Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 11:14 AM EDT

PDB ID	:	2UWQ
Title	:	Solution structure of ASPP2 N-terminus
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Deposited on	:	2007-03-22

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

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

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

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

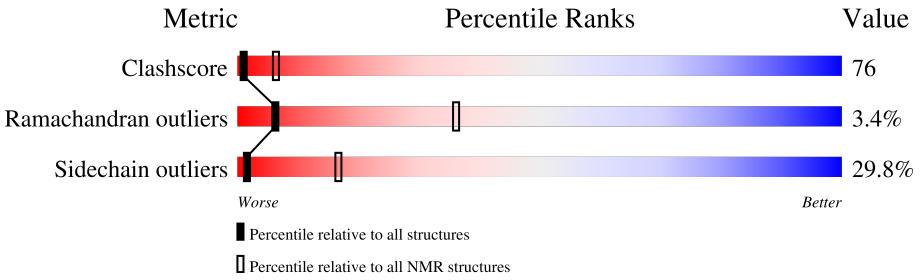
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	86	24% 44% 10% • 20%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 19 as representative.

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:10, A:14-A:36, A:43-A:81 (69)	0.39	10

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1354 atoms, of which 658 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called APOPTOSIS-STIMULATING OF P53 PROTEIN 2.

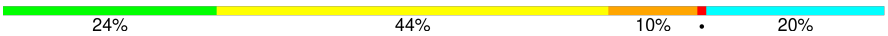
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	86	1354	432	658	122	134	8	0

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: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

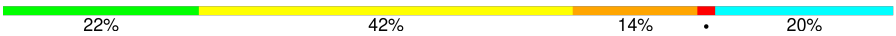
Chain A: 

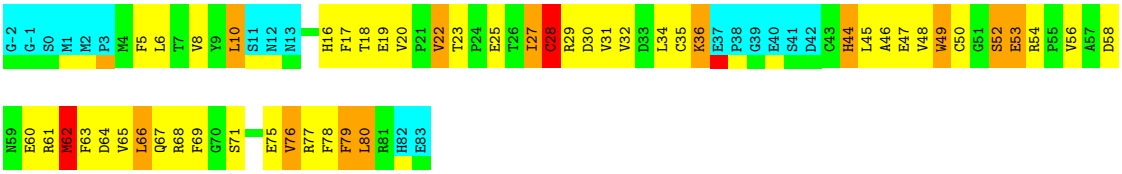
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

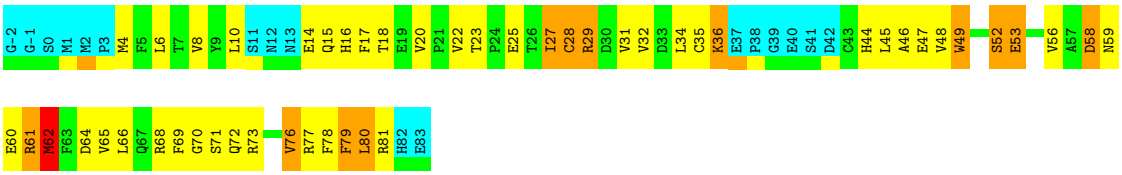
Chain A: 



4.2.2 Score per residue for model 2

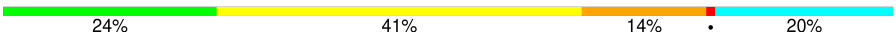
• Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

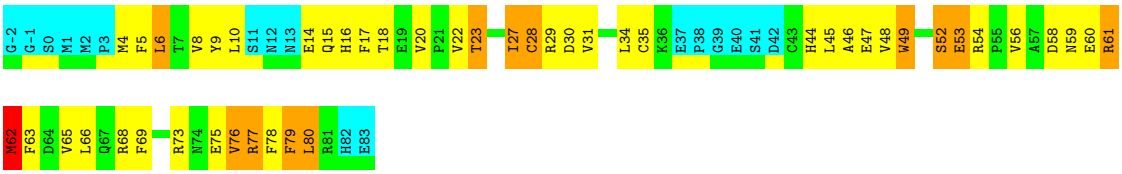
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

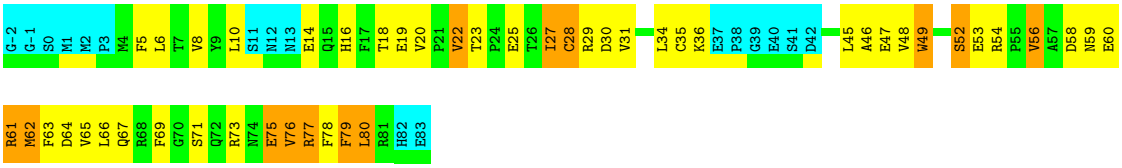
Chain A: 



4.2.4 Score per residue for model 4

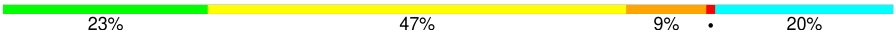
- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

Chain A: 

4.2.6 Score per residue for model 6

- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

Chain A: 26% 38% 15% • 20%

G-2 G-1 S0 M1 M2 P3 M4 F5 L6 T7 V8 Y9 L10 S11 N12 N13 E14 Q15 H16 F17 T18 E19 V20 P21 V22 T23 I27 C28 R29 D30 V31 L34 C35 K36 E37 P38 G39 E40 S41 D42 C43 H44 L45 A46 E47 V48 W49 S52 E53 R54 P55 V56 A57 D58 N59 E60 R61

M62 F63 D64 V65 L66 Q67 R68 F69 R73 N74 E75 V76 R77 F78 F79 L80 R81 H82 E83

4.2.7 Score per residue for model 7

- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

Chain A: 22% 41% 16% • 20%

G-2 G-1 S0 M1 M2 P3 M4 F5 L6 T7 V8 Y9 L10 S11 N12 N13 E14 Q15 H16 F17 T18 E19 V20 P21 V22 E25 T26 I27 C28 R29 D30 V31 V32 D33 L34 C35 K36 E37 P38 G39 E40 S41 D42 C43 H44 L45 A46 E47 V48 W49 C50 G51 S52 E53 R54 P55 V56 A57 D58

N59 E60 R61 M62 F63 D64 V65 L66 Q67 R68 F69 R73 N74 E75 V76 R77 F78 F79 L80 R81 H82 E83

4.2.8 Score per residue for model 8

- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

Chain A: 24% 38% 16% • 20%

G-2 G-1 S0 M1 M2 P3 L6 T7 V8 Y9 L10 S11 N12 N13 E14 Q15 H16 F17 T18 E19 V20 P21 V22 T23 P24 E25 T26 I27 C28 R29 D30 V31 V32 D33 L34 C35 K36 E37 P38 G39 E40 S41 D42 C43 H44 L45 A46 E47 V48 W49 S52 E53 R54 P55 V56 A57 D58 N59

