Full wwPDB NMR Structure Validation Report (i)

Feb 26, 2022 – 08:07 AM EST

PDB ID	:	2AL3
Title	:	Solution structure and backbone dynamics of an N-terminal ubiquitin-like domain in the GLUT4-tethering protein, TUG
Authors	:	Tettamanzi, M.C.; Yu, C.; Bogan, J.S.; Hodsdon, M.E.
Deposited on	:	2005-08-04

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:

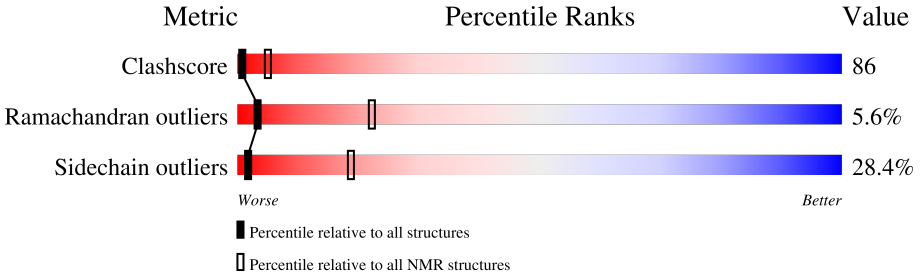
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	90	13% 51% 16% • • 16%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 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:10-A:82 (73)	0.13	4

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 5 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1237 atoms, of which 625 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TUG long isoform.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	76	1237	383	625	115	112	2	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: TUG long isoform

Chain A: 13% 51% 16% • • 16%

MET ALA ALA PRO ALA GLY GLY GLY S10 A11 V12 S13 V14 L15 A16 P17 N18 G19 R20 R21 H22 T23 V24 K25 V26 T27 P28 V31 L32 L33 Q34 V35 L36 E37 D38 T39 C40 R41 R42 Q43 D44 F45 N46 P47 S48 E49 Y50 D51 L52 K53 F54 Q55 R56 L59 D60 L61 S62

L63 Q64 W65 A68 N69 L70 P71 N72 N73 A74 K75 L76 E77 M78 V79 P80 V81 S82 R83 S84 R85 GLU GLY PRO GLU ASN

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: TUG long isoform

Chain A: 14% 42% 23% • • 16%

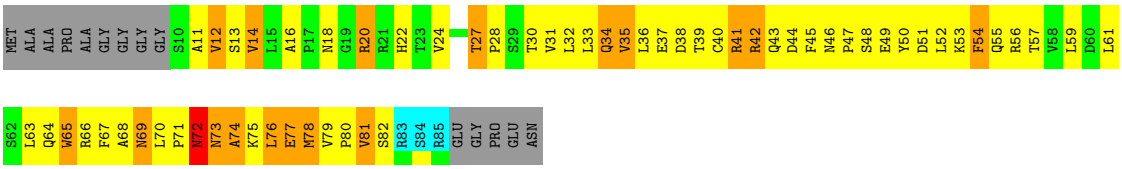
MET ALA ALA PRO ALA GLY GLY GLY S10 A11 V12 S13 V14 L15 A16 P17 N18 G19 R20 R21 H22 T23 V24 K25 V26 T27 P28 V31 L32 L33 Q34 V35 L36 E37 D38 T39 C40 R41 R42 Q43 D44 F45 N46 P47 S48 E49 Y50 D51 L52 K53 F54 V58 L59 D60 L61 S62 L63

Q64 W65 R66 F67 A68 N69 L70 P71 N72 N73 A74 K75 L76 E77 M78 V79 P80 V81 S82 R83 S84 R85 GLU GLY PRO GLU ASN

4.2.2 Score per residue for model 2

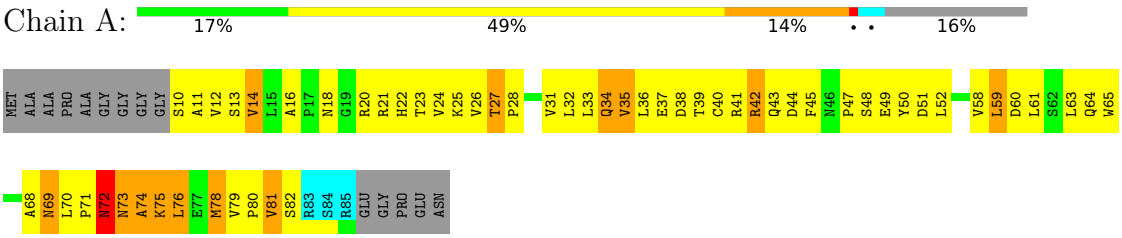
• Molecule 1: TUG long isoform

Chain A: 13% 48% 19% • • 16%



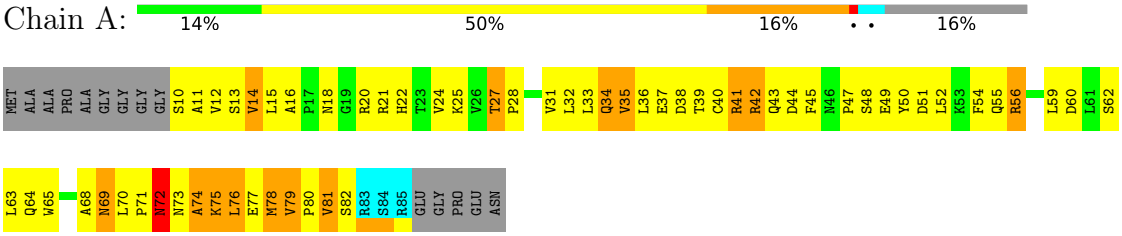
4.2.3 Score per residue for model 3

- Molecule 1: TUG long isoform



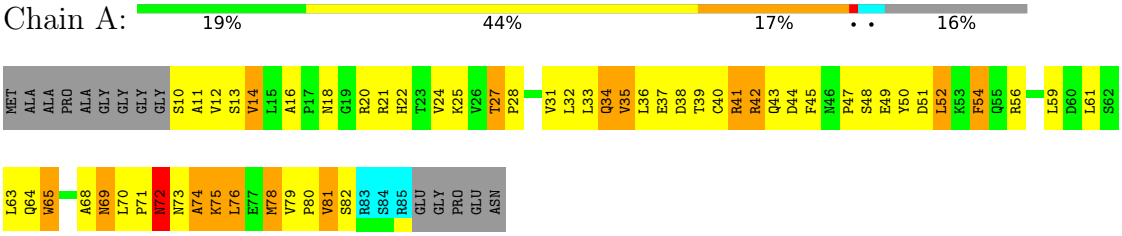
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: TUG long isoform



