Full wwPDB NMR Structure Validation Report (i)

Feb 22, 2022 – 02:27 PM EST

PDB ID	:	1VNA
Title	:	PROTON NUCLEAR MAGNETIC RESONANCE AND DISTANCE GEOMETRY(SLASH)SIMULATED ANNEALING STUDIES ON THE VARIANT-1 NEUROTOXIN FROM THE NEW WORLD SCORPION CENTRUROIDES SCULPTURATUS EWING
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Deposited on	:	1993-10-26

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

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

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

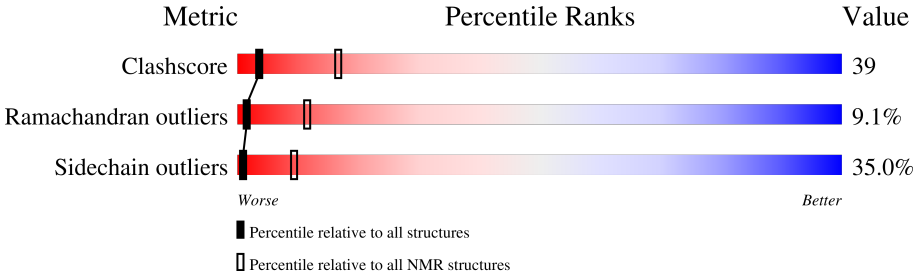
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	65	14% 77% 9%

2 Ensemble composition and analysis (i)

This entry contains 26 models. Model 20 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:1-A:65 (65)	0.91	20

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 5, 6, 9, 10, 11, 13, 14, 16, 18, 19, 20, 22, 24
2	2, 3, 7, 8, 12, 21, 23, 25, 26
3	15, 17
Single-model clusters	4

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 975 atoms, of which 465 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NEUROTOXIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	65	975	322	465	82	98	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: NEUROTOXIN

Chain A: 14% 77% 9%

K1 E2 G3 Y4 L5 V6 K7 K8 S9 D10 G11 C12 K13 Y14 D15 C16 F17 W18 L19 G20 K21 N22 E23 H24 C25 N26 T27 E28 C29 K30 A31 K32 N33 Q34 G35 G36 S37 Y38 G39 Y40 C41 Y42 A43 F44 A45 C46 W47 C48 E49 G50 L51 S54 T55 P56 T57 Y58 P59 L60 P61

N62 K63 S64 C65

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: NEUROTOXIN

Chain A: 31% 54% 14%

K1 E2 G3 Y4 L5 V6 K7 K8 S9 D10 G11 C12 K13 Y14 D15 C16 F17 W18 L19 N22 E23 H24 C25 N26 T27 E28 C29 K30 A31 K32 N33 Q34 S37 Y38 Y42 A43 F44 A45 C46 W47 C48 L51 P52 E53 S54 T55 P56 T57 Y58 P59 S64 C65

4.2.2 Score per residue for model 2

• Molecule 1: NEUROTOXIN

Chain A: 29% 46% 22%

K1 Y4 L5 V6 K7 K8 S9 D10 G11 C12 K13 Y14 D15 C16 F17 W18 L19 G20 K21 N22 E23 H24 C25 N26 T27 E28 C29 K30 A31 K32 N33 Q34 G35 G36 Y40 C41 Y42 A43 F44 A45 L51 P52 E53 S54 T55 P56 T57 Y58 P59 L60 K63 S64 C65

4.2.3 Score per residue for model 3

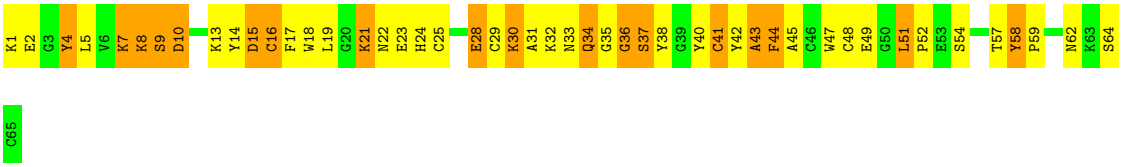
- Molecule 1: NEUROTOXIN

Chain A: 28% 58% 14%

4.2.4 Score per residue for model 4

- Molecule 1: NEUROTOXIN

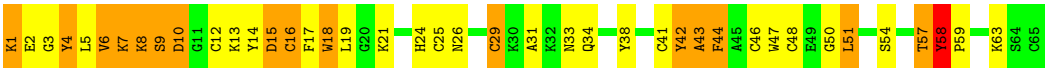
Chain A: 26% 46% 28%



4.2.5 Score per residue for model 5

- Molecule 1: NEUROTOXIN

Chain A: 37% 37% 25% •



4.2.6 Score per residue for model 6

- Molecule 1: NEUROTOXIN

Chain A: 40% 42% 14% 5%

4.2.7 Score per residue for model 7

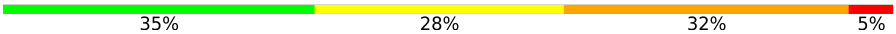
- Molecule 1: NEUROTOXIN

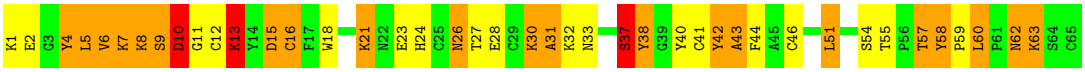
Chain A: 34% 49% 15% •

4.2.8 Score per residue for model 8

- Molecule 1: NEUROTOXIN

Chain A:

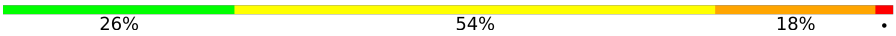


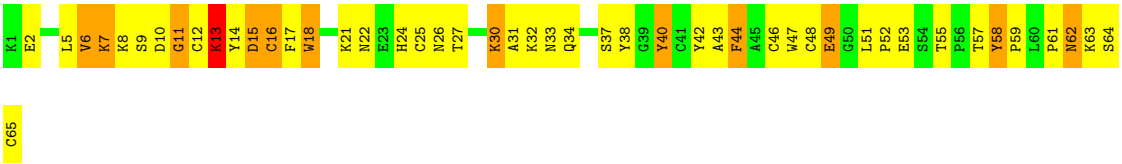


4.2.9 Score per residue for model 9

- Molecule 1: NEUROTOXIN

Chain A:

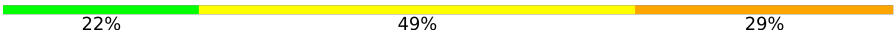




4.2.10 Score per residue for model 10

- Molecule 1: NEUROTOXIN

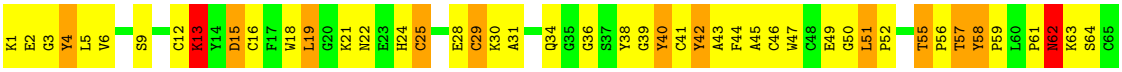
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: NEUROTOXIN

Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: NEUROTOXIN

Chain A: 35% 45% 18% •

K1 V6 K7 K8 S9 D10 G11 C12 K13 Y14 D15 C16 F17 W18 L19 G20 K21 N22 E23 E28 C29 K30 A31 K32 N33 Q34 G35 G36 S37 Y38 Y42 A43 F44 A45 C46 W47 C48 E49 G50 L51 T55 P56 T57 Y58 P59 L60 P61 N62 K63 S64 C65

4.2.13 Score per residue for model 13

- Molecule 1: NEUROTOXIN

Chain A: 26% 48% 23% •

K1 Y4 L5 V6 K7 K8 S9 D10 G11 C12 K13 Y14 D15 C16 F17 W18 L19 G20 K21 N22 E23 H24 C25 N26 T27 E28 C29 K30 A31 K32 N33 Q34 Y38 G39 Y40 C41 Y42 A43 F44 A45 C46 W47 E53 S54 T55 P56 T57 Y58 P59 L60 P61 N62 K63 S64 C65