E60 R61 M62 F63 D64 V65 L66 Q67 R68 F69 Q72 E75 V76 R77 F78 F79 L80 R81 H82 E83

4.2.9 Score per residue for model 9

- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

Chain A: 20% 47% 13% • 20%

G-2 G-1 S0 M1 M2 P3 L6 T7 V8 Y9 L10 S11 N12 N13 E14 Q15 H16 F17 T18 E19 V20 P21 V22 E25 T26 I27 C28 R29 D30 V31 V32 D33 L34 C35 K36 E37 P38 G39 E40 S41 D42 C43 H44 L45 A46 E47 V48 W49 C50 G51 S52 E53 R54 P55 V56 A57 D58 N59

E60 R61 M62 F63 D64 V65 L66 Q67 R68 F69 G70 S71 Q72 R73 N74 E75 V76 R77 F78 F79 L80 R81 H82 E83

4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

Chain A: 29% 34% 17% 20%

G-2 G-1 S0 M1 M2 P3 M4 F5 L6 T7 V8 Y9 L10 S11 N12 N13 E14 Q15 H16 F17 T18 E19 V20 P21 V22 T23 I27 C28 R29 D30 V31 V32 D33 L34 C35 K36 E37 P38 G39 E40 S41 D42 C43 H44 L45 A46 E47 V48 W49 S52 V56 A57 D58 N59 E60 R61 M62

F63 D64 V65 L66 Q67 R68 F69 Q72 E75 V76 R77 F78 F79 L80 R81 H82 E83

4.2.11 Score per residue for model 11

- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

Chain A: 23% 44% 12% • 20%

G-2 G-1 S0 M1 M2 P3 L6 T7 V8 Y9 L10 S11 N12 N13 H16 F17 T18 E19 V20 P21 V22 T23 P24 I27 C28 R29 D30 V31 V32 D33 L34 C35 K36 E37 P38 G39 E40 S41 D42 C43 H44 L45 A46 E47 V48 W49 C50 G51 S52 E53 R54 P55 V56 A57 D58 N59 E60

R61 M62 F63 D64 V65 L66 Q67 R68 F69 R73 N74 E75 V76 R77 F78 F79 L80 R81 H82 E83

4.2.12 Score per residue for model 12

- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

Chain A: 28% 34% 17% • 20%

G-2 G-1 S0 M1 M2 P3 L6 T7 V8 Y9 L10 S11 N12 N13 E14 Q15 H16 F17 T18 E19 V20 P21 V22 I27 C28 R29 D30 V31 L34 C35 K36 E37 P38 G39 E40 S41 D42 C43 H44 L45 A46 E47 V48 W49 S52 E53 V56 A57 D58 N59 E60 R61 M62 F63 D64

V65 L66 Q67 R68 F69 Q72 R73 N74 E75 V76 R77 F78 F79 L80 R81 H82 E83

4.2.13 Score per residue for model 13

- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

Chain A: 24% 41% 14% • 20%

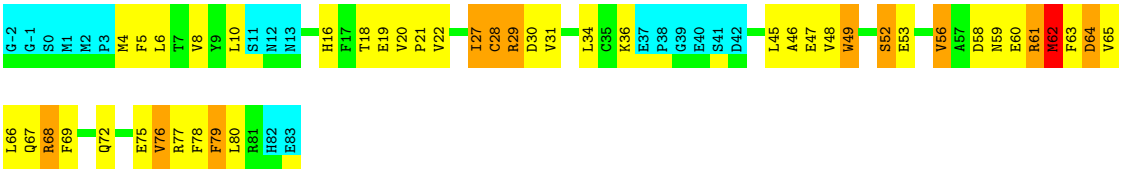
G-2 G-1 S0 M1 M2 P3 M4 F5 L6 T7 V8 Y9 L10 S11 N12 N13 H16 F17 T18 E19 V20 P21 V22 T23 P24 I27 C28 R29 D30 V31 L34 C35 K36 E37 P38 G39 E40 S41 D42 C43 H44 L45 A46 E47 V48 W49 S52 E53 R54 P55 V56 A57 D58 N59 E60 R61

M62 F63 D64 V65 L66 Q67 R68 F69 Q72 R73 N74 E75 V76 R77 F78 F79 L80 R81 H82 E83

4.2.14 Score per residue for model 14

- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

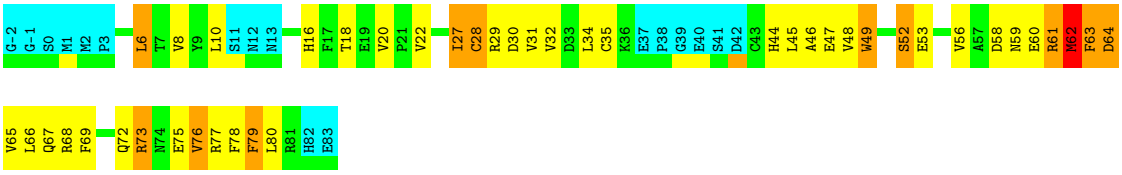
Chain A: 28% 38% 13% • 20%



4.2.15 Score per residue for model 15

- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

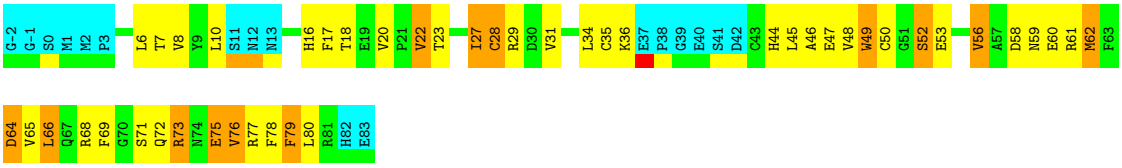
Chain A: 29% 37% 13% • 20%



4.2.16 Score per residue for model 16

- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

Chain A: 27% 38% 15% 20%



4.2.17 Score per residue for model 17

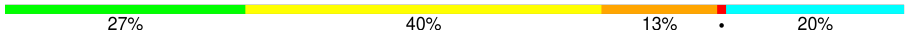
- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

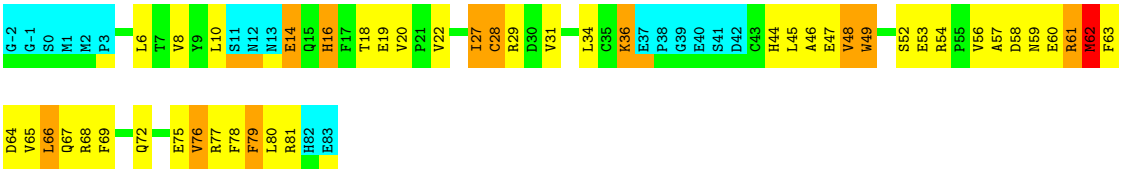
Chain A: 22% 38% 19% • 20%

4.2.18 Score per residue for model 18

- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

Chain A:





4.2.19 Score per residue for model 19

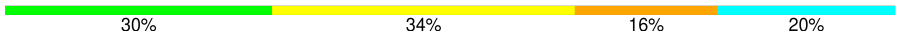
- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

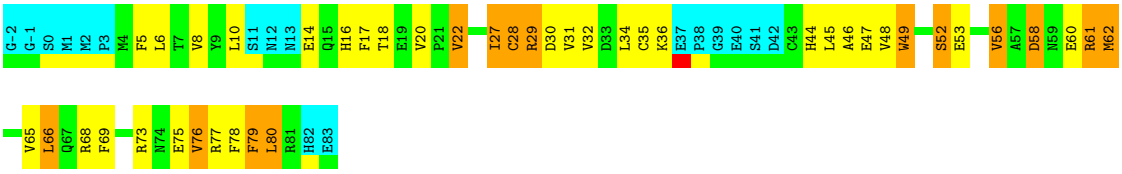
Chain A:

4.2.20 Score per residue for model 20

- Molecule 1: APOPTOSIS-STIMULATING OF P53 PROTEIN 2

Chain A:





5 Refinement protocol and experimental data overview (i)

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

Of the 90 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY, NO VIOLATIONS*.

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

Software name	Classification	Version
CNS	refinement	
CNS	structure solution	

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	574	558	556	86±5
All	All	11480	11160	11120	1717

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 76.

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:VAL:HG11	1:A:45:LEU:HD22	0.95	1.34	2	18
1:A:6:LEU:HD21	1:A:31:VAL:HG22	0.92	1.41	9	7
1:A:10:LEU:HD13	1:A:16:HIS:CD2	0.88	2.03	13	6
1:A:49:TRP:HB2	1:A:76:VAL:HA	0.86	1.48	3	20
1:A:6:LEU:HD22	1:A:78:PHE:CE1	0.86	2.05	10	9
1:A:6:LEU:HD22	1:A:78:PHE:CE2	0.86	2.06	4	3
1:A:6:LEU:HD11	1:A:31:VAL:HG22	0.84	1.48	8	9
1:A:31:VAL:CG1	1:A:45:LEU:HD13	0.83	2.03	12	11
1:A:45:LEU:HD23	1:A:56:VAL:HG21	0.83	1.50	10	16
1:A:10:LEU:HD22	1:A:16:HIS:CE1	0.82	2.10	13	5
1:A:6:LEU:HD13	1:A:78:PHE:CD2	0.82	2.10	4	3
1:A:8:VAL:HG21	1:A:31:VAL:HA	0.82	1.49	9	14
1:A:45:LEU:HD22	1:A:79:PHE:O	0.81	1.74	1	1
1:A:10:LEU:HD13	1:A:16:HIS:CE1	0.81	2.10	12	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:MET:CE	1:A:66:LEU:HD22	0.80	2.05	1	5
1:A:48:VAL:HG23	1:A:53:GLU:CB	0.79	2.08	18	1
1:A:20:VAL:HG11	1:A:30:ASP:HB3	0.78	1.55	15	6
1:A:47:GLU:HG2	1:A:56:VAL:HG12	0.78	1.56	7	8
1:A:69:PHE:CZ	1:A:76:VAL:HG21	0.78	2.13	6	20
1:A:45:LEU:HD12	1:A:79:PHE:O	0.78	1.79	7	12
1:A:27:ILE:HG22	1:A:61:ARG:CA	0.78	2.08	2	14
1:A:20:VAL:HG21	1:A:30:ASP:CB	0.77	2.09	11	5
1:A:6:LEU:HD12	1:A:78:PHE:CG	0.77	2.14	6	5
1:A:48:VAL:HG23	1:A:79:PHE:CE1	0.76	2.14	15	6
1:A:6:LEU:HD23	1:A:6:LEU:O	0.76	1.80	15	3
1:A:20:VAL:HG21	1:A:30:ASP:HB2	0.76	1.55	1	3
1:A:60:GLU:HB3	1:A:65:VAL:HG22	0.76	1.56	19	16
1:A:6:LEU:HD13	1:A:78:PHE:CD1	0.75	2.17	18	8
1:A:18:THR:HG21	1:A:34:LEU:HB3	0.75	1.58	17	20
1:A:27:ILE:HG22	1:A:61:ARG:HA	0.75	1.58	8	18
1:A:6:LEU:HD12	1:A:78:PHE:CD2	0.75	2.17	17	5
1:A:45:LEU:O	1:A:56:VAL:HG13	0.74	1.82	14	19
1:A:45:LEU:HD21	1:A:78:PHE:CD1	0.74	2.17	12	11
1:A:62:MET:HG2	1:A:63:PHE:H	0.74	1.41	11	1
1:A:10:LEU:HD13	1:A:16:HIS:NE2	0.74	1.98	20	7
1:A:31:VAL:HG11	1:A:45:LEU:CD2	0.73	2.13	3	14
1:A:69:PHE:CE2	1:A:76:VAL:HB	0.73	2.19	1	9
1:A:6:LEU:HD23	1:A:62:MET:SD	0.73	2.24	4	5
1:A:31:VAL:HG11	1:A:45:LEU:HD13	0.72	1.61	16	11
1:A:18:THR:OG1	1:A:34:LEU:HD13	0.72	1.85	12	5
1:A:20:VAL:HG21	1:A:30:ASP:HB3	0.72	1.58	17	8
1:A:69:PHE:CE1	1:A:76:VAL:HB	0.71	2.19	10	11
1:A:49:TRP:CE3	1:A:69:PHE:HD2	0.71	2.03	5	9
1:A:77:ARG:O	1:A:79:PHE:CE2	0.71	2.44	20	12
1:A:6:LEU:HD22	1:A:62:MET:SD	0.70	2.25	15	1
1:A:27:ILE:CD1	1:A:27:ILE:O	0.70	2.39	19	5
1:A:48:VAL:HG23	1:A:79:PHE:CE2	0.70	2.21	7	12
1:A:63:PHE:HA	1:A:66:LEU:HB2	0.70	1.61	4	3
1:A:79:PHE:CD1	1:A:79:PHE:N	0.70	2.59	15	8
1:A:49:TRP:CE3	1:A:69:PHE:HD1	0.70	2.04	18	11
1:A:6:LEU:HD12	1:A:78:PHE:CD1	0.69	2.21	9	4
1:A:8:VAL:CG1	1:A:31:VAL:HG13	0.69	2.18	9	15
1:A:18:THR:HG21	1:A:34:LEU:CB	0.69	2.17	17	11
1:A:79:PHE:N	1:A:79:PHE:CD2	0.69	2.60	9	12
1:A:8:VAL:HG11	1:A:31:VAL:HG13	0.68	1.65	17	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LEU:HD13	1:A:16:HIS:ND1	0.68	2.03	10	3
1:A:45:LEU:HD13	1:A:46:ALA:N	0.68	2.03	1	1
1:A:20:VAL:HG21	1:A:30:ASP:CG	0.67	2.10	11	2
1:A:77:ARG:O	1:A:79:PHE:CE1	0.67	2.47	2	8
1:A:6:LEU:HD11	1:A:30:ASP:OD1	0.67	1.90	1	1
1:A:48:VAL:HG22	1:A:53:GLU:HG3	0.67	1.66	16	2
1:A:31:VAL:HG21	1:A:45:LEU:HD22	0.66	1.67	5	7
1:A:45:LEU:HD11	1:A:78:PHE:HB3	0.66	1.67	9	5
1:A:31:VAL:HG12	1:A:80:LEU:HD23	0.66	1.65	5	3
1:A:10:LEU:HD21	1:A:16:HIS:CE1	0.66	2.26	17	2
1:A:6:LEU:HD12	1:A:6:LEU:O	0.65	1.92	2	10
1:A:69:PHE:CD2	1:A:76:VAL:HB	0.65	2.27	3	3
1:A:5:PHE:O	1:A:66:LEU:HD11	0.65	1.91	3	1
1:A:45:LEU:HD23	1:A:56:VAL:HG11	0.64	1.67	18	1
1:A:28:CYS:CB	1:A:58:ASP:HA	0.64	2.22	5	19
1:A:45:LEU:HD12	1:A:56:VAL:HG21	0.64	1.69	1	1
1:A:27:ILE:HD13	1:A:27:ILE:H	0.63	1.53	5	14
1:A:45:LEU:HD21	1:A:78:PHE:CD2	0.63	2.28	4	3
1:A:27:ILE:O	1:A:27:ILE:HD12	0.63	1.93	20	5
1:A:49:TRP:CB	1:A:76:VAL:HA	0.63	2.24	5	20
1:A:48:VAL:HG13	1:A:53:GLU:HB3	0.63	1.71	3	9
1:A:61:ARG:O	1:A:65:VAL:HG23	0.63	1.94	20	13
1:A:47:GLU:CG	1:A:56:VAL:HG12	0.62	2.22	9	7
1:A:27:ILE:HG22	1:A:61:ARG:N	0.62	2.09	1	4
1:A:66:LEU:HD23	1:A:73:ARG:HB2	0.62	1.70	12	4
1:A:20:VAL:HG11	1:A:30:ASP:CB	0.62	2.25	15	2
1:A:6:LEU:HD22	1:A:62:MET:CE	0.62	2.24	15	1
1:A:48:VAL:HG23	1:A:53:GLU:HB2	0.62	1.71	18	1
1:A:22:VAL:HG13	1:A:62:MET:HG3	0.62	1.72	10	1
1:A:22:VAL:HG13	1:A:62:MET:CG	0.61	2.24	10	1
1:A:62:MET:HE2	1:A:66:LEU:HD11	0.61	1.72	14	1
1:A:6:LEU:HD23	1:A:62:MET:HG2	0.61	1.72	10	1
1:A:31:VAL:HG12	1:A:80:LEU:CD2	0.61	2.26	5	5
1:A:47:GLU:HB2	1:A:69:PHE:CZ	0.61	2.31	17	20
1:A:45:LEU:HD23	1:A:56:VAL:CG2	0.61	2.23	10	9
1:A:57:ALA:HB3	1:A:60:GLU:HG2	0.61	1.71	18	1
1:A:31:VAL:CG1	1:A:45:LEU:HD22	0.60	2.23	3	8
1:A:6:LEU:HD21	1:A:31:VAL:CG2	0.60	2.24	9	2
1:A:62:MET:CE	1:A:66:LEU:HD11	0.60	2.26	4	2
1:A:6:LEU:CD1	1:A:8:VAL:HG22	0.60	2.26	20	6
1:A:48:VAL:HG22	1:A:53:GLU:CG	0.60	2.26	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:MET:HE3	1:A:66:LEU:HD13	0.60	1.72	20	1
1:A:30:ASP:O	1:A:34:LEU:HD12	0.60	1.97	9	2
1:A:8:VAL:HG23	1:A:18:THR:O	0.60	1.97	20	2
1:A:8:VAL:CG2	1:A:31:VAL:HG13	0.60	2.27	2	2
1:A:45:LEU:HB3	1:A:56:VAL:HG22	0.59	1.73	1	11
1:A:30:ASP:O	1:A:34:LEU:HD13	0.59	1.96	8	1
1:A:6:LEU:HG	1:A:78:PHE:CD2	0.59	2.32	5	1
1:A:36:LYS:HE3	1:A:36:LYS:HA	0.59	1.73	19	1
1:A:20:VAL:HG11	1:A:34:LEU:CD1	0.59	2.28	9	2
1:A:8:VAL:HG21	1:A:31:VAL:HG22	0.59	1.73	17	1
1:A:62:MET:O	1:A:65:VAL:HG22	0.58	1.98	12	3
1:A:69:PHE:CD1	1:A:76:VAL:HB	0.58	2.32	14	7
1:A:27:ILE:N	1:A:27:ILE:CD1	0.58	2.65	14	15
1:A:48:VAL:HG23	1:A:79:PHE:CZ	0.58	2.34	15	13
1:A:27:ILE:CD1	1:A:27:ILE:H	0.58	2.12	14	2
1:A:77:ARG:HB3	1:A:79:PHE:CE1	0.58	2.34	13	11
1:A:20:VAL:HG12	1:A:21:PRO:HD2	0.57	1.74	7	2
1:A:47:GLU:HB2	1:A:69:PHE:HZ	0.57	1.58	10	5
1:A:45:LEU:C	1:A:56:VAL:HG13	0.57	2.19	13	14
1:A:76:VAL:HG23	1:A:77:ARG:N	0.57	2.14	10	19
1:A:77:ARG:O	1:A:79:PHE:CZ	0.57	2.58	3	20
1:A:60:GLU:CB	1:A:65:VAL:HG22	0.57	2.30	6	13
1:A:27:ILE:HG12	1:A:59:ASN:HA	0.57	1.75	14	15
1:A:22:VAL:HG21	1:A:62:MET:HB2	0.57	1.77	8	1
1:A:62:MET:CG	1:A:63:PHE:H	0.57	2.12	11	1
1:A:6:LEU:HD12	1:A:6:LEU:C	0.57	2.20	2	1
1:A:31:VAL:HB	1:A:45:LEU:HD13	0.56	1.76	14	1
1:A:27:ILE:HG22	1:A:60:GLU:C	0.56	2.19	11	4
1:A:27:ILE:CG1	1:A:59:ASN:HA	0.56	2.30	14	15
1:A:45:LEU:CD2	1:A:56:VAL:HG21	0.56	2.30	19	5
1:A:6:LEU:HD21	1:A:8:VAL:HG22	0.56	1.75	7	1
1:A:62:MET:HE3	1:A:63:PHE:CD1	0.56	2.35	11	1
1:A:47:GLU:HG2	1:A:54:ARG:O	0.56	2.01	4	6
1:A:22:VAL:HG21	1:A:62:MET:SD	0.56	2.41	17	2
1:A:4:MET:HB2	1:A:62:MET:HE1	0.56	1.76	10	1
1:A:49:TRP:CE3	1:A:69:PHE:CD1	0.55	2.95	14	3
1:A:48:VAL:HG23	1:A:53:GLU:CG	0.55	2.32	18	1
1:A:8:VAL:HG21	1:A:31:VAL:HG13	0.55	1.77	2	3
1:A:46:ALA:CA	1:A:56:VAL:HG13	0.55	2.32	20	15
1:A:6:LEU:CD2	1:A:31:VAL:HG22	0.55	2.31	7	3
1:A:22:VAL:HG23	1:A:23:THR:O	0.55	2.02	2	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:CD1	1:A:78:PHE:CG	0.55	2.90	3	5
1:A:8:VAL:HG13	1:A:31:VAL:HG13	0.55	1.77	9	5
1:A:18:THR:OG1	1:A:34:LEU:HD23	0.55	2.02	8	1
1:A:32:VAL:HG12	1:A:36:LYS:HG3	0.54	1.79	11	5
1:A:65:VAL:O	1:A:69:PHE:CE1	0.54	2.60	11	8
1:A:6:LEU:HD12	1:A:78:PHE:CE2	0.54	2.37	17	3
1:A:8:VAL:CG2	1:A:31:VAL:HG12	0.54	2.32	14	1
1:A:62:MET:HE3	1:A:66:LEU:HD22	0.54	1.79	18	4
1:A:27:ILE:H	1:A:27:ILE:HD13	0.54	1.62	14	1
1:A:61:ARG:CB	1:A:64:ASP:HB2	0.54	2.32	14	7
1:A:77:ARG:HB3	1:A:79:PHE:CE2	0.54	2.38	15	8
1:A:27:ILE:HD13	1:A:27:ILE:O	0.54	2.01	14	14
1:A:10:LEU:C	1:A:10:LEU:HD22	0.54	2.23	1	2
1:A:31:VAL:HG12	1:A:80:LEU:CD1	0.54	2.33	13	3
1:A:28:CYS:HB3	1:A:58:ASP:O	0.54	2.03	17	13
1:A:65:VAL:O	1:A:69:PHE:CE2	0.54	2.61	9	11
1:A:62:MET:CE	1:A:66:LEU:HD13	0.54	2.33	20	3
1:A:18:THR:HG22	1:A:35:CYS:SG	0.53	2.43	4	11
1:A:20:VAL:CG1	1:A:34:LEU:HD12	0.53	2.33	10	4
1:A:27:ILE:H	1:A:27:ILE:CD1	0.53	2.17	10	13
1:A:45:LEU:HD21	1:A:78:PHE:HD1	0.53	1.63	2	4
1:A:76:VAL:CG2	1:A:77:ARG:N	0.53	2.72	10	20
1:A:6:LEU:CD1	1:A:31:VAL:HG22	0.53	2.30	8	5
1:A:36:LYS:HA	1:A:36:LYS:CE	0.52	2.34	19	3
1:A:45:LEU:O	1:A:56:VAL:HG23	0.52	2.05	18	1
1:A:62:MET:HG2	1:A:63:PHE:N	0.52	2.16	11	1
1:A:65:VAL:O	1:A:69:PHE:CD2	0.52	2.62	12	8
1:A:63:PHE:HA	1:A:66:LEU:HD12	0.52	1.82	14	1
1:A:20:VAL:CG1	1:A:34:LEU:HD22	0.52	2.35	8	1
1:A:10:LEU:HD13	1:A:10:LEU:O	0.52	2.05	17	2
1:A:49:TRP:CE3	1:A:52:SER:HB3	0.52	2.40	4	10
1:A:31:VAL:HG11	1:A:45:LEU:CD1	0.52	2.34	3	11
1:A:8:VAL:HG22	1:A:31:VAL:HG12	0.52	1.80	14	1
1:A:8:VAL:CG2	1:A:31:VAL:HG22	0.51	2.34	17	1
1:A:76:VAL:HG22	1:A:78:PHE:CE2	0.51	2.40	2	1
1:A:22:VAL:CG2	1:A:62:MET:HB2	0.51	2.34	8	6
1:A:61:ARG:HB2	1:A:64:ASP:HB2	0.51	1.83	5	4
1:A:6:LEU:HD22	1:A:62:MET:HE1	0.51	1.83	15	1
1:A:49:TRP:CE3	1:A:52:SER:HB2	0.51	2.41	9	7
1:A:27:ILE:O	1:A:29:ARG:N	0.50	2.44	3	20
1:A:27:ILE:HD13	1:A:27:ILE:N	0.50	2.21	15	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LEU:HD22	1:A:16:HIS:NE2	0.50	2.21	13	1
1:A:69:PHE:CZ	1:A:76:VAL:CG2	0.50	2.94	9	18
1:A:10:LEU:CD1	1:A:16:HIS:CE1	0.50	2.95	11	7
1:A:28:CYS:SG	1:A:32:VAL:HG23	0.50	2.47	17	4
1:A:27:ILE:HG22	1:A:61:ARG:CB	0.50	2.36	2	3
1:A:46:ALA:O	1:A:79:PHE:CD2	0.49	2.65	19	12
1:A:28:CYS:HB3	1:A:58:ASP:HA	0.49	1.84	11	11
1:A:31:VAL:CB	1:A:45:LEU:HD13	0.49	2.36	14	1
1:A:22:VAL:CG2	1:A:23:THR:N	0.49	2.75	13	2
1:A:65:VAL:O	1:A:69:PHE:CD1	0.49	2.65	13	7
1:A:20:VAL:HG11	1:A:34:LEU:HD12	0.49	1.84	10	4
1:A:22:VAL:HG22	1:A:62:MET:CB	0.49	2.37	13	5
1:A:27:ILE:HG22	1:A:61:ARG:HG3	0.49	1.85	12	3
1:A:46:ALA:O	1:A:79:PHE:CD1	0.49	2.66	2	8
1:A:5:PHE:CA	1:A:62:MET:HE2	0.49	2.37	4	1
1:A:62:MET:CE	1:A:66:LEU:CD1	0.49	2.90	14	1
1:A:69:PHE:CE1	1:A:76:VAL:CB	0.49	2.95	10	11
1:A:10:LEU:HD21	1:A:35:CYS:HA	0.49	1.82	9	1
1:A:7:THR:O	1:A:78:PHE:HB2	0.49	2.07	11	9
1:A:22:VAL:HG13	1:A:62:MET:HB2	0.49	1.85	19	3
1:A:49:TRP:CH2	1:A:69:PHE:O	0.48	2.66	12	12
1:A:46:ALA:HA	1:A:56:VAL:HG13	0.48	1.84	20	6
1:A:49:TRP:HB2	1:A:75:GLU:O	0.48	2.07	10	14
1:A:69:PHE:CE2	1:A:76:VAL:CB	0.48	2.96	5	8
1:A:6:LEU:CD2	1:A:8:VAL:HG22	0.48	2.38	7	1
1:A:20:VAL:HG13	1:A:34:LEU:HD22	0.48	1.84	8	1
1:A:22:VAL:HG22	1:A:62:MET:CG	0.48	2.39	11	1
1:A:10:LEU:O	1:A:10:LEU:HD22	0.48	2.08	17	1
1:A:48:VAL:HG12	1:A:79:PHE:CZ	0.48	2.43	18	1
1:A:76:VAL:CG2	1:A:78:PHE:CE2	0.48	2.97	2	1
1:A:6:LEU:HD11	1:A:31:VAL:HG12	0.48	1.84	20	1
1:A:20:VAL:CG2	1:A:34:LEU:HD12	0.48	2.38	5	1
1:A:22:VAL:HG22	1:A:62:MET:HB2	0.48	1.85	13	4
1:A:66:LEU:HD21	1:A:73:ARG:HB2	0.48	1.85	16	1
1:A:62:MET:SD	1:A:62:MET:N	0.48	2.87	11	1
1:A:61:ARG:O	1:A:62:MET:C	0.47	2.51	12	20
1:A:24:PRO:HA	1:A:62:MET:SD	0.47	2.49	11	1
1:A:44:HIS:CD2	1:A:45:LEU:O	0.47	2.68	18	6
1:A:35:CYS:HB2	1:A:80:LEU:HG	0.47	1.86	1	2
1:A:47:GLU:HB2	1:A:69:PHE:CE2	0.47	2.44	1	7
1:A:62:MET:HA	1:A:62:MET:HE2	0.47	1.87	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LEU:HD11	1:A:78:PHE:CD1	0.47	2.45	1	1
1:A:31:VAL:HG11	1:A:45:LEU:CG	0.47	2.40	3	4
1:A:27:ILE:N	1:A:27:ILE:HD13	0.47	2.25	4	2
1:A:63:PHE:N	1:A:63:PHE:CD1	0.47	2.83	6	1
1:A:35:CYS:O	1:A:80:LEU:HD22	0.47	2.10	8	2
1:A:49:TRP:CE3	1:A:52:SER:CB	0.47	2.97	8	3
1:A:49:TRP:CE3	1:A:69:PHE:CD2	0.47	3.00	11	1
1:A:28:CYS:HB2	1:A:58:ASP:O	0.47	2.10	1	2
1:A:7:THR:HG22	1:A:17:PHE:HB2	0.47	1.86	16	1
1:A:60:GLU:HB3	1:A:65:VAL:HG13	0.46	1.86	14	2
1:A:48:VAL:HG23	1:A:53:GLU:CA	0.46	2.40	18	1
1:A:48:VAL:CG2	1:A:79:PHE:CZ	0.46	2.98	15	4
1:A:5:PHE:HB3	1:A:21:PRO:HA	0.46	1.87	14	2
1:A:32:VAL:HA	1:A:80:LEU:HD21	0.46	1.86	11	3
1:A:27:ILE:HG22	1:A:60:GLU:O	0.46	2.10	11	1
1:A:45:LEU:O	1:A:56:VAL:O	0.46	2.32	13	5
1:A:47:GLU:HB2	1:A:69:PHE:CE1	0.46	2.46	4	5
1:A:57:ALA:HB3	1:A:60:GLU:CG	0.46	2.40	18	1
1:A:28:CYS:SG	1:A:31:VAL:HG21	0.46	2.51	1	1
1:A:77:ARG:CB	1:A:79:PHE:CE1	0.46	2.98	19	8
1:A:60:GLU:CB	1:A:65:VAL:CG2	0.46	2.94	3	2
1:A:35:CYS:CB	1:A:80:LEU:HD22	0.46	2.41	8	2
1:A:6:LEU:HD11	1:A:31:VAL:CG2	0.46	2.35	19	2
1:A:69:PHE:CE1	1:A:76:VAL:HG11	0.46	2.46	5	1
1:A:45:LEU:O	1:A:56:VAL:CB	0.46	2.63	18	1
1:A:31:VAL:HG21	1:A:45:LEU:CD2	0.46	2.41	5	1
1:A:32:VAL:HG22	1:A:80:LEU:HD11	0.46	1.88	9	1
1:A:66:LEU:HD13	1:A:73:ARG:CD	0.45	2.41	4	1
1:A:48:VAL:N	1:A:79:PHE:CE2	0.45	2.84	12	2
1:A:49:TRP:CD1	1:A:75:GLU:HB3	0.45	2.46	8	5
1:A:10:LEU:CB	1:A:16:HIS:CD2	0.45	2.99	16	1
1:A:49:TRP:HB2	1:A:76:VAL:CA	0.45	2.41	8	7
1:A:47:GLU:CD	1:A:56:VAL:HG12	0.45	2.32	1	1
1:A:27:ILE:O	1:A:27:ILE:HD13	0.45	2.10	19	3
1:A:27:ILE:HD12	1:A:27:ILE:H	0.45	1.71	11	3
1:A:27:ILE:HG22	1:A:61:ARG:HB3	0.45	1.88	2	1
1:A:69:PHE:CE2	1:A:76:VAL:CG2	0.45	3.00	3	1
1:A:8:VAL:O	1:A:18:THR:N	0.45	2.45	20	11
1:A:22:VAL:O	1:A:63:PHE:CZ	0.45	2.70	15	4
1:A:49:TRP:CZ3	1:A:52:SER:CB	0.45	3.00	10	1
1:A:66:LEU:HD13	1:A:73:ARG:HD3	0.45	1.88	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:VAL:HG12	1:A:79:PHE:HZ	0.45	1.70	18	1
1:A:32:VAL:HG12	1:A:36:LYS:HE2	0.45	1.88	20	1
1:A:44:HIS:ND1	1:A:45:LEU:O	0.44	2.50	19	3
1:A:6:LEU:CD1	1:A:8:VAL:CG2	0.44	2.95	2	5
1:A:8:VAL:O	1:A:17:PHE:CA	0.44	2.65	16	8
1:A:18:THR:O	1:A:18:THR:HG23	0.44	2.12	7	9
1:A:20:VAL:CG1	1:A:34:LEU:CD1	0.44	2.96	2	8
1:A:66:LEU:HA	1:A:69:PHE:CD1	0.44	2.47	5	1
1:A:22:VAL:CG2	1:A:62:MET:CG	0.44	2.94	15	3
1:A:22:VAL:HG23	1:A:23:THR:N	0.44	2.28	13	1
1:A:20:VAL:HG21	1:A:30:ASP:OD1	0.44	2.12	1	1
1:A:30:ASP:O	1:A:34:LEU:CD1	0.44	2.66	8	1
1:A:8:VAL:HG11	1:A:31:VAL:HB	0.44	1.88	1	2
1:A:32:VAL:HG12	1:A:36:LYS:CE	0.44	2.43	20	1
1:A:62:MET:HE1	1:A:66:LEU:HD22	0.44	1.88	1	2
1:A:77:ARG:CB	1:A:79:PHE:CE2	0.44	3.00	1	5
1:A:62:MET:CG	1:A:63:PHE:N	0.44	2.79	11	1
1:A:65:VAL:O	1:A:68:ARG:HG2	0.44	2.12	14	1
1:A:6:LEU:HG	1:A:78:PHE:CD1	0.44	2.47	7	1
1:A:35:CYS:HB3	1:A:80:LEU:HB2	0.44	1.90	4	2
1:A:10:LEU:HB3	1:A:16:HIS:CE1	0.44	2.47	8	1
1:A:22:VAL:CG2	1:A:62:MET:CB	0.44	2.96	8	3
1:A:6:LEU:CD1	1:A:78:PHE:CD1	0.44	2.99	9	1
1:A:6:LEU:HD23	1:A:6:LEU:C	0.44	2.33	15	1
1:A:6:LEU:CD1	1:A:31:VAL:HG12	0.44	2.43	20	1
1:A:8:VAL:HG11	1:A:80:LEU:HD23	0.43	1.89	2	1
1:A:62:MET:HE2	1:A:66:LEU:HD22	0.43	1.89	5	1
1:A:8:VAL:O	1:A:17:PHE:CB	0.43	2.66	9	8
1:A:31:VAL:HG23	1:A:32:VAL:N	0.43	2.28	1	2
1:A:10:LEU:HB3	1:A:16:HIS:CD2	0.43	2.48	16	1
1:A:45:LEU:CD2	1:A:79:PHE:O	0.43	2.59	1	1
1:A:22:VAL:CG1	1:A:62:MET:HB3	0.43	2.42	11	1
1:A:62:MET:O	1:A:65:VAL:CG2	0.43	2.66	13	1
1:A:27:ILE:HG12	1:A:58:ASP:O	0.43	2.14	17	9
1:A:45:LEU:O	1:A:56:VAL:CG2	0.43	2.67	18	1
1:A:22:VAL:HG13	1:A:62:MET:HG2	0.43	1.90	6	2
1:A:69:PHE:CE1	1:A:76:VAL:CG2	0.43	3.02	8	3
1:A:32:VAL:O	1:A:36:LYS:HB2	0.43	2.14	20	1
1:A:47:GLU:OE2	1:A:65:VAL:HG12	0.43	2.13	8	2
1:A:32:VAL:HG12	1:A:36:LYS:CD	0.43	2.44	19	1
1:A:28:CYS:HB3	1:A:58:ASP:CA	0.43	2.43	5	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:PHE:N	1:A:5:PHE:CD2	0.43	2.86	20	1
1:A:27:ILE:C	1:A:29:ARG:N	0.43	2.72	15	14
1:A:8:VAL:HA	1:A:78:PHE:HB2	0.43	1.91	2	1
1:A:9:TYR:CD1	1:A:17:PHE:HB3	0.43	2.49	3	1
1:A:6:LEU:HD12	1:A:78:PHE:CE1	0.43	2.48	9	1
1:A:4:MET:HB2	1:A:62:MET:CE	0.43	2.44	14	1
1:A:66:LEU:HD12	1:A:78:PHE:CZ	0.42	2.49	6	1
1:A:35:CYS:O	1:A:80:LEU:CD2	0.42	2.67	15	2
1:A:18:THR:OG1	1:A:34:LEU:HD22	0.42	2.14	16	1
1:A:44:HIS:HD2	1:A:45:LEU:O	0.42	1.97	18	1
1:A:45:LEU:HD22	1:A:46:ALA:H	0.42	1.73	1	1
1:A:61:ARG:O	1:A:64:ASP:HB2	0.42	2.13	15	2
1:A:31:VAL:CG2	1:A:45:LEU:HD22	0.42	2.43	5	1
1:A:47:GLU:OE1	1:A:65:VAL:HG12	0.42	2.14	7	1
1:A:10:LEU:CD2	1:A:35:CYS:HA	0.42	2.44	9	1
1:A:4:MET:CG	1:A:63:PHE:CZ	0.42	3.01	3	1
1:A:20:VAL:HG11	1:A:34:LEU:HD11	0.42	1.89	9	1
1:A:46:ALA:HB2	1:A:81:ARG:HG3	0.42	1.92	18	1
1:A:6:LEU:HD12	1:A:8:VAL:HG22	0.42	1.91	20	1
1:A:48:VAL:HB	1:A:79:PHE:CZ	0.42	2.49	15	4
1:A:48:VAL:HG13	1:A:53:GLU:HB2	0.42	1.90	15	2
1:A:6:LEU:HB2	1:A:78:PHE:CZ	0.42	2.49	2	1
1:A:45:LEU:HD12	1:A:56:VAL:CG2	0.42	2.40	1	1
1:A:6:LEU:HB3	1:A:62:MET:HG3	0.42	1.91	17	2
1:A:22:VAL:CG2	1:A:62:MET:HG2	0.42	2.45	15	1
1:A:9:TYR:N	1:A:78:PHE:O	0.42	2.52	9	1
1:A:45:LEU:HD11	1:A:78:PHE:CB	0.42	2.42	9	1
1:A:45:LEU:HD23	1:A:56:VAL:CG1	0.42	2.41	18	1
1:A:61:ARG:HG2	1:A:64:ASP:HB2	0.42	1.92	2	1
1:A:29:ARG:O	1:A:33:ASP:CB	0.42	2.68	9	2
1:A:49:TRP:CZ3	1:A:52:SER:HB3	0.42	2.49	10	2
1:A:19:GLU:O	1:A:20:VAL:HG13	0.42	2.14	17	3
1:A:5:PHE:N	1:A:62:MET:HE3	0.42	2.29	14	1
1:A:49:TRP:CZ3	1:A:69:PHE:HA	0.42	2.49	14	1
1:A:6:LEU:HD23	1:A:62:MET:HG3	0.42	1.91	2	1
1:A:22:VAL:CG2	1:A:62:MET:CE	0.41	2.98	15	1
1:A:5:PHE:CD1	1:A:5:PHE:N	0.41	2.88	13	2
1:A:8:VAL:HB	1:A:35:CYS:SG	0.41	2.56	1	1
1:A:31:VAL:HG11	1:A:45:LEU:HG	0.41	1.92	1	1
1:A:77:ARG:HB2	1:A:79:PHE:CZ	0.41	2.49	4	7
1:A:6:LEU:CD1	1:A:78:PHE:CD2	0.41	3.00	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:VAL:CG1	1:A:62:MET:HB2	0.41	2.45	19	2
1:A:60:GLU:HB3	1:A:65:VAL:CG2	0.41	2.45	3	1
1:A:47:GLU:OE2	1:A:69:PHE:CZ	0.41	2.74	5	1
1:A:22:VAL:HG22	1:A:62:MET:SD	0.41	2.56	11	1
1:A:27:ILE:CG2	1:A:61:ARG:CD	0.41	2.99	14	2
1:A:45:LEU:CB	1:A:56:VAL:HG22	0.41	2.46	15	1
1:A:18:THR:HG21	1:A:34:LEU:HB2	0.41	1.92	1	1
1:A:62:MET:SD	1:A:63:PHE:CD1	0.41	3.14	1	1
1:A:22:VAL:O	1:A:63:PHE:CE1	0.41	2.73	6	1
1:A:48:VAL:N	1:A:79:PHE:CE1	0.41	2.89	1	1
1:A:24:PRO:HD3	1:A:63:PHE:CE1	0.41	2.50	13	1
1:A:63:PHE:CA	1:A:66:LEU:HB2	0.41	2.43	14	1
1:A:32:VAL:CG1	1:A:36:LYS:CD	0.41	2.99	19	1
1:A:10:LEU:HB3	1:A:35:CYS:CB	0.41	2.45	1	1
1:A:48:VAL:HA	1:A:52:SER:O	0.41	2.16	3	2
1:A:48:VAL:HG22	1:A:53:GLU:HG2	0.41	1.93	4	1
1:A:8:VAL:O	1:A:17:PHE:HA	0.41	2.15	16	1
1:A:23:THR:HB	1:A:24:PRO:HD2	0.41	1.92	19	1
1:A:35:CYS:CB	1:A:80:LEU:HB2	0.41	2.46	20	1
1:A:8:VAL:HG11	1:A:31:VAL:CG1	0.41	2.43	17	1
1:A:45:LEU:HD13	1:A:45:LEU:C	0.40	2.36	1	1
1:A:31:VAL:HG23	1:A:62:MET:HE3	0.40	1.92	2	1
1:A:23:THR:O	1:A:25:GLU:N	0.40	2.48	8	1
1:A:28:CYS:HB2	1:A:58:ASP:HA	0.40	1.93	14	1
1:A:48:VAL:HG22	1:A:53:GLU:CB	0.40	2.47	14	1
1:A:66:LEU:HD22	1:A:73:ARG:HB2	0.40	1.93	15	1
1:A:31:VAL:HG13	1:A:45:LEU:HD13	0.40	1.89	18	1
1:A:45:LEU:O	1:A:56:VAL:HB	0.40	2.16	18	1
1:A:5:PHE:CD2	1:A:5:PHE:N	0.40	2.90	1	1
1:A:8:VAL:O	1:A:17:PHE:HB2	0.40	2.17	1	1
1:A:10:LEU:HD11	1:A:18:THR:HB	0.40	1.93	12	1
1:A:5:PHE:HB2	1:A:20:VAL:O	0.40	2.17	14	1
1:A:8:VAL:HA	1:A:78:PHE:O	0.40	2.16	17	1
1:A:46:ALA:HB3	1:A:79:PHE:CD1	0.40	2.52	18	1
1:A:47:GLU:CG	1:A:47:GLU:O	0.40	2.69	18	1
1:A:48:VAL:CB	1:A:79:PHE:CZ	0.40	3.05	1	2
1:A:24:PRO:HD3	1:A:63:PHE:CE2	0.40	2.52	5	1
1:A:66:LEU:HD12	1:A:78:PHE:HZ	0.40	1.76	6	1
1:A:18:THR:HG23	1:A:18:THR:O	0.40	2.17	8	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	69/86 (80%)	62±2 (90±3%)	4±2 (6±2%)	2±1 (3±1%)	6 36
All	All	1380/1720 (80%)	1247 (90%)	86 (6%)	47 (3%)	6 36

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	28	CYS	20
1	A	62	MET	20
1	A	14	GLU	4
1	A	71	SER	2
1	A	70	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	65/79 (82%)	46±3 (70±4%)	19±3 (30±4%)	1 17
All	All	1300/1580 (82%)	913 (70%)	387 (30%)	1 17

All 44 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	27	ILE	20
1	A	49	TRP	20
1	A	52	SER	20
1	A	76	VAL	20
1	A	79	PHE	20

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Mol	Chain	Res	Type	Models (Total)
1	A	68	ARG	19
1	A	80	LEU	18
1	A	36	LYS	15
1	A	22	VAL	13
1	A	44	HIS	13
1	A	62	MET	13
1	A	66	LEU	13
1	A	61	ARG	13
1	A	73	ARG	12
1	A	56	VAL	12
1	A	72	GLN	11
1	A	14	GLU	10
1	A	67	GLN	9
1	A	15	GLN	9
1	A	29	ARG	8
1	A	25	GLU	7
1	A	53	GLU	7
1	A	54	ARG	7
1	A	75	GLU	7
1	A	19	GLU	7
1	A	63	PHE	7
1	A	50	CYS	6
1	A	64	ASP	6
1	A	71	SER	5
1	A	58	ASP	5
1	A	6	LEU	5
1	A	23	THR	4
1	A	16	HIS	4
1	A	10	LEU	3
1	A	28	CYS	3
1	A	81	ARG	3
1	A	77	ARG	3
1	A	20	VAL	2
1	A	74	ASN	2
1	A	59	ASN	2
1	A	4	MET	1
1	A	5	PHE	1
1	A	34	LEU	1
1	A	48	VAL	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