4.2.5 Score per residue for model 5

- Molecule 1: TUG long isoform



4.2.6 Score per residue for model 6

- Molecule 1: TUG long isoform

Chain A: 13% 47% 20% • • 16%

MET ALA ALA PRO ALA GLY GLY GLY GLY S10 A11 V12 S13 V14 L15 A16 P17 N18 G19 R20 R21 H22 T23 V24 K25 V26 T27 P28 S29 T30 V31 L32 L33 Q34 V35 L36 E37 D38 T39 C40 R41 R42 Q43 D44 F45 N46 P47 S48 E49 Y50 D51 L52 K53 F54 Q55 R56 L59 D60 L61

S62 L63 Q64 W65 A68 N69 L70 P71 N72 N73 A74 K75 L76 E77 M78 V79 P80 V81 S82 R83 S84 R85 GLU GLY PRO GLU ASN

4.2.7 Score per residue for model 7

- Molecule 1: TUG long isoform

Chain A: 14% 49% 17% • • 16%

MET ALA ALA PRO ALA GLY GLY GLY GLY S10 A11 V12 S13 V14 L15 A16 P17 N18 G19 R20 R21 H22 T23 V24 K25 V26 T27 P28 V31 L32 L33 Q34 V35 L36 E37 D38 T39 C40 R41 R42 Q43 D44 F45 N46 P47 S48 E49 Y50 D51 L52 V58 L59 D60 L61 S62 L63 Q64 W65

A68 N69 L70 P71 N72 N73 A74 K75 L76 E77 M78 V79 P80 V81 S82 R83 S84 R85 GLU GLY PRO GLU ASN

4.2.8 Score per residue for model 8

- Molecule 1: TUG long isoform

Chain A: 17% 47% 17% • • 16%

MET ALA ALA PRO ALA GLY GLY GLY GLY S10 A11 V12 S13 V14 L15 A16 P17 N18 G19 R20 R21 H22 T23 V24 T27 P28 V31 L32 L33 Q34 V35 L36 E37 D38 T39 C40 R41 R42 Q43 D44 F45 N46 P47 S48 E49 Y50 D51 L52 K53 F54 Q55 R56 T57 V58 L59 D60 L61 S62

L63 Q64 W65 A68 N69 L70 P71 N72 N73 A74 K75 L76 E77 M78 V79 P80 V81 S82 R83 S84 R85 GLU GLY PRO GLU ASN

4.2.9 Score per residue for model 9

- Molecule 1: TUG long isoform

Chain A: 12% 50% 17% • • 16%

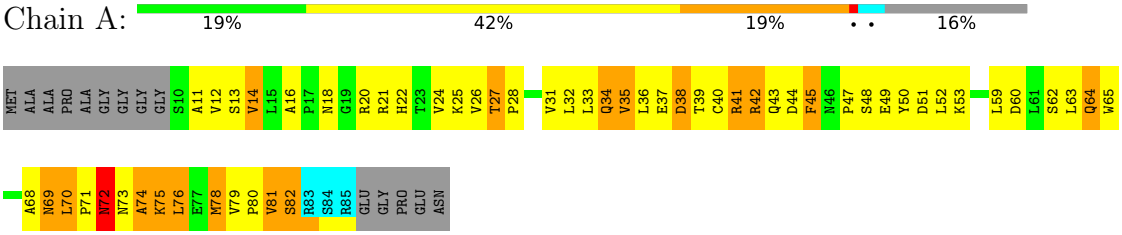
MET ALA ALA PRO ALA GLY GLY GLY GLY S10 A11 V12 S13 V14 L15 A16 P17 N18 G19 R20 R21 H22 T23 V24 K25 V26 T27 P28 V31 L32 L33 Q34 V35 L36 E37 D38 T39 C40 R41 R42 Q43 D44 F45 W46 P47 S48 E49 Y50 D51 L52 K53 F54 Q55 R56 T57 V58 L59 D60 L61

S62 L63 Q64 W65 A68 N69 L70 P71 N72 N73 A74 K75 L76 E77 M78 V79 P80 V81 S82 R83 S84 R85 GLU GLY PRO GLU ASN

4.2.10 Score per residue for model 10

- Molecule 1: TUG long isoform

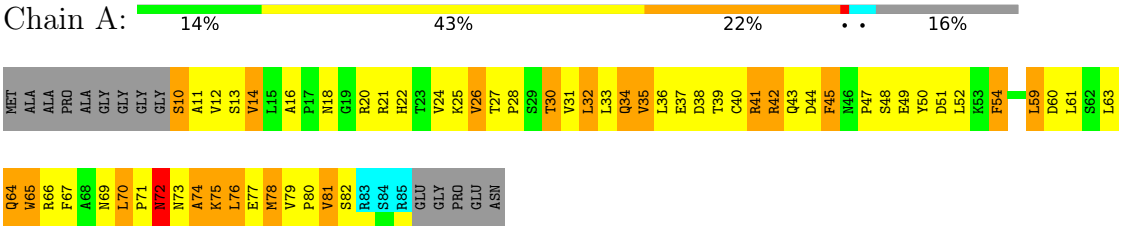
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: TUG long isoform

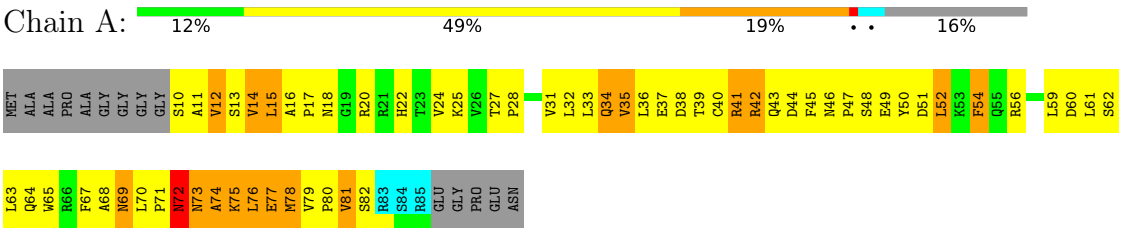
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: TUG long isoform