4.2.14 Score per residue for model 14

- Molecule 1: NEUROTOXIN

Chain A: 45% 42% 14%

K1 Y4 L5 V6 K7 K8 S9 D10 G11 C12 K13 Y14 D15 C16 K21 N22 E23 H24 C25 N26 T27 E28 C29 K30 A31 K32 G39 Y40 C41 Y42 A43 F44 A45 C46 W47 E53 P56 T57 Y58 P59 L60 P61 N62 K63 S64 C65

4.2.15 Score per residue for model 15

- Molecule 1: NEUROTOXIN

Chain A: 28% 42% 25% 6%

K1 E2 G3 Y4 L5 V6 K7 K8 S9 D10 G11 C12 K13 Y14 D15 C16 F17 W18 L19 G20 K21 N22 E23 H24 C25 N26 T27 E28 C29 K30 A31 K32 G36 S37 Y38 G39 Y40 C41 Y42 A43 F44 A45 C46 W47 L51 P52 E53 S54 T57 Y58 P59 L60 P61 N62 K63 S64 C65

4.2.16 Score per residue for model 16

- Molecule 1: NEUROTOXIN

Chain A: 42% 48% 11%

K1 E2 G3 Y4 L5 V6 K7 K8 C12 K13 Y14 D15 C16 L19 H24 C25 N26 T27 E28 C29 K30 A31 K32 N33 Q34 Y38 G39 Y40 C41 Y42 A43 F44 A45 C46 W47 C48 E49 G50 L51 S54 T57 Y58 P59 N62 K63 S64 C65

4.2.17 Score per residue for model 17

- Molecule 1: NEUROTOXIN

Chain A: 31% 46% 20% •

K1 E2 G3 Y4 L5 V6 K7 K8 S9 D10 G11 C12 K13 Y14 D15 C16 N22 E23 H24 C25 N26 T27 E28 C29 K30 A31 K32 N33 Q34 Y38 G39 Y40 C41 Y42 A43 F44 W47 C48 E49 G50 L51 P52 T55 P56 T57 Y58 P59 L60 P61 N62 K63 S64 C65

4.2.18 Score per residue for model 18

- Molecule 1: NEUROTOXIN

Chain A: 37% 42% 22%

K1 E2 L5 V6 K7 K8 S9 D10 K13 Y14 D15 C16 F17 W18 N22 N26 T27 E28 C29 K30 A31 K32 G35 G36 S37 Y42 A43 F44 A45 C46 W47 C48 E49 G50 L51 T57 Y58 P59 L60 P61 N62 K63 S64 C65

4.2.19 Score per residue for model 19

- Molecule 1: NEUROTOXIN

Chain A: 26% 58% 14% •

K1 E2 G3 Y4 L5 V6 K7 K8 S9 C12 K13 Y14 D15 C16 L19 G20 K21 H24 C25 N26 T27 E28 C29 K30 A31 K32 G35 G36 S37 Y38 G39 Y40 C41 Y42 A43 F44 A45 C46 W47 C48 E49 G50 L51 P52 E53 S54 T55 P56 T57 Y58 P59 L60 P61 N62 K63 S64

C65

4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: NEUROTOXIN

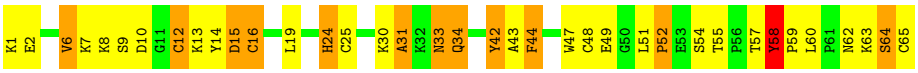
Chain A: 31% 54% 15%

K1 E2 G3 Y4 L5 V6 K7 K8 S9 D10 G11 C12 K13 Y14 D15 C16 F17 W18 L19 G20 K21 C25 N26 T27 E28 C29 K32 N33 Q34 G35 G36 S37 Y38 C41 Y42 A43 F44 A45 C46 W47 C48 L51 S54 T55 P56 T57 Y58 P59 L60 P61 N62 K63 S64 C65

4.2.21 Score per residue for model 21

- Molecule 1: NEUROTOXIN

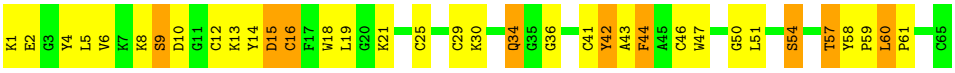
Chain A: 43% 37% 18% •



4.2.22 Score per residue for model 22

- Molecule 1: NEUROTOXIN

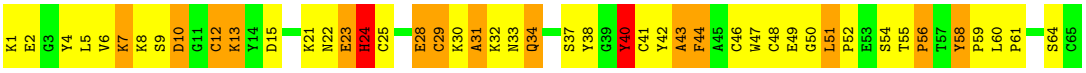
Chain A: 46% 40% 14%



4.2.23 Score per residue for model 23

- Molecule 1: NEUROTOXIN

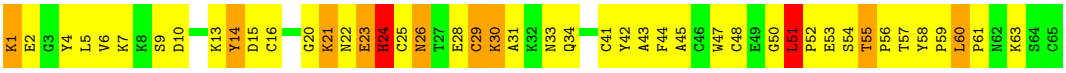
Chain A: 29% 46% 22% •



4.2.24 Score per residue for model 24

- Molecule 1: NEUROTOXIN

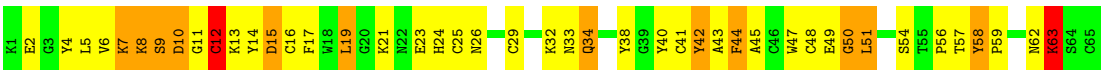
Chain A: 31% 52% 14% •



4.2.25 Score per residue for model 25

- Molecule 1: NEUROTOXIN

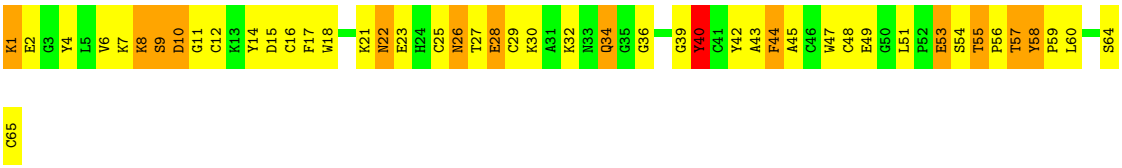
Chain A: 32% 46% 18% •



4.2.26 Score per residue for model 26

- Molecule 1: NEUROTOXIN

Chain A: 28% 51% 20% •


K1
E2
G3
Y4
L5
V6
K7
K8
S9
D10
G11
C12
K13
Y14
D15
C16
F17
W18
K21
N22
E23
H24
C25
N26
T27
E28
C29
K30
A31
K32
N33
Q34
G35
G36
G39
Y40
C41
Y42
A43
F44
A45
C46
W47
C48
E49
G50
L51
P52
E53
S54
T55
P56
T57
Y58
P59
L60
S64
C65

5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 26 were deposited, based on the following criterion: *?*.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	510	465	465	38±9
All	All	13260	12090	12090	995

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:GLY:C	1:A:51:LEU:HD13	0.94	1.82	10	1
1:A:6:VAL:HG23	1:A:12:CYS:O	0.91	1.63	2	6
1:A:51:LEU:HD12	1:A:51:LEU:O	0.89	1.67	7	1
1:A:51:LEU:O	1:A:51:LEU:HD22	0.88	1.69	5	3
1:A:60:LEU:HD12	1:A:65:CYS:O	0.86	1.70	17	1
1:A:51:LEU:HD12	1:A:52:PRO:O	0.85	1.72	21	1
1:A:51:LEU:HD23	1:A:57:THR:HG21	0.84	1.48	15	1
1:A:60:LEU:HD13	1:A:61:PRO:HD2	0.84	1.49	24	2
1:A:51:LEU:HD12	1:A:55:THR:HG21	0.84	1.47	1	2
1:A:5:LEU:HD12	1:A:46:CYS:HB3	0.82	1.49	20	4
1:A:19:LEU:HD21	1:A:43:ALA:O	0.81	1.75	21	10
1:A:56:PRO:O	1:A:57:THR:HG23	0.77	1.80	14	4
1:A:51:LEU:HD22	1:A:51:LEU:N	0.76	1.95	10	4
1:A:51:LEU:HD23	1:A:55:THR:CG2	0.76	2.10	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:VAL:HG11	1:A:60:LEU:HD23	0.76	1.57	24	1
1:A:51:LEU:HD23	1:A:51:LEU:N	0.76	1.96	6	4
1:A:51:LEU:HD22	1:A:51:LEU:H	0.75	1.40	10	1
1:A:19:LEU:HD23	1:A:41:CYS:SG	0.75	2.21	19	2
1:A:8:LYS:O	1:A:10:ASP:N	0.74	2.21	7	2
1:A:51:LEU:C	1:A:51:LEU:HD22	0.73	2.04	11	2
1:A:51:LEU:HD22	1:A:51:LEU:C	0.73	2.04	17	3
1:A:5:LEU:HD12	1:A:46:CYS:HB2	0.72	1.61	23	1
1:A:40:TYR:CE2	1:A:47:TRP:CH2	0.72	2.78	6	1
1:A:6:VAL:HG21	1:A:58:TYR:CD1	0.71	2.20	11	1
1:A:58:TYR:CE1	1:A:60:LEU:HD12	0.71	2.20	23	1
1:A:6:VAL:HG11	1:A:60:LEU:CD2	0.71	2.16	24	1
1:A:51:LEU:HD13	1:A:51:LEU:N	0.71	2.00	10	1
1:A:40:TYR:CZ	1:A:47:TRP:CH2	0.70	2.80	6	1
1:A:4:TYR:CE2	1:A:47:TRP:CZ3	0.70	2.80	25	3
1:A:34:GLN:HG2	1:A:51:LEU:HD12	0.69	1.64	24	1
1:A:4:TYR:CZ	1:A:45:ALA:HB3	0.69	2.22	2	3
1:A:48:CYS:HB2	1:A:51:LEU:HD11	0.69	1.63	25	2
1:A:27:THR:O	1:A:31:ALA:HB2	0.68	1.88	9	2
1:A:51:LEU:HD22	1:A:52:PRO:O	0.67	1.90	17	3
1:A:42:TYR:O	1:A:43:ALA:HB3	0.67	1.90	4	15
1:A:51:LEU:HD11	1:A:57:THR:HG21	0.67	1.63	3	1
1:A:5:LEU:HD12	1:A:25:CYS:SG	0.67	2.30	10	4
1:A:4:TYR:CD1	1:A:47:TRP:CB	0.66	2.79	6	1
1:A:51:LEU:CD1	1:A:57:THR:HG21	0.66	2.20	6	2
1:A:51:LEU:O	1:A:51:LEU:HD13	0.65	1.91	17	4
1:A:40:TYR:CZ	1:A:47:TRP:CZ3	0.65	2.84	6	1
1:A:40:TYR:CD1	1:A:40:TYR:N	0.65	2.64	9	8
1:A:51:LEU:HD11	1:A:55:THR:HG22	0.65	1.69	24	1
1:A:43:ALA:O	1:A:44:PHE:CG	0.65	2.50	23	26
1:A:60:LEU:HD22	1:A:63:LYS:CE	0.63	2.23	17	1
1:A:50:GLY:C	1:A:51:LEU:HD23	0.63	2.14	25	2
1:A:51:LEU:HD22	1:A:51:LEU:O	0.63	1.94	11	2
1:A:55:THR:O	1:A:55:THR:HG23	0.63	1.94	21	2
1:A:4:TYR:CE1	1:A:45:ALA:HB1	0.63	2.29	1	2
1:A:6:VAL:HG13	1:A:13:LYS:HA	0.62	1.70	9	2
1:A:51:LEU:HD12	1:A:57:THR:HG21	0.62	1.70	25	2
1:A:1:LYS:O	1:A:51:LEU:HD11	0.62	1.95	5	1
1:A:5:LEU:HD21	1:A:34:GLN:NE2	0.62	2.09	13	2
1:A:40:TYR:CE2	1:A:47:TRP:CZ3	0.61	2.88	6	1
1:A:47:TRP:O	1:A:47:TRP:CE3	0.61	2.53	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ALA:HB3	1:A:33:ASN:OD1	0.61	1.95	4	4
1:A:7:LYS:O	1:A:8:LYS:C	0.61	2.39	7	13
1:A:51:LEU:HD12	1:A:55:THR:CG2	0.61	2.25	1	1
1:A:5:LEU:HD12	1:A:46:CYS:CB	0.61	2.24	23	4
1:A:59:PRO:O	1:A:60:LEU:HD23	0.61	1.95	13	2
1:A:19:LEU:HD21	1:A:43:ALA:C	0.61	2.15	21	2
1:A:60:LEU:HD22	1:A:63:LYS:HE2	0.61	1.71	17	1
1:A:60:LEU:HD12	1:A:65:CYS:C	0.60	2.15	17	1
1:A:60:LEU:CB	1:A:61:PRO:CD	0.60	2.79	13	1
1:A:47:TRP:CD1	1:A:48:CYS:N	0.60	2.69	12	7
1:A:6:VAL:HG13	1:A:13:LYS:CA	0.60	2.25	9	1
1:A:9:SER:O	1:A:10:ASP:CB	0.60	2.48	26	9
1:A:43:ALA:O	1:A:44:PHE:CD1	0.60	2.54	5	10
1:A:6:VAL:HG21	1:A:58:TYR:CE1	0.60	2.31	11	1
1:A:51:LEU:CD1	1:A:51:LEU:N	0.60	2.65	23	5
1:A:4:TYR:CE2	1:A:45:ALA:HB3	0.60	2.32	20	1
1:A:6:VAL:HG11	1:A:60:LEU:HD21	0.60	1.74	20	2
1:A:18:TRP:CD1	1:A:21:LYS:O	0.59	2.55	4	1
1:A:43:ALA:O	1:A:44:PHE:CD2	0.59	2.55	21	9
1:A:42:TYR:O	1:A:43:ALA:C	0.59	2.41	5	11
1:A:17:PHE:CD1	1:A:17:PHE:O	0.59	2.56	9	1
1:A:42:TYR:O	1:A:43:ALA:CB	0.58	2.52	4	15
1:A:60:LEU:CB	1:A:61:PRO:HD2	0.58	2.29	13	1
1:A:51:LEU:N	1:A:51:LEU:HD13	0.58	2.13	5	4
1:A:59:PRO:O	1:A:60:LEU:HD22	0.58	1.98	19	1
1:A:6:VAL:HG13	1:A:13:LYS:N	0.58	2.14	9	1
1:A:8:LYS:O	1:A:9:SER:C	0.58	2.42	25	13
1:A:57:THR:O	1:A:58:TYR:C	0.58	2.41	13	16
1:A:2:GLU:OE1	1:A:47:TRP:CZ2	0.58	2.57	5	1
1:A:51:LEU:HD12	1:A:51:LEU:C	0.57	2.18	7	1
1:A:4:TYR:CE1	1:A:45:ALA:HB3	0.57	2.34	13	4
1:A:2:GLU:CB	1:A:47:TRP:CZ2	0.57	2.88	17	4
1:A:4:TYR:CD1	1:A:47:TRP:HB2	0.57	2.35	6	1
1:A:14:TYR:CD1	1:A:46:CYS:SG	0.57	2.98	22	1
1:A:5:LEU:HD21	1:A:34:GLN:OE1	0.57	2.00	2	2
1:A:5:LEU:HD11	1:A:29:CYS:SG	0.57	2.40	15	2
1:A:4:TYR:CE1	1:A:45:ALA:CB	0.57	2.88	1	3
1:A:34:GLN:HG3	1:A:51:LEU:HD11	0.57	1.77	26	1
1:A:4:TYR:CE1	1:A:47:TRP:CD2	0.57	2.93	10	1
1:A:51:LEU:HD23	1:A:57:THR:HG23	0.56	1.76	26	1
1:A:6:VAL:HG11	1:A:58:TYR:HB2	0.56	1.76	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:VAL:CG2	1:A:7:LYS:N	0.56	2.68	20	3
1:A:3:GLY:O	1:A:47:TRP:CE3	0.56	2.59	19	1
1:A:2:GLU:OE1	1:A:47:TRP:CE2	0.56	2.58	10	1
1:A:22:ASN:O	1:A:23:GLU:O	0.56	2.24	13	1
1:A:4:TYR:CG	1:A:47:TRP:HB3	0.56	2.36	6	1
1:A:23:GLU:O	1:A:25:CYS:N	0.56	2.38	13	1
1:A:4:TYR:CZ	1:A:47:TRP:CE3	0.56	2.94	25	6
1:A:51:LEU:HD13	1:A:55:THR:CG2	0.56	2.31	21	1
1:A:51:LEU:HD23	1:A:51:LEU:H	0.55	1.59	4	1
1:A:51:LEU:N	1:A:51:LEU:CD2	0.55	2.69	19	5
1:A:22:ASN:O	1:A:24:HIS:N	0.55	2.40	24	2
1:A:28:GLU:O	1:A:31:ALA:HB3	0.55	2.01	15	1
1:A:7:LYS:HG3	1:A:14:TYR:CE2	0.55	2.37	20	2
1:A:16:CYS:SG	1:A:16:CYS:O	0.55	2.65	16	10
1:A:60:LEU:HD13	1:A:63:LYS:HD3	0.55	1.76	15	1
1:A:6:VAL:HG22	1:A:7:LYS:N	0.55	2.17	20	4
1:A:2:GLU:HB2	1:A:47:TRP:CZ2	0.55	2.37	24	4
1:A:51:LEU:CD2	1:A:57:THR:HG21	0.55	2.31	21	1
1:A:55:THR:HG23	1:A:56:PRO:HD2	0.55	1.78	12	3
1:A:47:TRP:CE3	1:A:47:TRP:C	0.54	2.81	6	1
1:A:19:LEU:HD23	1:A:42:TYR:O	0.54	2.03	7	1
1:A:47:TRP:C	1:A:47:TRP:CD1	0.54	2.80	23	3
1:A:61:PRO:O	1:A:62:ASN:CB	0.54	2.55	18	4
1:A:38:TYR:CD2	1:A:49:GLU:OE2	0.54	2.61	17	1
1:A:58:TYR:CG	1:A:59:PRO:HA	0.54	2.37	7	9
1:A:4:TYR:OH	1:A:42:TYR:CD2	0.54	2.59	23	2
1:A:10:ASP:O	1:A:11:GLY:C	0.54	2.45	9	1
1:A:6:VAL:O	1:A:14:TYR:CG	0.54	2.59	18	1
1:A:4:TYR:CG	1:A:47:TRP:CB	0.54	2.91	6	1
1:A:62:ASN:N	1:A:62:ASN:OD1	0.54	2.40	10	1
1:A:5:LEU:HD22	1:A:34:GLN:HG2	0.54	1.77	4	1
1:A:43:ALA:C	1:A:44:PHE:CD2	0.54	2.82	10	2
1:A:16:CYS:SG	1:A:45:ALA:N	0.54	2.81	11	4
1:A:47:TRP:C	1:A:47:TRP:CD2	0.53	2.81	6	1
1:A:60:LEU:HB3	1:A:61:PRO:HD2	0.53	1.79	13	2
1:A:9:SER:O	1:A:11:GLY:N	0.53	2.41	7	2
1:A:2:GLU:HB3	1:A:47:TRP:CE2	0.53	2.39	4	3
1:A:34:GLN:O	1:A:52:PRO:CD	0.53	2.56	17	1
1:A:58:TYR:CE1	1:A:65:CYS:O	0.53	2.61	17	1
1:A:6:VAL:CG2	1:A:11:GLY:O	0.53	2.57	20	1
1:A:7:LYS:HG3	1:A:14:TYR:CD2	0.53	2.38	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LEU:HB2	1:A:55:THR:HG21	0.53	1.79	7	1
1:A:22:ASN:O	1:A:23:GLU:C	0.53	2.47	13	3
1:A:3:GLY:O	1:A:47:TRP:CB	0.53	2.56	10	1
1:A:33:ASN:ND2	1:A:34:GLN:OE1	0.53	2.42	23	1
1:A:51:LEU:CD1	1:A:55:THR:HG21	0.52	2.34	8	2
1:A:29:CYS:O	1:A:34:GLN:CB	0.52	2.57	23	2
1:A:6:VAL:O	1:A:14:TYR:CD2	0.52	2.62	18	1
1:A:55:THR:O	1:A:55:THR:CG2	0.52	2.57	21	1
1:A:2:GLU:HB3	1:A:47:TRP:CZ2	0.52	2.39	4	4
1:A:39:GLY:CA	1:A:47:TRP:O	0.52	2.56	14	2
1:A:37:SER:O	1:A:38:TYR:CD1	0.52	2.63	12	3
1:A:9:SER:O	1:A:60:LEU:HD22	0.52	2.04	8	1
1:A:4:TYR:CZ	1:A:47:TRP:CZ3	0.52	2.98	25	2
1:A:27:THR:CG2	1:A:28:GLU:N	0.52	2.72	13	1
1:A:21:LYS:O	1:A:22:ASN:ND2	0.52	2.43	2	1
1:A:10:ASP:O	1:A:63:LYS:CD	0.52	2.58	3	1
1:A:6:VAL:O	1:A:8:LYS:N	0.52	2.42	5	3
1:A:5:LEU:C	1:A:6:VAL:CG1	0.52	2.78	10	1
1:A:8:LYS:O	1:A:9:SER:O	0.52	2.27	26	2
1:A:58:TYR:CZ	1:A:63:LYS:HE3	0.52	2.39	8	1
1:A:51:LEU:CD2	1:A:52:PRO:O	0.52	2.57	23	3
1:A:26:ASN:OD1	1:A:27:THR:N	0.52	2.42	14	1
1:A:24:HIS:CE1	1:A:25:CYS:SG	0.52	3.03	15	1
1:A:51:LEU:HD23	1:A:55:THR:HB	0.52	1.82	23	1
1:A:12:CYS:O	1:A:13:LYS:HB2	0.52	2.04	8	3
1:A:26:ASN:OD1	1:A:30:LYS:CE	0.52	2.58	24	1
1:A:2:GLU:HB3	1:A:49:GLU:CB	0.51	2.35	21	2
1:A:22:ASN:O	1:A:26:ASN:ND2	0.51	2.42	14	1
1:A:42:TYR:O	1:A:44:PHE:N	0.51	2.44	5	2
1:A:5:LEU:CD1	1:A:25:CYS:SG	0.51	2.97	10	1
1:A:60:LEU:HD13	1:A:63:LYS:HB2	0.51	1.81	10	1
1:A:33:ASN:OD1	1:A:34:GLN:N	0.51	2.43	25	4
1:A:51:LEU:N	1:A:51:LEU:CD1	0.51	2.70	10	1
1:A:56:PRO:O	1:A:57:THR:CG2	0.51	2.56	14	3
1:A:22:ASN:N	1:A:22:ASN:OD1	0.51	2.44	4	1
1:A:2:GLU:HB2	1:A:47:TRP:NE1	0.51	2.19	6	1
1:A:58:TYR:CD1	1:A:59:PRO:HA	0.51	2.41	5	5
1:A:4:TYR:CE2	1:A:45:ALA:CB	0.51	2.93	20	1
1:A:29:CYS:SG	1:A:34:GLN:NE2	0.51	2.84	22	1
1:A:37:SER:OG	1:A:38:TYR:N	0.51	2.43	20	3
1:A:23:GLU:O	1:A:24:HIS:C	0.51	2.49	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:GLU:O	1:A:34:GLN:NE2	0.51	2.43	17	1
1:A:4:TYR:CE1	1:A:47:TRP:CE3	0.51	2.99	10	3
1:A:51:LEU:CD1	1:A:52:PRO:O	0.51	2.56	21	1
1:A:15:ASP:CG	1:A:16:CYS:N	0.51	2.64	4	22
1:A:6:VAL:HG11	1:A:60:LEU:HD11	0.51	1.81	23	1
1:A:57:THR:O	1:A:59:PRO:O	0.51	2.29	24	13
1:A:28:GLU:O	1:A:31:ALA:CB	0.51	2.59	15	1
1:A:1:LYS:NZ	1:A:51:LEU:CD2	0.51	2.74	24	1
1:A:17:PHE:CG	1:A:18:TRP:N	0.50	2.79	26	3
1:A:11:GLY:O	1:A:12:CYS:O	0.50	2.29	25	4
1:A:51:LEU:HD23	1:A:55:THR:HG21	0.50	1.82	11	1
1:A:39:GLY:O	1:A:40:TYR:CB	0.50	2.59	19	2
1:A:39:GLY:C	1:A:40:TYR:CG	0.50	2.83	26	2
1:A:19:LEU:HD21	1:A:43:ALA:CA	0.50	2.36	20	2
1:A:19:LEU:HD22	1:A:43:ALA:O	0.50	2.07	25	1
1:A:51:LEU:O	1:A:51:LEU:CD2	0.50	2.56	17	3
1:A:26:ASN:O	1:A:30:LYS:CB	0.50	2.59	16	2
1:A:31:ALA:CB	1:A:33:ASN:OD1	0.50	2.60	4	1
1:A:58:TYR:CD2	1:A:59:PRO:HA	0.50	2.42	17	4
1:A:60:LEU:HD13	1:A:63:LYS:CE	0.50	2.37	15	1
1:A:39:GLY:O	1:A:40:TYR:CD2	0.50	2.65	19	1
1:A:5:LEU:HD13	1:A:28:GLU:OE2	0.50	2.06	23	1
1:A:2:GLU:HB3	1:A:47:TRP:CD2	0.50	2.42	10	1
1:A:9:SER:O	1:A:10:ASP:HB3	0.50	2.07	26	9
1:A:14:TYR:CD2	1:A:28:GLU:OE1	0.50	2.64	4	1
1:A:4:TYR:HE1	1:A:45:ALA:HB3	0.50	1.65	13	2
1:A:5:LEU:CD2	1:A:34:GLN:OE1	0.49	2.60	2	1
1:A:40:TYR:CD2	1:A:41:CYS:N	0.49	2.80	15	3
1:A:17:PHE:CD2	1:A:18:TRP:N	0.49	2.80	6	1
1:A:10:ASP:O	1:A:63:LYS:CE	0.49	2.60	25	1
1:A:50:GLY:O	1:A:51:LEU:C	0.49	2.50	5	2
1:A:6:VAL:HG21	1:A:60:LEU:CD1	0.49	2.38	26	1
1:A:23:GLU:O	1:A:27:THR:HG23	0.49	2.06	2	1
1:A:6:VAL:HG23	1:A:11:GLY:O	0.49	2.07	20	2
1:A:10:ASP:O	1:A:63:LYS:O	0.49	2.31	7	1
1:A:1:LYS:O	1:A:51:LEU:CD2	0.49	2.61	10	1
1:A:5:LEU:O	1:A:6:VAL:HG12	0.49	2.08	10	1
1:A:40:TYR:CG	1:A:41:CYS:N	0.49	2.80	23	1
1:A:23:GLU:O	1:A:26:ASN:N	0.49	2.46	13	1
1:A:37:SER:O	1:A:38:TYR:CD2	0.49	2.66	1	1
1:A:23:GLU:O	1:A:27:THR:HG22	0.49	2.08	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:VAL:HG12	1:A:13:LYS:HA	0.49	1.84	6	1
1:A:34:GLN:OE1	1:A:55:THR:HG21	0.49	2.08	20	1
1:A:30:LYS:O	1:A:31:ALA:O	0.48	2.32	8	7
1:A:51:LEU:HD23	1:A:55:THR:HG22	0.48	1.85	17	2
1:A:51:LEU:HD23	1:A:55:THR:HG23	0.48	1.85	11	1
1:A:5:LEU:HD21	1:A:29:CYS:SG	0.48	2.48	25	1
1:A:5:LEU:O	1:A:14:TYR:HB2	0.48	2.08	5	1
1:A:9:SER:O	1:A:10:ASP:OD1	0.48	2.30	25	1
1:A:4:TYR:CD2	1:A:47:TRP:HB3	0.48	2.44	6	1
1:A:37:SER:HB2	1:A:38:TYR:CE2	0.48	2.43	12	1
1:A:40:TYR:CE1	1:A:47:TRP:HB3	0.48	2.43	25	3
1:A:42:TYR:O	1:A:42:TYR:CD2	0.48	2.67	24	2
1:A:4:TYR:O	1:A:5:LEU:C	0.48	2.52	1	9
1:A:5:LEU:HD22	1:A:34:GLN:CG	0.48	2.37	4	1
1:A:1:LYS:O	1:A:51:LEU:CD1	0.48	2.61	5	1
1:A:60:LEU:HB3	1:A:61:PRO:CD	0.48	2.36	13	1
1:A:2:GLU:HB2	1:A:47:TRP:CD1	0.48	2.43	6	1
1:A:55:THR:HG22	1:A:55:THR:O	0.48	2.08	26	1
1:A:11:GLY:O	1:A:12:CYS:C	0.48	2.50	10	4
1:A:29:CYS:O	1:A:36:GLY:O	0.48	2.32	22	4
1:A:35:GLY:O	1:A:36:GLY:O	0.48	2.32	12	5
1:A:2:GLU:HB3	1:A:47:TRP:NE1	0.48	2.24	9	1
1:A:4:TYR:CD1	1:A:47:TRP:HB3	0.48	2.44	10	2
1:A:10:ASP:N	1:A:10:ASP:OD1	0.48	2.47	15	1
1:A:1:LYS:O	1:A:50:GLY:O	0.48	2.32	24	1
1:A:11:GLY:O	1:A:12:CYS:SG	0.48	2.72	26	2
1:A:39:GLY:HA3	1:A:47:TRP:O	0.48	2.09	14	2
1:A:58:TYR:CZ	1:A:65:CYS:O	0.47	2.67	17	1
1:A:41:CYS:HA	1:A:45:ALA:O	0.47	2.09	24	5
1:A:40:TYR:CE1	1:A:47:TRP:CZ3	0.47	3.02	6	1
1:A:24:HIS:HA	1:A:27:THR:CG2	0.47	2.38	14	1
1:A:5:LEU:O	1:A:6:VAL:O	0.47	2.32	20	1
1:A:57:THR:O	1:A:60:LEU:HD12	0.47	2.09	26	1
1:A:48:CYS:SG	1:A:51:LEU:HD21	0.47	2.49	9	1
1:A:50:GLY:O	1:A:51:LEU:O	0.47	2.32	24	2
1:A:33:ASN:OD1	1:A:34:GLN:OE1	0.47	2.33	21	1
1:A:9:SER:O	1:A:10:ASP:OD2	0.47	2.32	26	1
1:A:6:VAL:HG22	1:A:7:LYS:H	0.47	1.69	7	1
1:A:25:CYS:SG	1:A:25:CYS:O	0.47	2.73	4	1
1:A:26:ASN:OD1	1:A:39:GLY:O	0.47	2.33	13	2
1:A:6:VAL:HG21	1:A:60:LEU:HD13	0.47	1.85	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:TRP:O	1:A:41:CYS:SG	0.47	2.73	11	2
1:A:52:PRO:O	1:A:55:THR:HG22	0.47	2.09	11	1
1:A:60:LEU:HD13	1:A:63:LYS:CD	0.47	2.39	15	1
1:A:6:VAL:O	1:A:6:VAL:HG23	0.47	2.09	22	1
1:A:12:CYS:O	1:A:13:LYS:HD3	0.47	2.09	9	3
1:A:16:CYS:SG	1:A:45:ALA:O	0.47	2.73	14	3
1:A:51:LEU:HD22	1:A:57:THR:HG21	0.47	1.87	21	1
1:A:58:TYR:HA	1:A:59:PRO:C	0.47	2.30	18	14
1:A:12:CYS:HA	1:A:65:CYS:CB	0.47	2.40	21	1
1:A:11:GLY:O	1:A:65:CYS:CA	0.47	2.63	7	1
1:A:2:GLU:OE1	1:A:47:TRP:NE1	0.47	2.48	10	1
1:A:24:HIS:HA	1:A:27:THR:HG22	0.47	1.87	14	1
1:A:29:CYS:O	1:A:34:GLN:HB2	0.47	2.10	23	1
1:A:10:ASP:OD1	1:A:65:CYS:SG	0.46	2.73	3	1
1:A:15:ASP:OD1	1:A:16:CYS:N	0.46	2.48	7	2
1:A:5:LEU:C	1:A:6:VAL:CG2	0.46	2.84	9	1
1:A:57:THR:O	1:A:58:TYR:O	0.46	2.33	13	1
1:A:5:LEU:HD12	1:A:46:CYS:SG	0.46	2.50	19	1
1:A:10:ASP:OD1	1:A:12:CYS:SG	0.46	2.73	22	1
1:A:6:VAL:HG22	1:A:58:TYR:HB2	0.46	1.85	1	1
1:A:14:TYR:CD1	1:A:15:ASP:O	0.46	2.68	10	1
1:A:19:LEU:CD2	1:A:43:ALA:HA	0.46	2.39	10	1
1:A:25:CYS:SG	1:A:26:ASN:N	0.46	2.88	17	1
1:A:36:GLY:CA	1:A:50:GLY:O	0.46	2.64	18	1
1:A:2:GLU:OE1	1:A:48:CYS:O	0.46	2.32	26	1
1:A:4:TYR:CZ	1:A:45:ALA:CB	0.46	2.98	2	1
1:A:62:ASN:O	1:A:62:ASN:CG	0.46	2.54	8	1
1:A:43:ALA:C	1:A:44:PHE:CG	0.46	2.89	10	1
1:A:62:ASN:O	1:A:63:LYS:CB	0.46	2.63	25	1
1:A:22:ASN:O	1:A:26:ASN:OD1	0.46	2.34	26	1
1:A:55:THR:CG2	1:A:56:PRO:HD2	0.46	2.41	12	3
1:A:41:CYS:SG	1:A:45:ALA:O	0.46	2.74	20	3
1:A:6:VAL:CG2	1:A:12:CYS:O	0.46	2.55	17	2
1:A:9:SER:C	1:A:10:ASP:OD1	0.46	2.54	17	2
1:A:36:GLY:HA2	1:A:50:GLY:O	0.46	2.10	18	1
1:A:8:LYS:HG3	1:A:9:SER:N	0.46	2.26	15	1
1:A:35:GLY:O	1:A:36:GLY:C	0.46	2.54	19	3
1:A:1:LYS:HG2	1:A:51:LEU:HD11	0.46	1.87	7	1
1:A:6:VAL:CG1	1:A:13:LYS:N	0.46	2.79	9	1
1:A:4:TYR:HA	1:A:47:TRP:HB2	0.46	1.86	6	1
1:A:10:ASP:OD2	1:A:65:CYS:SG	0.46	2.74	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:GLU:O	1:A:24:HIS:O	0.46	2.33	23	1
1:A:10:ASP:OD1	1:A:10:ASP:C	0.46	2.54	26	2
1:A:51:LEU:HD13	1:A:51:LEU:H	0.46	1.69	11	1
1:A:58:TYR:CD1	1:A:59:PRO:CA	0.46	2.99	16	1
1:A:49:GLU:OE1	1:A:49:GLU:O	0.46	2.34	26	1
1:A:51:LEU:C	1:A:51:LEU:CD2	0.46	2.79	2	4
1:A:4:TYR:HA	1:A:47:TRP:HB3	0.46	1.88	10	1
1:A:6:VAL:CG2	1:A:11:GLY:HA2	0.45	2.40	3	1
1:A:34:GLN:O	1:A:52:PRO:HD2	0.45	2.11	17	1
1:A:17:PHE:O	1:A:18:TRP:C	0.45	2.54	3	4
1:A:11:GLY:O	1:A:13:LYS:N	0.45	2.49	10	1
1:A:8:LYS:O	1:A:63:LYS:NZ	0.45	2.50	17	1
1:A:40:TYR:O	1:A:46:CYS:SG	0.45	2.74	3	2
1:A:26:ASN:O	1:A:30:LYS:HB3	0.45	2.11	9	1
1:A:27:THR:HG23	1:A:28:GLU:N	0.45	2.26	14	1
1:A:47:TRP:O	1:A:48:CYS:SG	0.45	2.74	19	1
1:A:58:TYR:CE1	1:A:63:LYS:HE3	0.45	2.47	8	1
1:A:1:LYS:O	1:A:51:LEU:HD22	0.45	2.11	10	1
1:A:56:PRO:C	1:A:57:THR:CG2	0.45	2.83	17	1
1:A:51:LEU:HD23	1:A:51:LEU:O	0.45	2.12	20	1
1:A:19:LEU:CD2	1:A:41:CYS:O	0.45	2.64	22	1
1:A:29:CYS:SG	1:A:34:GLN:OE1	0.45	2.74	24	1
1:A:2:GLU:CB	1:A:49:GLU:HB3	0.45	2.42	3	1
1:A:26:ASN:C	1:A:26:ASN:ND2	0.45	2.70	24	1
1:A:6:VAL:CG1	1:A:58:TYR:HB2	0.45	2.41	13	2
1:A:9:SER:O	1:A:10:ASP:C	0.45	2.53	7	2
1:A:63:LYS:O	1:A:64:SER:CB	0.45	2.64	15	2
1:A:54:SER:OG	1:A:55:THR:N	0.45	2.49	13	1
1:A:62:ASN:O	1:A:63:LYS:CG	0.45	2.65	25	1
1:A:60:LEU:HD22	1:A:63:LYS:CD	0.45	2.41	10	1
1:A:37:SER:C	1:A:38:TYR:CG	0.45	2.90	12	1
1:A:18:TRP:CE3	1:A:18:TRP:HA	0.45	2.47	2	6
1:A:15:ASP:HA	1:A:44:PHE:O	0.45	2.12	20	4
1:A:40:TYR:O	1:A:46:CYS:HA	0.45	2.12	6	1
1:A:10:ASP:OD1	1:A:10:ASP:N	0.45	2.49	13	3
1:A:60:LEU:HD12	1:A:60:LEU:O	0.45	2.12	10	1
1:A:34:GLN:O	1:A:52:PRO:HD3	0.45	2.13	24	1
1:A:12:CYS:O	1:A:13:LYS:CB	0.44	2.65	8	3
1:A:2:GLU:CB	1:A:49:GLU:CB	0.44	2.96	19	2
1:A:24:HIS:O	1:A:28:GLU:OE1	0.44	2.35	10	2
1:A:18:TRP:HB3	1:A:21:LYS:CD	0.44	2.41	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ASN:CB	1:A:25:CYS:HB3	0.44	2.42	1	1
1:A:9:SER:C	1:A:11:GLY:N	0.44	2.71	7	2
1:A:47:TRP:HA	1:A:47:TRP:CE3	0.44	2.47	16	1
1:A:54:SER:O	1:A:54:SER:OG	0.44	2.33	22	1
1:A:26:ASN:ND2	1:A:30:LYS:HD3	0.44	2.28	24	1
1:A:26:ASN:O	1:A:26:ASN:OD1	0.44	2.35	2	1
1:A:13:LYS:CD	1:A:13:LYS:C	0.44	2.86	3	1
1:A:16:CYS:O	1:A:16:CYS:SG	0.44	2.75	9	1
1:A:47:TRP:CD1	1:A:47:TRP:N	0.44	2.83	10	1
1:A:59:PRO:C	1:A:60:LEU:HD23	0.44	2.31	13	1
1:A:2:GLU:CB	1:A:49:GLU:HA	0.44	2.42	19	1
1:A:5:LEU:O	1:A:14:TYR:CB	0.44	2.65	5	1
1:A:40:TYR:C	1:A:40:TYR:CD1	0.44	2.90	11	2
1:A:8:LYS:O	1:A:10:ASP:CG	0.44	2.55	7	2
1:A:38:TYR:O	1:A:49:GLU:OE2	0.44	2.35	9	1
1:A:29:CYS:O	1:A:34:GLN:HB3	0.44	2.12	13	1
1:A:15:ASP:OD1	1:A:15:ASP:C	0.44	2.55	25	1
1:A:10:ASP:CB	1:A:62:ASN:OD1	0.44	2.65	6	1
1:A:62:ASN:O	1:A:63:LYS:C	0.44	2.56	8	1
1:A:50:GLY:C	1:A:51:LEU:HD22	0.44	2.32	19	2
1:A:37:SER:OG	1:A:38:TYR:CE1	0.44	2.71	8	1
1:A:58:TYR:OH	1:A:65:CYS:OXT	0.44	2.36	13	1
1:A:17:PHE:CD1	1:A:17:PHE:C	0.44	2.90	9	2
1:A:23:GLU:O	1:A:27:THR:CG2	0.44	2.66	14	1
1:A:42:TYR:O	1:A:42:TYR:CG	0.44	2.71	24	1
1:A:14:TYR:CE2	1:A:28:GLU:OE1	0.44	2.71	4	1
1:A:18:TRP:O	1:A:23:GLU:OE2	0.44	2.36	7	1
1:A:34:GLN:NE2	1:A:55:THR:HG21	0.44	2.28	21	1
1:A:25:CYS:O	1:A:25:CYS:SG	0.44	2.75	23	1
1:A:30:LYS:O	1:A:31:ALA:C	0.43	2.56	7	8
1:A:12:CYS:O	1:A:13:LYS:O	0.43	2.35	15	1
1:A:19:LEU:CD2	1:A:43:ALA:C	0.43	2.86	21	1
1:A:16:CYS:SG	1:A:17:PHE:N	0.43	2.91	1	3
1:A:50:GLY:O	1:A:51:LEU:HD13	0.43	2.11	10	1
1:A:60:LEU:HD12	1:A:60:LEU:C	0.43	2.34	10	1
1:A:28:GLU:O	1:A:34:GLN:OE1	0.43	2.36	26	1
1:A:54:SER:O	1:A:56:PRO:HD3	0.43	2.13	24	3
1:A:30:LYS:HA	1:A:36:GLY:O	0.43	2.14	2	1
1:A:31:ALA:CB	1:A:33:ASN:ND2	0.43	2.82	9	1
1:A:26:ASN:OD1	1:A:26:ASN:C	0.43	2.56	1	2
1:A:63:LYS:O	1:A:63:LYS:HG3	0.43	2.14	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:SER:O	1:A:10:ASP:CG	0.43	2.57	26	1
1:A:64:SER:O	1:A:65:CYS:C	0.43	2.57	1	1
1:A:61:PRO:O	1:A:62:ASN:HB2	0.43	2.12	9	2
1:A:58:TYR:OH	1:A:65:CYS:SG	0.43	2.73	10	1
1:A:13:LYS:N	1:A:13:LYS:CD	0.43	2.80	13	1
1:A:63:LYS:O	1:A:64:SER:HB2	0.43	2.13	15	1
1:A:10:ASP:O	1:A:63:LYS:HG2	0.43	2.14	20	1
1:A:7:LYS:O	1:A:9:SER:N	0.43	2.52	25	1
1:A:4:TYR:HA	1:A:47:TRP:CB	0.43	2.43	6	1
1:A:47:TRP:CD1	1:A:47:TRP:C	0.43	2.92	12	1
1:A:6:VAL:O	1:A:7:LYS:C	0.43	2.57	15	2
1:A:1:LYS:O	1:A:1:LYS:CG	0.43	2.65	5	1
1:A:4:TYR:CA	1:A:47:TRP:HB2	0.43	2.43	6	1
1:A:13:LYS:HD3	1:A:58:TYR:CE2	0.43	2.48	8	1
1:A:6:VAL:HG12	1:A:7:LYS:H	0.43	1.72	9	1
1:A:13:LYS:HE2	1:A:58:TYR:CD2	0.43	2.49	13	1
1:A:10:ASP:O	1:A:63:LYS:CG	0.43	2.66	20	1
1:A:49:GLU:O	1:A:49:GLU:HG3	0.43	2.13	21	1
1:A:60:LEU:C	1:A:60:LEU:HD23	0.43	2.33	18	1
1:A:28:GLU:N	1:A:28:GLU:OE1	0.43	2.52	24	1
1:A:17:PHE:O	1:A:17:PHE:CG	0.43	2.72	4	1
1:A:9:SER:OG	1:A:10:ASP:N	0.43	2.50	22	3
1:A:21:LYS:N	1:A:21:LYS:HD2	0.43	2.28	8	1
1:A:37:SER:OG	1:A:38:TYR:CD1	0.43	2.72	8	1
1:A:10:ASP:O	1:A:12:CYS:N	0.43	2.52	9	1
1:A:3:GLY:C	1:A:47:TRP:CB	0.43	2.87	10	1
1:A:16:CYS:SG	1:A:44:PHE:C	0.43	2.98	24	3
1:A:26:ASN:O	1:A:30:LYS:HB2	0.43	2.13	16	1
1:A:12:CYS:O	1:A:13:LYS:C	0.42	2.56	1	3
1:A:5:LEU:CD2	1:A:34:GLN:HG2	0.42	2.44	4	1
1:A:39:GLY:HA2	1:A:47:TRP:O	0.42	2.14	6	1
1:A:47:TRP:CE3	1:A:47:TRP:HA	0.42	2.48	15	1
1:A:7:LYS:HD3	1:A:14:TYR:CE1	0.42	2.49	24	1
1:A:10:ASP:OD2	1:A:10:ASP:O	0.42	2.36	4	1
1:A:11:GLY:O	1:A:65:CYS:HA	0.42	2.15	7	1
1:A:58:TYR:OH	1:A:65:CYS:HB2	0.42	2.14	18	1
1:A:54:SER:O	1:A:55:THR:C	0.42	2.56	13	1
1:A:33:ASN:OD1	1:A:33:ASN:C	0.42	2.58	25	1
1:A:34:GLN:OE1	1:A:51:LEU:HD22	0.42	2.14	25	1
1:A:20:GLY:O	1:A:21:LYS:C	0.42	2.57	24	3
1:A:5:LEU:HD21	1:A:34:GLN:CD	0.42	2.35	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:TRP:CG	1:A:48:CYS:N	0.42	2.88	6	1
1:A:1:LYS:CG	1:A:2:GLU:N	0.42	2.83	23	1
1:A:3:GLY:HA3	1:A:48:CYS:HB2	0.42	1.92	5	1
1:A:4:TYR:O	1:A:58:TYR:HB2	0.42	2.15	10	1
1:A:6:VAL:HG21	1:A:60:LEU:HD21	0.42	1.92	13	1
1:A:6:VAL:HB	1:A:12:CYS:O	0.42	2.14	19	1
1:A:3:GLY:O	1:A:47:TRP:HA	0.42	2.14	5	1
1:A:19:LEU:CD2	1:A:43:ALA:O	0.42	2.68	12	1
1:A:38:TYR:HB2	1:A:49:GLU:OE2	0.42	2.15	25	1
1:A:3:GLY:HA2	1:A:47:TRP:CZ2	0.42	2.50	3	1
1:A:11:GLY:O	1:A:58:TYR:CE2	0.42	2.72	8	1
1:A:3:GLY:C	1:A:47:TRP:HB2	0.42	2.35	10	1
1:A:34:GLN:HG3	1:A:51:LEU:CD1	0.42	2.45	1	1
1:A:26:ASN:CG	1:A:27:THR:N	0.42	2.72	8	1
1:A:39:GLY:O	1:A:40:TYR:HB3	0.42	2.15	11	1
1:A:56:PRO:HB2	1:A:60:LEU:CD1	0.42	2.45	14	1
1:A:60:LEU:HD13	1:A:63:LYS:HE2	0.42	1.92	15	1
1:A:60:LEU:CD1	1:A:65:CYS:OXT	0.42	2.67	17	1
1:A:6:VAL:CG1	1:A:60:LEU:HD21	0.42	2.42	20	1
1:A:4:TYR:CD1	1:A:4:TYR:N	0.42	2.87	26	1
1:A:7:LYS:HG2	1:A:14:TYR:CD1	0.42	2.50	26	1
1:A:17:PHE:O	1:A:19:LEU:N	0.41	2.53	5	2
1:A:22:ASN:OD1	1:A:22:ASN:C	0.41	2.58	15	1
1:A:7:LYS:CG	1:A:14:TYR:CE2	0.41	3.03	20	1
1:A:36:GLY:O	1:A:37:SER:HB3	0.41	2.15	3	1
1:A:13:LYS:HD3	1:A:58:TYR:CZ	0.41	2.50	15	1
1:A:1:LYS:HB2	1:A:51:LEU:O	0.41	2.15	5	1
1:A:19:LEU:CD2	1:A:42:TYR:O	0.41	2.68	7	3
1:A:24:HIS:O	1:A:27:THR:HG22	0.41	2.15	7	2
1:A:40:TYR:OH	1:A:42:TYR:CD1	0.41	2.71	15	1
1:A:58:TYR:OH	1:A:65:CYS:C	0.41	2.59	17	1
1:A:6:VAL:HG23	1:A:11:GLY:C	0.41	2.36	3	1
1:A:8:LYS:HB3	1:A:10:ASP:OD2	0.41	2.16	8	1
1:A:21:LYS:O	1:A:21:LYS:HG3	0.41	2.14	14	1
1:A:15:ASP:O	1:A:16:CYS:CB	0.41	2.67	16	1
1:A:36:GLY:N	1:A:50:GLY:O	0.41	2.54	6	1
1:A:50:GLY:H	1:A:51:LEU:HD23	0.41	1.75	6	1
1:A:17:PHE:O	1:A:19:LEU:HG	0.41	2.16	7	1
1:A:18:TRP:O	1:A:41:CYS:CB	0.41	2.69	3	1
1:A:25:CYS:O	1:A:29:CYS:HB2	0.41	2.16	5	2
1:A:52:PRO:HG2	1:A:55:THR:OG1	0.41	2.15	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:GLY:O	1:A:47:TRP:CD1	0.41	2.74	11	1
1:A:6:VAL:N	1:A:14:TYR:HB2	0.41	2.31	18	1
1:A:60:LEU:HD12	1:A:63:LYS:HB2	0.41	1.93	20	1
1:A:1:LYS:HB3	1:A:51:LEU:CB	0.41	2.45	26	1
1:A:23:GLU:HA	1:A:23:GLU:OE1	0.41	2.16	26	1
1:A:53:GLU:O	1:A:54:SER:C	0.41	2.57	26	1
1:A:65:CYS:O	1:A:65:CYS:SG	0.41	2.78	26	1
1:A:10:ASP:O	1:A:65:CYS:HB2	0.41	2.16	9	1
1:A:19:LEU:CD2	1:A:43:ALA:CA	0.41	2.99	21	1
1:A:33:ASN:C	1:A:34:GLN:OE1	0.40	2.60	4	1
1:A:6:VAL:HG21	1:A:11:GLY:HA2	0.40	1.92	8	1
1:A:12:CYS:N	1:A:65:CYS:HB2	0.40	2.30	13	1
1:A:25:CYS:O	1:A:26:ASN:C	0.40	2.59	13	1
1:A:2:GLU:OE2	1:A:49:GLU:HG3	0.40	2.17	18	1
1:A:3:GLY:HA2	1:A:47:TRP:CZ3	0.40	2.51	19	1
1:A:14:TYR:O	1:A:45:ALA:HA	0.40	2.17	19	1
1:A:2:GLU:HB2	1:A:47:TRP:CH2	0.40	2.51	24	1
1:A:18:TRP:CE3	1:A:18:TRP:CA	0.40	3.03	2	1
1:A:7:LYS:O	1:A:8:LYS:O	0.40	2.40	7	1
1:A:38:TYR:CG	1:A:39:GLY:N	0.40	2.88	7	1
1:A:51:LEU:O	1:A:51:LEU:HG	0.40	2.16	21	1
1:A:49:GLU:OE1	1:A:49:GLU:C	0.40	2.59	26	1
1:A:28:GLU:CD	1:A:29:CYS:N	0.40	2.75	3	1
1:A:25:CYS:O	1:A:29:CYS:SG	0.40	2.79	10	1
1:A:60:LEU:CD1	1:A:62:ASN:O	0.40	2.69	10	1
1:A:52:PRO:O	1:A:55:THR:CG2	0.40	2.69	11	1
1:A:19:LEU:O	1:A:20:GLY:C	0.40	2.58	13	1
1:A:56:PRO:O	1:A:57:THR:HG22	0.40	2.16	17	1
1:A:6:VAL:HA	1:A:12:CYS:O	0.40	2.16	3	1
1:A:51:LEU:O	1:A:51:LEU:CD1	0.40	2.56	7	2
1:A:6:VAL:CG2	1:A:58:TYR:CD2	0.40	3.04	8	1
1:A:57:THR:C	1:A:59:PRO:O	0.40	2.60	8	1
1:A:22:ASN:O	1:A:22:ASN:CG	0.40	2.57	15	1
1:A:26:ASN:OD1	1:A:26:ASN:O	0.40	2.39	1	1
1:A:60:LEU:HD12	1:A:65:CYS:OXT	0.40	2.16	17	1
1:A:34:GLN:CG	1:A:51:LEU:HD12	0.40	2.42	24	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	63/65 (97%)	44±4 (69±7%)	14±3 (22±5%)	6±3 (9±4%)	1 11
All	All	1638/1690 (97%)	1132 (69%)	357 (22%)	149 (9%)	1 11

All 31 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	44	PHE	14
1	A	10	ASP	13
1	A	31	ALA	10
1	A	9	SER	10
1	A	36	GLY	8
1	A	12	CYS	7
1	A	40	TYR	7
1	A	43	ALA	7
1	A	37	SER	5
1	A	62	ASN	5
1	A	24	HIS	5
1	A	52	PRO	4
1	A	64	SER	4
1	A	7	LYS	4
1	A	50	GLY	4
1	A	8	LYS	4
1	A	5	LEU	4
1	A	13	LYS	4
1	A	61	PRO	4
1	A	18	TRP	3
1	A	58	TYR	3
1	A	22	ASN	3
1	A	6	VAL	3
1	A	56	PRO	3
1	A	23	GLU	3
1	A	21	LYS	2
1	A	51	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	17	PHE	1
1	A	11	GLY	1
1	A	54	SER	1
1	A	63	LYS	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	55/55 (100%)	36±3 (65±6%)	19±3 (35±6%)	1 9
All	All	1430/1430 (100%)	930 (65%)	500 (35%)	1 9

All 50 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	15	ASP	23
1	A	32	LYS	19
1	A	1	LYS	19
1	A	13	LYS	18
1	A	30	LYS	18
1	A	34	GLN	15
1	A	21	LYS	15
1	A	58	TYR	15
1	A	7	LYS	14
1	A	51	LEU	14
1	A	24	HIS	13
1	A	28	GLU	13
1	A	64	SER	13
1	A	16	CYS	13
1	A	8	LYS	12
1	A	29	CYS	12
1	A	62	ASN	12
1	A	26	ASN	12
1	A	57	THR	12
1	A	10	ASP	11
1	A	14	TYR	11

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Mol	Chain	Res	Type	Models (Total)
1	A	12	CYS	11
1	A	42	TYR	11
1	A	54	SER	11
1	A	63	LYS	11
1	A	41	CYS	11
1	A	25	CYS	10
1	A	53	GLU	10
1	A	9	SER	10
1	A	22	ASN	9
1	A	60	LEU	9
1	A	6	VAL	8
1	A	23	GLU	8
1	A	49	GLU	8
1	A	27	THR	8
1	A	48	CYS	7
1	A	4	TYR	6
1	A	46	CYS	6
1	A	38	TYR	6
1	A	33	ASN	5
1	A	2	GLU	5
1	A	40	TYR	5
1	A	47	TRP	4
1	A	55	THR	4
1	A	19	LEU	4
1	A	59	PRO	3
1	A	18	TRP	2
1	A	17	PHE	2
1	A	56	PRO	1
1	A	37	SER	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