1:A:26:THR:HG23	0.43	2.33	7	2
1:A:64:ASP:N	1:A:67:GLU:OE1	0.43	2.49	19	1
1:A:58:ASP:OD1	1:A:58:ASP:C	0.43	2.56	20	1
1:A:22:ASP:OD2	1:A:24:ASP:OD1	0.43	2.36	1	1
1:A:59:GLY:C	1:A:60:ASP:OD1	0.43	2.57	20	5
1:A:68:PHE:O	1:A:69:LEU:C	0.43	2.57	10	4
1:A:16:PHE:O	1:A:17:SER:C	0.43	2.57	6	3
1:A:4:LEU:O	1:A:8:GLN:N	0.43	2.49	13	1
1:A:20:ASP:O	1:A:21:LYS:C	0.42	2.57	5	1
1:A:28:THR:O	1:A:29:THR:C	0.42	2.58	16	3
1:A:16:PHE:CE1	1:A:27:ILE:HD11	0.42	2.49	2	1
1:A:12:PHE:O	1:A:15:ALA:N	0.42	2.52	10	1
1:A:58:ASP:OD2	1:A:60:ASP:OD1	0.42	2.37	20	2
1:A:19:PHE:O	1:A:27:ILE:HD12	0.42	2.14	17	1
1:A:24:ASP:OD1	1:A:25:GLY:N	0.42	2.52	20	1
1:A:58:ASP:CG	1:A:60:ASP:OD1	0.42	2.58	20	3
1:A:21:LYS:CE	1:A:35:VAL:CG2	0.42	2.95	11	1
1:A:65:PHE:CB	1:A:66:PRO:CD	0.42	2.98	3	2
1:A:8:GLN:O	1:A:9:ILE:C	0.42	2.59	4	1
1:A:56:ASP:OD1	1:A:58:ASP:OD1	0.42	2.38	5	3
1:A:75:LYS:HA	1:A:75:LYS:CE	0.42	2.45	18	1
1:A:58:ASP:OD2	1:A:67:GLU:OE1	0.41	2.38	3	1
1:A:15:ALA:C	1:A:17:SER:N	0.41	2.73	5	1
1:A:40:GLY:O	1:A:41:GLN:O	0.41	2.37	9	3
1:A:58:ASP:OD1	1:A:67:GLU:OE2	0.41	2.37	11	3
1:A:36:MET:HB3	1:A:43:PRO:CG	0.41	2.46	2	1
1:A:35:VAL:O	1:A:38:SER:N	0.41	2.53	10	2
1:A:27:ILE:N	1:A:27:ILE:CD1	0.41	2.82	20	2
1:A:60:ASP:OD1	1:A:60:ASP:N	0.41	2.54	20	1
1:A:76:MET:HG3	1:A:77:LYS:N	0.41	2.30	1	2
1:A:21:LYS:HE2	1:A:35:VAL:CG2	0.41	2.46	12	2
1:A:8:GLN:CG	1:A:9:ILE:N	0.41	2.83	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:ILE:O	1:A:64:ASP:OD1	0.41	2.38	20	2
1:A:58:ASP:CG	1:A:60:ASP:OD2	0.41	2.59	9	1
1:A:8:GLN:HG3	1:A:9:ILE:N	0.41	2.30	13	1
1:A:22:ASP:OD1	1:A:31:GLU:OE1	0.41	2.38	19	1
1:A:63:ILE:O	1:A:64:ASP:CG	0.41	2.59	1	1
1:A:29:THR:CG2	1:A:61:GLY:O	0.41	2.68	17	1
1:A:58:ASP:OD1	1:A:60:ASP:CG	0.41	2.59	20	1
1:A:58:ASP:OD2	1:A:60:ASP:OD2	0.41	2.38	2	2
1:A:15:ALA:CB	1:A:19:PHE:CZ	0.41	3.01	11	1
1:A:44:THR:O	1:A:48:LEU:CD2	0.41	2.64	14	1
1:A:62:THR:HG22	1:A:63:ILE:N	0.41	2.31	14	1
1:A:24:ASP:OD2	1:A:26:THR:OG1	0.41	2.38	5	1
1:A:59:GLY:O	1:A:60:ASP:OD1	0.41	2.38	11	2
1:A:35:VAL:O	1:A:38:SER:CB	0.41	2.69	12	1
1:A:21:LYS:CG	1:A:31:GLU:HG3	0.41	2.46	17	1
1:A:24:ASP:OD1	1:A:24:ASP:N	0.41	2.53	3	1
1:A:24:ASP:OD1	1:A:26:THR:OG1	0.41	2.39	5	1
1:A:14:GLU:O	1:A:15:ALA:C	0.41	2.58	6	1
1:A:59:GLY:O	1:A:60:ASP:CB	0.41	2.69	19	2
1:A:37:ARG:HG3	1:A:38:SER:N	0.41	2.30	15	1
1:A:64:ASP:OD1	1:A:67:GLU:OE1	0.41	2.38	15	1
1:A:22:ASP:CG	1:A:31:GLU:OE2	0.41	2.59	19	1
1:A:60:ASP:OD2	1:A:62:THR:N	0.41	2.52	19	1
1:A:59:GLY:C	1:A:60:ASP:CG	0.41	2.80	20	1
1:A:63:ILE:HG21	1:A:68:PHE:HD1	0.40	1.76	9	1
1:A:21:LYS:O	1:A:22:ASP:C	0.40	2.59	15	1
1:A:19:PHE:HA	1:A:35:VAL:CG2	0.40	2.46	17	1
1:A:20:ASP:OD2	1:A:25:GLY:C	0.40	2.60	8	1
1:A:58:ASP:OD1	1:A:59:GLY:O	0.40	2.39	14	1
1:A:19:PHE:CE2	1:A:35:VAL:HG11	0.40	2.51	15	1
1:A:69:LEU:C	1:A:69:LEU:CD1	0.40	2.87	7	1
1:A:58:ASP:N	1:A:58:ASP:OD1	0.40	2.53	18	1
1:A:8:GLN:OE1	1:A:12:PHE:CD2	0.40	2.74	8	1
1:A:64:ASP:O	1:A:68:PHE:HB2	0.40	2.17	11	1
1:A:55:VAL:CG1	1:A:71:MET:HB2	0.40	2.47	12	1
1:A:58:ASP:OD1	1:A:67:GLU:CD	0.40	2.60	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	75/79 (95%)	61±2 (81±3%)	12±3 (16±4%)	3±1 (3±1%)	6 35
All	All	1500/1580 (95%)	1212 (81%)	236 (16%)	52 (3%)	6 35