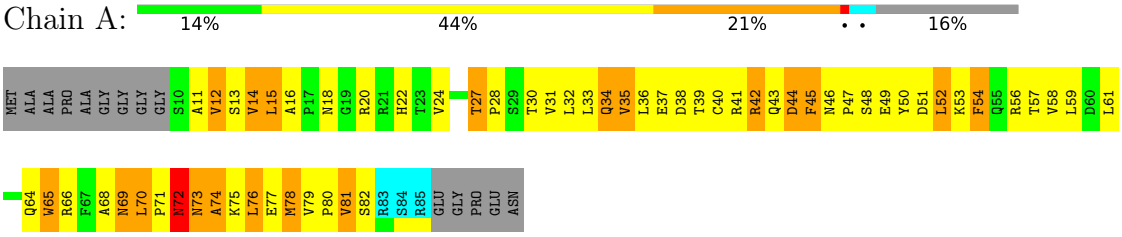
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: TUG long isoform

Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: TUG long isoform

Chain A: 17% 44% 19% 16%

MET ALA ALA PRO ALA GLY GLY GLY GLY S10 A11 V12 S13 V14 L15 A16 R20 R21 H22 T23 V24 K25 V26 T27 P28 V31 L32 L33 Q34 V35 L36 E37 D38 T39 C40 R41 R42 Q43 D44 F45 N46 P47 S48 E49 Y50 D51 L52 K53 F54 Q55 R56 L59 D60 L61 S62 L63 Q64

W65 R66 F67 A68 N69 L70 P71 N72 N73 A74 K75 L76 E77 M78 V79 P80 V81 S82 R83 S84 R85 GLU GLY PRO GLU ASN

4.2.15 Score per residue for model 15

- Molecule 1: TUG long isoform

Chain A: 10% 49% 21% 16%

MET ALA ALA PRO ALA GLY GLY GLY GLY S10 A11 V12 S13 V14 L15 A16 P17 N18 G19 R20 R21 H22 T23 V24 K25 V26 T27 P28 V31 L32 L33 Q34 V35 L36 E37 D38 T39 C40 R41 R42 Q43 D44 F45 N46 P47 S48 E49 Y50 D51 L52 K53 F54 Q55 R56 T57 V58 L59 D60 L61

S62 L63 Q64 W65 R66 F67 A68 N69 L70 P71 N72 N73 A74 K75 L76 E77 M78 V79 P80 V81 S82 R83 S84 R85 GLU GLY PRO GLU ASN

4.2.16 Score per residue for model 16

- Molecule 1: TUG long isoform

Chain A: 16% 46% 19% 16%

MET ALA ALA PRO ALA GLY GLY GLY GLY S10 A11 V12 S13 V14 L15 A16 P17 N18 G19 R20 R21 H22 T23 V24 K25 V26 T27 P28 S29 T30 V31 L32 L33 Q34 V35 L36 E37 D38 T39 C40 R41 R42 Q43 D44 F45 N46 P47 S48 E49 Y50 D51 L52 K53 F54 Q55 R56 T57 V58 L59 D60

L61 Q64 W65 R66 F67 A68 N69 L70 P71 N72 N73 A74 K75 L76 E77 M78 V79 P80 V81 S82 R83 S84 R85 GLU GLY PRO GLU ASN

4.2.17 Score per residue for model 17

- Molecule 1: TUG long isoform

Chain A: 10% 47% 22% 16%

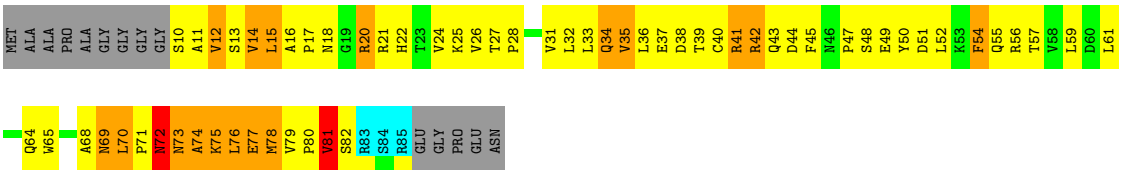
MET ALA ALA PRO ALA GLY GLY GLY GLY S10 A11 V12 S13 V14 L15 A16 P17 N18 G19 R20 R21 H22 T23 V24 K25 V26 T27 P28 V31 L32 L33 Q34 V35 L36 E37 D38 T39 C40 R41 R42 Q43 D44 F45 N46 P47 S48 E49 Y50 D51 L52 K53 F54 Q55 R56 L59 D60 L61 S62

L63 Q64 W65 R66 F67 A68 N69 L70 P71 N72 N73 A74 K75 L76 E77 M78 V79 P80 V81 S82 R83 S84 R85 GLU GLY PRO GLU ASN

4.2.18 Score per residue for model 18

- Molecule 1: TUG long isoform

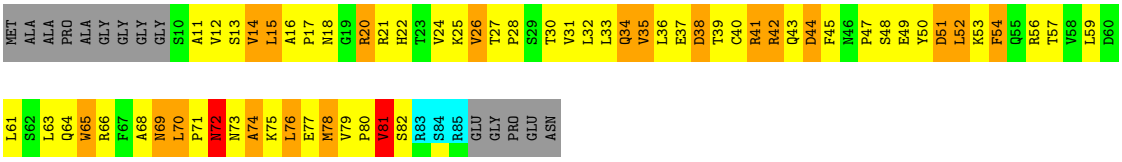
Chain A: 13% 47% 19% • • 16%



4.2.19 Score per residue for model 19

- Molecule 1: TUG long isoform

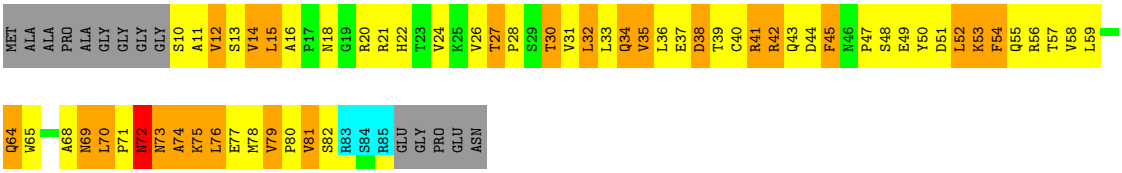
Chain A: 11% 47% 21% • • 16%



4.2.20 Score per residue for model 20

- Molecule 1: TUG long isoform

Chain A: 13% 40% 27% • • 16%



5 Refinement protocol and experimental data overview (i)

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	refinement	1.0.5
CYANA	structure solution	1.0.5
TALOS	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	584	594	593	102±10
All	All	11680	11880	11860	2032

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 86.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:VAL:HG12	1:A:76:LEU:HD21	1.09	1.23	15	4
1:A:36:LEU:HD22	1:A:61:LEU:HD21	0.99	1.31	9	4
1:A:16:ALA:HB1	1:A:18:ASN:OD1	0.96	1.60	5	7
1:A:80:PRO:O	1:A:81:VAL:HG13	0.94	1.60	18	4
1:A:75:LYS:C	1:A:76:LEU:HD13	0.93	1.83	17	17
1:A:32:LEU:HD11	1:A:70:LEU:HD21	0.90	1.41	14	5
1:A:12:VAL:CG1	1:A:76:LEU:HD21	0.90	1.97	6	5
1:A:32:LEU:HD12	1:A:63:LEU:O	0.88	1.67	15	11
1:A:13:SER:O	1:A:76:LEU:HD22	0.86	1.69	15	16
1:A:59:LEU:HD11	1:A:70:LEU:HD21	0.86	1.47	15	5
1:A:31:VAL:HG12	1:A:64:GLN:CG	0.86	2.00	3	14
1:A:12:VAL:HG12	1:A:76:LEU:HD11	0.85	1.46	9	1
1:A:16:ALA:HB3	1:A:20:ARG:O	0.85	1.70	15	20
1:A:45:PHE:CD2	1:A:50:TYR:CE2	0.84	2.66	14	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:VAL:HG11	1:A:33:LEU:HD23	0.83	1.50	6	6
1:A:12:VAL:HG21	1:A:26:VAL:HG22	0.83	1.50	19	6
1:A:15:LEU:HD22	1:A:15:LEU:O	0.83	1.74	17	8
1:A:12:VAL:HG22	1:A:76:LEU:HD21	0.82	1.51	12	11
1:A:12:VAL:CG1	1:A:76:LEU:HD11	0.82	2.03	9	1
1:A:80:PRO:O	1:A:81:VAL:HB	0.82	1.75	15	16
1:A:52:LEU:O	1:A:59:LEU:N	0.81	2.13	11	20
1:A:31:VAL:HG12	1:A:64:GLN:HG2	0.81	1.52	18	11
1:A:12:VAL:O	1:A:24:VAL:O	0.80	2.00	18	20
1:A:59:LEU:HG	1:A:76:LEU:HD22	0.80	1.52	9	3
1:A:51:ASP:C	1:A:52:LEU:HD13	0.79	1.97	1	3
1:A:12:VAL:CG2	1:A:26:VAL:HG22	0.79	2.08	19	6
1:A:32:LEU:HD13	1:A:59:LEU:HD12	0.79	1.55	17	9
1:A:15:LEU:C	1:A:15:LEU:HD22	0.78	2.00	13	2
1:A:47:PRO:CG	1:A:61:LEU:HD11	0.78	2.09	13	15
1:A:62:SER:C	1:A:63:LEU:HD22	0.77	1.99	1	8
1:A:80:PRO:C	1:A:81:VAL:HG22	0.77	1.98	17	4
1:A:11:ALA:O	1:A:73:ASN:C	0.77	2.22	19	20
1:A:76:LEU:HD13	1:A:76:LEU:N	0.76	1.94	11	17
1:A:31:VAL:HG13	1:A:64:GLN:HG3	0.76	1.58	12	6
1:A:59:LEU:HD21	1:A:70:LEU:HD21	0.75	1.59	3	2
1:A:47:PRO:HG3	1:A:61:LEU:HD11	0.75	1.59	11	12
1:A:54:PHE:HB2	1:A:76:LEU:HD23	0.75	1.57	13	2
1:A:65:TRP:CE3	1:A:70:LEU:HD12	0.75	2.16	6	3
1:A:27:THR:HG22	1:A:28:PRO:HD2	0.74	1.58	10	13
1:A:45:PHE:CD2	1:A:50:TYR:CD2	0.74	2.74	11	19
1:A:59:LEU:HD13	1:A:76:LEU:HB3	0.74	1.60	6	1
1:A:81:VAL:HG22	1:A:82:SER:H	0.73	1.43	3	16
1:A:80:PRO:O	1:A:81:VAL:CG1	0.73	2.36	18	4
1:A:41:ARG:HG3	1:A:42:ARG:N	0.72	1.98	10	4
1:A:32:LEU:HD13	1:A:59:LEU:CD1	0.71	2.15	9	2
1:A:31:VAL:HG12	1:A:64:GLN:HG3	0.70	1.60	3	4
1:A:80:PRO:O	1:A:81:VAL:HG22	0.70	1.87	17	4
1:A:51:ASP:N	1:A:79:VAL:O	0.70	2.21	1	20
1:A:12:VAL:HG22	1:A:76:LEU:HD11	0.69	1.65	2	2
1:A:11:ALA:O	1:A:72:ASN:O	0.68	2.12	14	20
1:A:50:TYR:CD1	1:A:78:MET:CE	0.68	2.77	19	13
1:A:15:LEU:O	1:A:15:LEU:HD13	0.67	1.90	19	7
1:A:13:SER:O	1:A:76:LEU:N	0.67	2.21	9	9
1:A:54:PHE:CB	1:A:76:LEU:HD23	0.67	2.20	13	2
1:A:36:LEU:HD22	1:A:61:LEU:CD2	0.67	2.19	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:PHE:CE2	1:A:50:TYR:CE2	0.67	2.82	11	17
1:A:12:VAL:HG13	1:A:76:LEU:HD21	0.67	1.65	17	6
1:A:15:LEU:HD22	1:A:15:LEU:C	0.67	2.09	12	6
1:A:30:THR:HG23	1:A:34:GLN:HG2	0.66	1.67	2	6
1:A:39:THR:HG22	1:A:43:GLN:CD	0.66	2.09	16	5
1:A:49:GLU:CA	1:A:81:VAL:O	0.66	2.43	10	20
1:A:65:TRP:CE3	1:A:70:LEU:HD23	0.66	2.26	9	2
1:A:32:LEU:HD13	1:A:59:LEU:HD23	0.66	1.68	3	1
1:A:31:VAL:HG13	1:A:64:GLN:CG	0.66	2.20	16	3
1:A:14:VAL:HG11	1:A:52:LEU:HD23	0.65	1.65	13	2
1:A:45:PHE:CG	1:A:50:TYR:CE2	0.64	2.86	2	17
1:A:45:PHE:CE2	1:A:50:TYR:CZ	0.64	2.85	6	13
1:A:16:ALA:CB	1:A:20:ARG:O	0.64	2.46	15	20
1:A:59:LEU:HD11	1:A:70:LEU:HD11	0.64	1.69	7	2
1:A:60:ASP:HB3	1:A:63:LEU:HD23	0.64	1.70	1	6
1:A:52:LEU:O	1:A:59:LEU:O	0.64	2.16	3	20
1:A:50:TYR:CD1	1:A:78:MET:HE1	0.63	2.28	15	6
1:A:65:TRP:CZ3	1:A:74:ALA:HB2	0.63	2.28	17	3
1:A:15:LEU:HD21	1:A:77:GLU:CD	0.63	2.13	15	2
1:A:41:ARG:CD	1:A:41:ARG:C	0.63	2.67	9	4
1:A:38:ASP:O	1:A:42:ARG:CD	0.62	2.48	8	20
1:A:36:LEU:HD23	1:A:40:CYS:SG	0.62	2.34	8	5
1:A:65:TRP:CH2	1:A:74:ALA:HB2	0.62	2.29	17	7
1:A:12:VAL:CG2	1:A:76:LEU:HD11	0.62	2.25	13	2
1:A:52:LEU:N	1:A:52:LEU:HD22	0.62	2.09	5	5
1:A:12:VAL:CG1	1:A:76:LEU:CD2	0.61	2.76	11	2
1:A:40:CYS:O	1:A:44:ASP:N	0.61	2.33	20	20
1:A:71:PRO:O	1:A:74:ALA:HB2	0.61	1.94	3	18
1:A:60:ASP:CB	1:A:63:LEU:HD23	0.61	2.26	8	9
1:A:73:ASN:O	1:A:74:ALA:C	0.61	2.38	3	20
1:A:54:PHE:O	1:A:54:PHE:CG	0.61	2.54	6	9
1:A:51:ASP:O	1:A:52:LEU:HD13	0.60	1.94	1	6
1:A:51:ASP:CG	1:A:81:VAL:CG1	0.60	2.70	1	16
1:A:12:VAL:HG12	1:A:76:LEU:CD2	0.60	2.25	6	5
1:A:12:VAL:HG22	1:A:65:TRP:HZ3	0.60	1.54	19	3
1:A:59:LEU:HD21	1:A:70:LEU:CD2	0.60	2.26	3	1
1:A:50:TYR:CD1	1:A:78:MET:HE2	0.60	2.31	18	5
1:A:32:LEU:CD1	1:A:59:LEU:HD12	0.60	2.26	17	5
1:A:14:VAL:O	1:A:22:HIS:O	0.60	2.20	9	20
1:A:28:PRO:HA	1:A:65:TRP:CG	0.60	2.32	1	20
1:A:59:LEU:HD11	1:A:70:LEU:CD2	0.60	2.27	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:PRO:HA	1:A:65:TRP:CD1	0.59	2.32	19	9
1:A:12:VAL:HG21	1:A:26:VAL:CG2	0.59	2.25	19	4
1:A:11:ALA:HB3	1:A:73:ASN:HA	0.59	1.74	5	8
1:A:39:THR:HG22	1:A:43:GLN:OE1	0.59	1.97	16	1
1:A:12:VAL:HG23	1:A:74:ALA:CB	0.59	2.28	12	6
1:A:33:LEU:HD12	1:A:34:GLN:N	0.59	2.12	16	4
1:A:52:LEU:HD12	1:A:52:LEU:N	0.58	2.13	13	2
1:A:39:THR:HG23	1:A:43:GLN:NE2	0.58	2.13	8	3
1:A:76:LEU:N	1:A:76:LEU:CD1	0.58	2.66	6	15
1:A:11:ALA:O	1:A:74:ALA:HB3	0.57	2.00	10	3
1:A:12:VAL:HA	1:A:74:ALA:HB3	0.57	1.75	17	3
1:A:34:GLN:HG3	1:A:35:VAL:N	0.57	2.14	14	20
1:A:54:PHE:C	1:A:54:PHE:CD1	0.57	2.77	6	1
1:A:49:GLU:C	1:A:81:VAL:O	0.57	2.42	10	20
1:A:33:LEU:O	1:A:37:GLU:CG	0.57	2.52	7	20
1:A:41:ARG:CG	1:A:42:ARG:N	0.57	2.68	6	18
1:A:65:TRP:HA	1:A:70:LEU:HD22	0.57	1.76	20	4
1:A:33:LEU:HD12	1:A:33:LEU:C	0.56	2.20	16	2
1:A:13:SER:N	1:A:74:ALA:O	0.56	2.37	6	18
1:A:59:LEU:HD22	1:A:76:LEU:HG	0.56	1.76	11	2
1:A:31:VAL:CG1	1:A:33:LEU:HD23	0.56	2.27	6	4
1:A:32:LEU:HD13	1:A:59:LEU:HD13	0.56	1.75	9	1
1:A:58:VAL:O	1:A:63:LEU:HD13	0.56	2.01	3	1
1:A:12:VAL:HG12	1:A:76:LEU:CD1	0.56	2.27	9	1
1:A:10:SER:OG	1:A:65:TRP:CZ2	0.56	2.51	5	3
1:A:26:VAL:CG1	1:A:27:THR:N	0.56	2.69	14	1
1:A:36:LEU:C	1:A:36:LEU:HD23	0.56	2.21	2	2
1:A:54:PHE:N	1:A:57:THR:O	0.55	2.37	2	6
1:A:15:LEU:C	1:A:15:LEU:CD2	0.55	2.75	19	7
1:A:70:LEU:HD13	1:A:70:LEU:N	0.55	2.15	10	5
1:A:12:VAL:HG23	1:A:74:ALA:HB3	0.55	1.78	12	7
1:A:59:LEU:CD2	1:A:76:LEU:HD22	0.55	2.31	2	1
1:A:12:VAL:HG22	1:A:65:TRP:CZ3	0.55	2.35	19	1
1:A:51:ASP:HB2	1:A:81:VAL:HG12	0.55	1.77	8	16
1:A:40:CYS:O	1:A:44:ASP:CA	0.55	2.54	10	19
1:A:59:LEU:CG	1:A:76:LEU:HD22	0.55	2.31	2	2
1:A:64:GLN:NE2	1:A:67:PHE:CD2	0.55	2.74	11	1
1:A:12:VAL:HA	1:A:74:ALA:O	0.55	2.01	15	16
1:A:62:SER:O	1:A:63:LEU:HD22	0.55	2.02	9	1
1:A:51:ASP:CG	1:A:81:VAL:HG13	0.55	2.22	6	16
1:A:50:TYR:N	1:A:81:VAL:O	0.55	2.39	9	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LEU:HD23	1:A:21:ARG:NH2	0.55	2.17	17	1
1:A:15:LEU:HD21	1:A:77:GLU:OE1	0.54	2.01	1	3
1:A:48:SER:C	1:A:81:VAL:O	0.54	2.45	6	20
1:A:16:ALA:CB	1:A:18:ASN:OD1	0.54	2.56	16	6
1:A:39:THR:HG23	1:A:43:GLN:OE1	0.54	2.01	6	2
1:A:80:PRO:C	1:A:81:VAL:CG2	0.54	2.69	17	4
1:A:32:LEU:O	1:A:35:VAL:HG22	0.54	2.03	5	19
1:A:39:THR:O	1:A:43:GLN:CG	0.54	2.56	4	19
1:A:15:LEU:HD13	1:A:77:GLU:HA	0.54	1.78	13	7
1:A:36:LEU:O	1:A:39:THR:HG22	0.54	2.02	14	2
1:A:69:ASN:C	1:A:70:LEU:HD13	0.54	2.23	10	4
1:A:80:PRO:O	1:A:81:VAL:CG2	0.54	2.54	17	4
1:A:64:GLN:O	1:A:68:ALA:N	0.53	2.36	17	9
1:A:58:VAL:C	1:A:59:LEU:HD22	0.53	2.24	13	7
1:A:65:TRP:CE3	1:A:70:LEU:HB2	0.53	2.38	19	2
1:A:65:TRP:CZ3	1:A:74:ALA:CB	0.53	2.92	17	4
1:A:71:PRO:HD2	1:A:74:ALA:HA	0.53	1.80	6	19
1:A:16:ALA:N	1:A:20:ARG:O	0.53	2.40	13	7
1:A:30:THR:HG23	1:A:34:GLN:OE1	0.53	2.03	13	1
1:A:59:LEU:CD1	1:A:70:LEU:HD21	0.53	2.27	15	2
1:A:51:ASP:CG	1:A:81:VAL:HG23	0.53	2.24	9	2
1:A:31:VAL:HG11	1:A:33:LEU:CD2	0.53	2.30	6	3
1:A:47:PRO:CB	1:A:61:LEU:HD11	0.53	2.34	2	5
1:A:70:LEU:HB3	1:A:74:ALA:HB1	0.53	1.79	9	8
1:A:36:LEU:HD23	1:A:61:LEU:CD2	0.53	2.34	11	6
1:A:12:VAL:HG13	1:A:74:ALA:CB	0.53	2.33	15	2
1:A:12:VAL:O	1:A:24:VAL:N	0.52	2.43	5	7
1:A:35:VAL:CG2	1:A:36:LEU:N	0.52	2.73	1	20
1:A:49:GLU:N	1:A:81:VAL:O	0.52	2.43	5	20
1:A:51:ASP:HB2	1:A:81:VAL:HG23	0.52	1.82	9	4
1:A:31:VAL:HG22	1:A:64:GLN:HG2	0.52	1.81	16	1
1:A:39:THR:O	1:A:43:GLN:CB	0.52	2.58	4	16
1:A:41:ARG:HG2	1:A:42:ARG:N	0.52	2.19	2	14
1:A:60:ASP:N	1:A:63:LEU:HD12	0.52	2.19	3	1
1:A:43:GLN:O	1:A:44:ASP:C	0.51	2.48	13	14
1:A:36:LEU:HD23	1:A:61:LEU:HD23	0.51	1.81	13	3
1:A:80:PRO:O	1:A:81:VAL:CB	0.51	2.58	18	15
1:A:12:VAL:HG13	1:A:76:LEU:CD2	0.51	2.35	8	6
1:A:53:LYS:CG	1:A:57:THR:O	0.51	2.59	20	2
1:A:18:ASN:C	1:A:18:ASN:OD1	0.51	2.49	1	1
1:A:64:GLN:NE2	1:A:67:PHE:CE2	0.51	2.79	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:ARG:HG3	1:A:67:PHE:CD2	0.50	2.41	15	2
1:A:71:PRO:O	1:A:72:ASN:C	0.50	2.50	9	12
1:A:14:VAL:CG1	1:A:52:LEU:HD22	0.50	2.36	18	1
1:A:10:SER:HB3	1:A:65:TRP:CH2	0.50	2.41	3	9
1:A:75:LYS:O	1:A:76:LEU:HD13	0.50	2.05	12	4
1:A:14:VAL:HG11	1:A:52:LEU:HD22	0.50	1.83	18	1
1:A:39:THR:HA	1:A:42:ARG:CG	0.50	2.37	9	20
1:A:52:LEU:O	1:A:59:LEU:CA	0.50	2.60	11	16
1:A:36:LEU:CD1	1:A:52:LEU:HD13	0.49	2.37	6	1
1:A:51:ASP:CB	1:A:81:VAL:HG23	0.49	2.36	9	3
1:A:71:PRO:O	1:A:72:ASN:O	0.49	2.30	9	8
1:A:43:GLN:HG3	1:A:45:PHE:CG	0.49	2.42	7	20
1:A:39:THR:O	1:A:43:GLN:N	0.49	2.42	4	16
1:A:12:VAL:HG23	1:A:26:VAL:HG13	0.49	1.83	9	1
1:A:54:PHE:CZ	1:A:71:PRO:HD3	0.49	2.41	9	1
1:A:43:GLN:CG	1:A:45:PHE:HB2	0.49	2.37	7	19
1:A:65:TRP:C	1:A:65:TRP:CD1	0.49	2.86	16	7
1:A:65:TRP:CH2	1:A:71:PRO:O	0.49	2.65	17	8
1:A:73:ASN:O	1:A:74:ALA:O	0.49	2.30	7	7
1:A:32:LEU:CD1	1:A:59:LEU:CD1	0.49	2.89	9	2
1:A:36:LEU:HD12	1:A:52:LEU:HD13	0.49	1.83	6	1
1:A:54:PHE:CE1	1:A:55:GLN:OE1	0.48	2.67	17	1
1:A:15:LEU:CD1	1:A:77:GLU:HA	0.48	2.39	20	4
1:A:13:SER:HA	1:A:23:THR:HA	0.48	1.85	14	3
1:A:48:SER:O	1:A:82:SER:CB	0.48	2.61	10	1
1:A:32:LEU:CD2	1:A:59:LEU:HD23	0.48	2.39	6	1
1:A:15:LEU:O	1:A:15:LEU:CD2	0.48	2.56	17	7
1:A:12:VAL:HG13	1:A:74:ALA:HB3	0.48	1.85	9	2
1:A:39:THR:C	1:A:43:GLN:OE1	0.48	2.53	16	8
1:A:32:LEU:HD11	1:A:70:LEU:HD11	0.48	1.85	4	4
1:A:65:TRP:CZ3	1:A:70:LEU:HB2	0.48	2.44	19	1
1:A:36:LEU:CD1	1:A:40:CYS:SG	0.47	3.02	19	2
1:A:81:VAL:HG13	1:A:82:SER:N	0.47	2.22	6	12
1:A:32:LEU:HD11	1:A:70:LEU:CD2	0.47	2.37	18	2
1:A:35:VAL:O	1:A:39:THR:HG23	0.47	2.08	19	1
1:A:14:VAL:HB	1:A:22:HIS:CE1	0.47	2.44	13	13
1:A:81:VAL:HG22	1:A:82:SER:N	0.47	2.21	6	10
1:A:54:PHE:CE2	1:A:71:PRO:HD3	0.47	2.44	2	4
1:A:54:PHE:CZ	1:A:71:PRO:HG3	0.47	2.43	13	3
1:A:18:ASN:OD1	1:A:20:ARG:N	0.47	2.47	2	6
1:A:17:PRO:CD	1:A:78:MET:O	0.47	2.62	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:C	1:A:33:LEU:HD12	0.47	2.29	2	3
1:A:51:ASP:OD1	1:A:81:VAL:HG13	0.47	2.09	1	1
1:A:14:VAL:HG13	1:A:76:LEU:HB2	0.47	1.86	9	1
1:A:67:PHE:O	1:A:69:ASN:ND2	0.47	2.48	12	5
1:A:64:GLN:OE1	1:A:64:GLN:N	0.47	2.47	5	3
1:A:65:TRP:O	1:A:69:ASN:N	0.47	2.48	6	6
1:A:48:SER:HA	1:A:82:SER:HA	0.47	1.86	17	6
1:A:12:VAL:HB	1:A:26:VAL:HG13	0.46	1.87	10	2
1:A:68:ALA:C	1:A:69:ASN:ND2	0.46	2.69	13	7
1:A:69:ASN:O	1:A:69:ASN:ND2	0.46	2.49	19	8
1:A:55:GLN:CG	1:A:56:ARG:N	0.46	2.76	4	5
1:A:39:THR:O	1:A:43:GLN:HG2	0.46	2.10	7	8
1:A:68:ALA:O	1:A:69:ASN:O	0.46	2.34	2	15
1:A:12:VAL:HB	1:A:24:VAL:O	0.46	2.10	17	4
1:A:17:PRO:HD3	1:A:78:MET:O	0.46	2.10	17	5
1:A:72:ASN:OD1	1:A:72:ASN:N	0.46	2.48	4	11
1:A:12:VAL:CG2	1:A:76:LEU:HD21	0.46	2.34	12	2
1:A:54:PHE:CE1	1:A:55:GLN:HG3	0.45	2.46	8	2
1:A:12:VAL:HB	1:A:26:VAL:HG22	0.45	1.88	3	2
1:A:81:VAL:CG2	1:A:82:SER:H	0.45	2.21	2	7
1:A:32:LEU:CD1	1:A:63:LEU:O	0.45	2.64	2	1
1:A:36:LEU:CD2	1:A:40:CYS:SG	0.45	3.05	15	2
1:A:40:CYS:O	1:A:44:ASP:HA	0.45	2.12	10	5
1:A:31:VAL:O	1:A:35:VAL:HG13	0.45	2.12	12	11
1:A:47:PRO:O	1:A:50:TYR:O	0.45	2.35	14	20
1:A:68:ALA:O	1:A:69:ASN:CG	0.45	2.55	1	12
1:A:52:LEU:N	1:A:52:LEU:CD2	0.45	2.80	5	1
1:A:32:LEU:HD22	1:A:59:LEU:HD23	0.45	1.86	6	1
1:A:39:THR:HG22	1:A:43:GLN:NE2	0.45	2.27	16	2
1:A:50:TYR:CD1	1:A:78:MET:HE3	0.45	2.45	1	1
1:A:31:VAL:O	1:A:34:GLN:HG3	0.45	2.12	3	15
1:A:70:LEU:HB3	1:A:74:ALA:CB	0.45	2.42	9	4
1:A:66:ARG:HG3	1:A:67:PHE:CD1	0.45	2.46	11	1
1:A:18:ASN:OD1	1:A:18:ASN:C	0.44	2.55	13	6
1:A:12:VAL:HG12	1:A:24:VAL:O	0.44	2.12	10	4
1:A:78:MET:SD	1:A:79:VAL:N	0.44	2.90	19	4
1:A:30:THR:HG23	1:A:34:GLN:CG	0.44	2.42	2	2
1:A:34:GLN:OE1	1:A:34:GLN:C	0.44	2.56	7	9
1:A:65:TRP:CE3	1:A:70:LEU:CD2	0.44	2.99	9	2
1:A:49:GLU:C	1:A:81:VAL:H	0.44	2.16	18	4
1:A:53:LYS:O	1:A:77:GLU:CG	0.44	2.66	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:ASP:HB2	1:A:81:VAL:CG2	0.44	2.42	9	3
1:A:65:TRP:CD1	1:A:65:TRP:C	0.44	2.91	19	4
1:A:72:ASN:C	1:A:74:ALA:N	0.44	2.71	5	9
1:A:51:ASP:HB2	1:A:81:VAL:CG1	0.44	2.43	6	6
1:A:12:VAL:CG2	1:A:74:ALA:HB3	0.44	2.43	20	2
1:A:43:GLN:HG3	1:A:45:PHE:CD1	0.44	2.48	8	10
1:A:64:GLN:N	1:A:64:GLN:CD	0.44	2.71	3	1
1:A:36:LEU:HD13	1:A:61:LEU:HD23	0.44	1.88	14	1
1:A:54:PHE:CD1	1:A:54:PHE:C	0.43	2.90	14	2
1:A:65:TRP:CZ2	1:A:70:LEU:O	0.43	2.71	3	2
1:A:15:LEU:O	1:A:15:LEU:CD1	0.43	2.64	19	1
1:A:28:PRO:CA	1:A:65:TRP:CD1	0.43	3.00	19	1
1:A:40:CYS:HA	1:A:43:GLN:HG2	0.43	1.91	1	1
1:A:63:LEU:HD22	1:A:63:LEU:N	0.43	2.29	1	4
1:A:16:ALA:HB1	1:A:18:ASN:ND2	0.43	2.29	15	3
1:A:12:VAL:CG2	1:A:26:VAL:HG13	0.43	2.43	9	2
1:A:41:ARG:C	1:A:41:ARG:HD2	0.43	2.34	16	2
1:A:52:LEU:HD13	1:A:52:LEU:N	0.43	2.27	1	1
1:A:31:VAL:O	1:A:34:GLN:CG	0.43	2.67	13	2
1:A:68:ALA:O	1:A:69:ASN:C	0.43	2.56	12	2
1:A:20:ARG:O	1:A:20:ARG:CG	0.43	2.64	16	1
1:A:39:THR:O	1:A:43:GLN:OE1	0.43	2.36	19	1
1:A:39:THR:HA	1:A:42:ARG:HD3	0.42	1.91	17	2
1:A:55:GLN:HG2	1:A:56:ARG:N	0.42	2.29	2	2
1:A:31:VAL:CG2	1:A:33:LEU:HG	0.42	2.44	13	2
1:A:72:ASN:C	1:A:74:ALA:H	0.42	2.16	5	7
1:A:32:LEU:N	1:A:32:LEU:HD22	0.42	2.30	16	1
1:A:28:PRO:HA	1:A:65:TRP:CD2	0.42	2.49	11	1
1:A:64:GLN:OE1	1:A:67:PHE:CD2	0.42	2.73	2	1
1:A:32:LEU:HD11	1:A:70:LEU:CD1	0.42	2.44	4	1
1:A:14:VAL:HA	1:A:76:LEU:O	0.42	2.15	13	1
1:A:51:ASP:OD1	1:A:82:SER:O	0.42	2.37	8	3
1:A:11:ALA:N	1:A:72:ASN:O	0.42	2.48	5	2
1:A:52:LEU:N	1:A:52:LEU:CD1	0.42	2.83	13	1
1:A:69:ASN:O	1:A:69:ASN:OD1	0.42	2.38	12	7
1:A:54:PHE:CD2	1:A:57:THR:HB	0.42	2.49	19	2
1:A:51:ASP:HB2	1:A:79:VAL:CG1	0.42	2.44	17	1
1:A:71:PRO:CD	1:A:74:ALA:HA	0.42	2.45	18	6
1:A:40:CYS:HB3	1:A:45:PHE:O	0.42	2.15	20	3
1:A:18:ASN:OD1	1:A:20:ARG:HB2	0.42	2.13	4	2
1:A:62:SER:O	1:A:63:LEU:HD13	0.42	2.15	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:VAL:HG13	1:A:64:GLN:HG2	0.42	1.91	16	1
1:A:12:VAL:CA	1:A:24:VAL:O	0.41	2.68	14	1
1:A:36:LEU:HD12	1:A:40:CYS:SG	0.41	2.55	19	1
1:A:68:ALA:C	1:A:69:ASN:OD1	0.41	2.59	3	5
1:A:59:LEU:CD2	1:A:76:LEU:HG	0.41	2.44	6	1
1:A:13:SER:O	1:A:75:LYS:HA	0.41	2.16	19	1
1:A:33:LEU:O	1:A:37:GLU:CB	0.41	2.68	1	1
1:A:82:SER:O	1:A:82:SER:OG	0.41	2.38	10	1
1:A:68:ALA:O	1:A:69:ASN:OD1	0.41	2.38	12	2
1:A:12:VAL:CG2	1:A:26:VAL:HG21	0.41	2.45	10	1
1:A:36:LEU:O	1:A:40:CYS:SG	0.41	2.79	11	3
1:A:62:SER:O	1:A:63:LEU:HD23	0.41	2.15	14	1
1:A:48:SER:O	1:A:82:SER:HB2	0.41	2.16	1	1
1:A:54:PHE:HB3	1:A:59:LEU:CD1	0.41	2.46	6	1
1:A:72:ASN:ND2	1:A:72:ASN:H	0.41	2.14	10	1
1:A:18:ASN:OD1	1:A:18:ASN:N	0.41	2.48	11	1
1:A:30:THR:HG23	1:A:34:GLN:CD	0.41	2.36	13	1
1:A:12:VAL:N	1:A:24:VAL:O	0.41	2.54	14	1
1:A:59:LEU:HD11	1:A:70:LEU:CD1	0.41	2.42	7	1
1:A:31:VAL:HG12	1:A:33:LEU:H	0.40	1.76	8	1
1:A:60:ASP:HB3	1:A:63:LEU:CD2	0.40	2.45	10	1
1:A:15:LEU:HD11	1:A:77:GLU:OE1	0.40	2.15	15	1
1:A:16:ALA:CB	1:A:20:ARG:HG2	0.40	2.47	16	1
1:A:38:ASP:O	1:A:42:ARG:HD2	0.40	2.17	4	1
1:A:39:THR:O	1:A:43:GLN:HB3	0.40	2.17	12	1
1:A:69:ASN:O	1:A:69:ASN:CG	0.40	2.60	2	1
1:A:54:PHE:O	1:A:54:PHE:CD2	0.40	2.75	12	1
1:A:48:SER:C	1:A:82:SER:HA	0.40	2.37	18	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	72/90 (80%)	63±1 (87±1%)	5±1 (7±1%)	4±0 (6±0%)	3 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1440/1800 (80%)	1256 (87%)	104 (7%)	80 (6%)	3 22

All 4 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	69	ASN	20
1	A	72	ASN	20
1	A	74	ALA	20
1	A	81	VAL	20

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	68/77 (88%)	49±3 (72±4%)	19±3 (28±4%)	2 19
All	All	1360/1540 (88%)	974 (72%)	386 (28%)	2 19

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	14	VAL	20
1	A	27	THR	20
1	A	34	GLN	20
1	A	35	VAL	20
1	A	42	ARG	20
1	A	72	ASN	20
1	A	76	LEU	20
1	A	78	MET	20
1	A	75	LYS	19
1	A	41	ARG	18
1	A	54	PHE	17
1	A	25	LYS	16
1	A	21	ARG	14
1	A	70	LEU	11
1	A	65	TRP	9

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Mol	Chain	Res	Type	Models (Total)
1	A	73	ASN	9
1	A	20	ARG	8
1	A	12	VAL	8
1	A	56	ARG	8
1	A	15	LEU	8
1	A	45	PHE	7
1	A	64	GLN	7
1	A	38	ASP	7
1	A	52	LEU	6
1	A	77	GLU	6
1	A	32	LEU	5
1	A	46	ASN	5
1	A	26	VAL	5
1	A	79	VAL	4
1	A	81	VAL	4
1	A	53	LYS	4
1	A	59	LEU	3
1	A	44	ASP	3
1	A	66	ARG	3
1	A	30	THR	2
1	A	51	ASP	2
1	A	23	THR	1
1	A	61	LEU	1
1	A	60	ASP	1
1	A	82	SER	1
1	A	10	SER	1
1	A	24	VAL	1
1	A	55	GLN	1
1	A	33	LEU	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