All 9 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	60	ASP	18
1	A	4	LEU	13
1	A	41	GLN	8
1	A	40	GLY	7
1	A	5	THR	2
1	A	16	PHE	1
1	A	22	ASP	1
1	A	66	PRO	1
1	A	56	ASP	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	65/67 (97%)	49±4 (75±6%)	16±4 (25±6%)	2 25
All	All	1300/1340 (97%)	980 (75%)	320 (25%)	2 25

All 45 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	75	LYS	20

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Mol	Chain	Res	Type	Models (Total)
1	A	65	PHE	19
1	A	69	LEU	19
1	A	4	LEU	17
1	A	72	MET	15
1	A	13	LYS	14
1	A	77	LYS	13
1	A	38	SER	13
1	A	60	ASP	13
1	A	58	ASP	12
1	A	76	MET	12
1	A	51	MET	11
1	A	12	PHE	10
1	A	42	ASN	10
1	A	78	ASP	10
1	A	45	GLU	9
1	A	24	ASP	7
1	A	37	ARG	7
1	A	41	GLN	7
1	A	71	MET	6
1	A	14	GLU	6
1	A	30	LYS	6
1	A	54	GLU	5
1	A	74	ARG	5
1	A	68	PHE	5
1	A	7	GLU	5
1	A	44	THR	5
1	A	8	GLN	4
1	A	32	LEU	4
1	A	47	GLU	4
1	A	21	LYS	4
1	A	5	THR	4
1	A	17	SER	3
1	A	22	ASP	3
1	A	53	ASN	2
1	A	19	PHE	2
1	A	50	ASP	1
1	A	31	GLU	1
1	A	63	ILE	1
1	A	26	THR	1
1	A	6	GLU	1
1	A	11	GLU	1
1	A	16	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	20	ASP	1
1	A	9	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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided