



Full wwPDB NMR Structure Validation Report ⓘ

Feb 19, 2022 – 01:49 PM EST

PDB ID : 1RLP
Title : TWO BINDING ORIENTATIONS FOR PEPTIDES TO SRC SH3 DOMAIN:
DEVELOPMENT OF A GENERAL MODEL FOR SH3-LIGAND INTERAC-
TIONS
Authors : Feng, S.; Chen, J.K.; Yu, H.; Simon, J.A.; Schreiber, S.L.
Deposited on : 1994-10-10

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

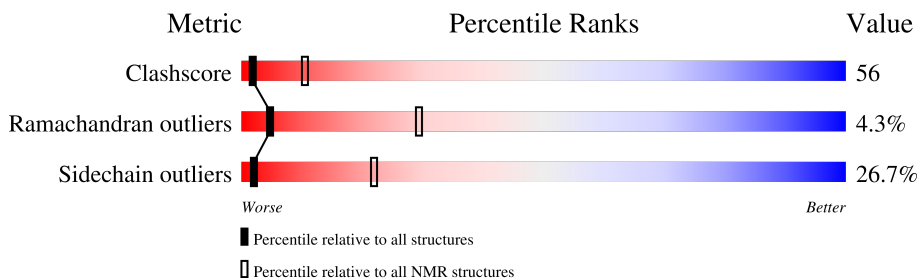
1 Overall quality at a glance

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	C	64	
2	R	9	

2 Ensemble composition and analysis

This entry contains 16 models. Model 11 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	C:9-C:64, R:71-R:76 (62)	0.64	11

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1035 atoms, of which 506 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called C-SRC TYROSINE KINASE SH3 DOMAIN.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	C	56	873	287	421	73	92	0

- Molecule 2 is a protein called PROLINE-RICH LIGAND RLP2 (RALPPLPRY).

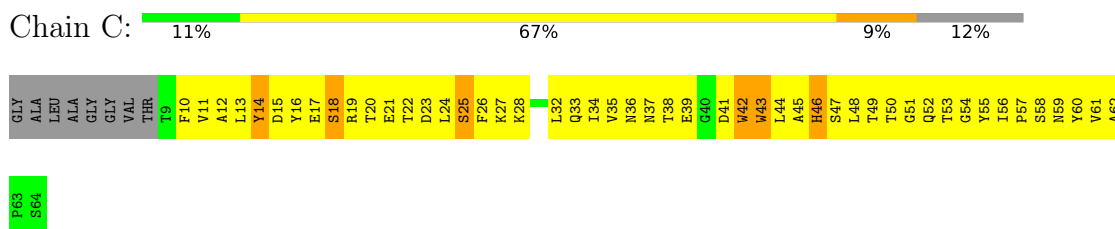
Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	R	9	162	51	85	15	11	0

4 Residue-property plots i

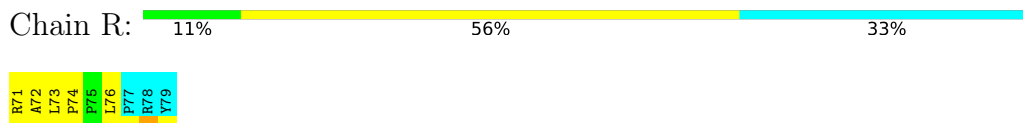
4.1 Average score per residue in the NMR ensemble

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: C-SRC TYROSINE KINASE SH3 DOMAIN



- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)

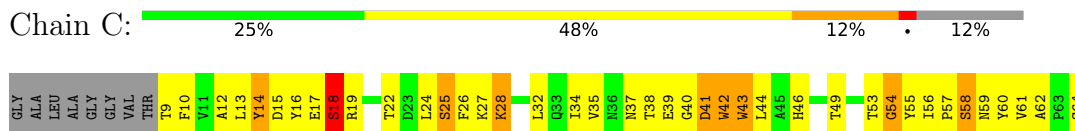


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

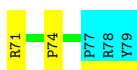
4.2.1 Score per residue for model 1

- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN



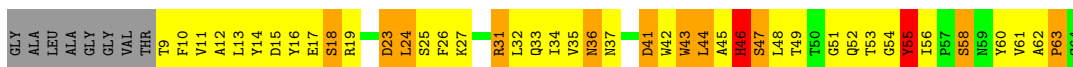
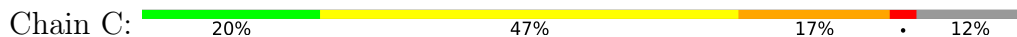
- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)



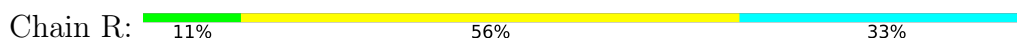


4.2.2 Score per residue for model 2

- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN

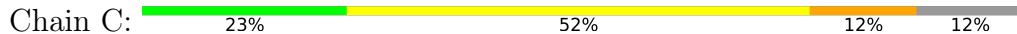


- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)

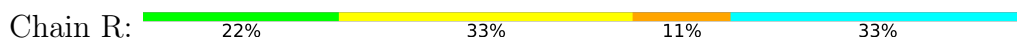


4.2.3 Score per residue for model 3

- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN

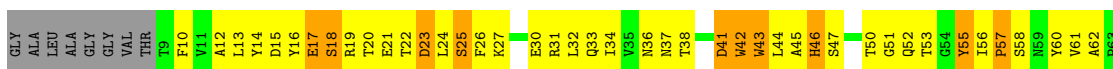
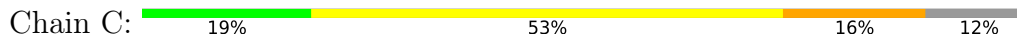


- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)

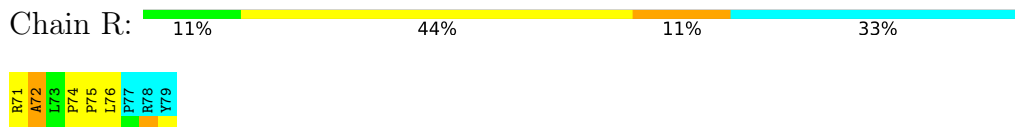


4.2.4 Score per residue for model 4

- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN

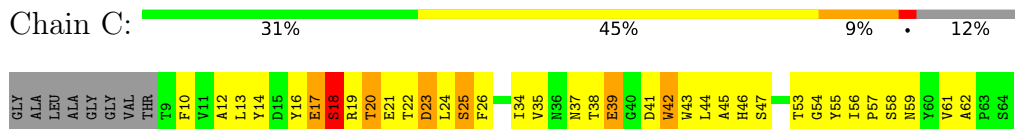


- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)

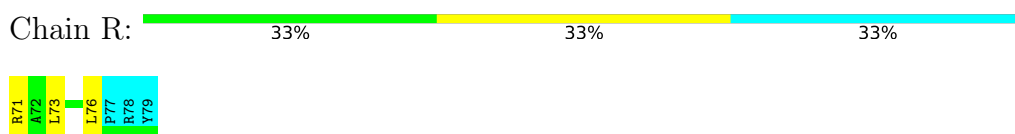


4.2.5 Score per residue for model 5

- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN

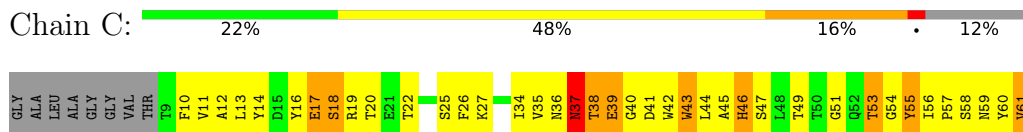


- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)

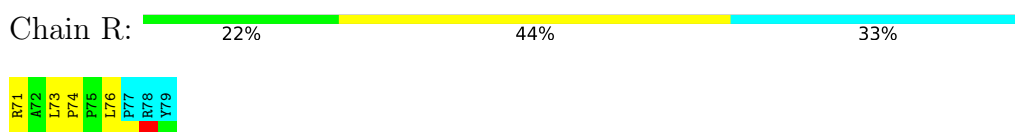


4.2.6 Score per residue for model 6

- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN

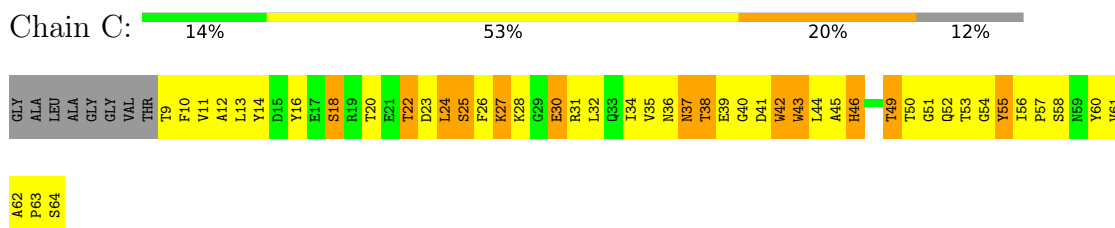


- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)

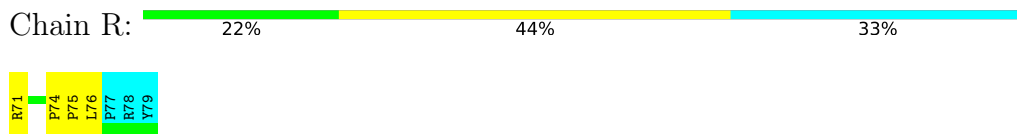


4.2.7 Score per residue for model 7

- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN

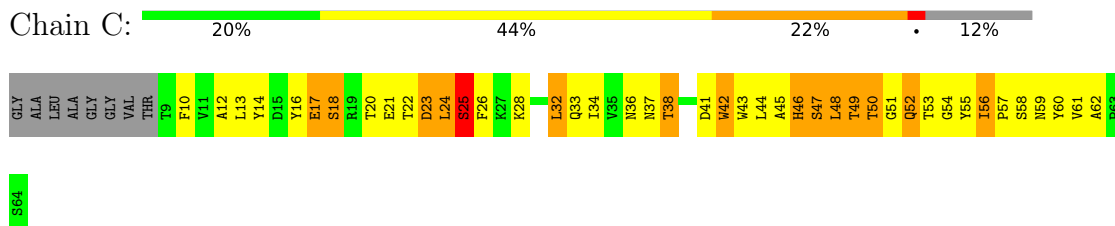


- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)



4.2.8 Score per residue for model 8

- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN

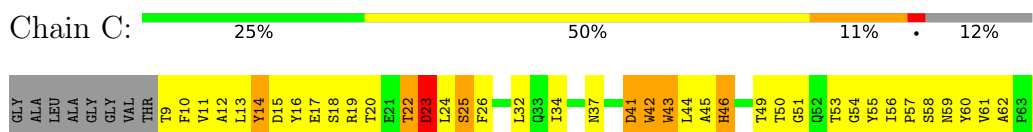


- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)

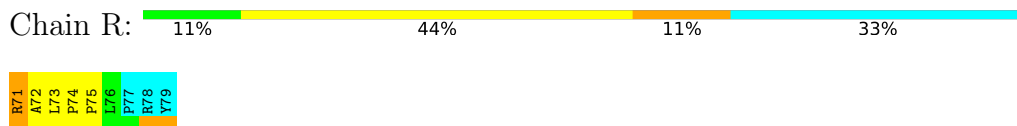


4.2.9 Score per residue for model 9

- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN

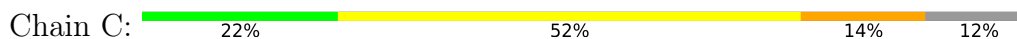


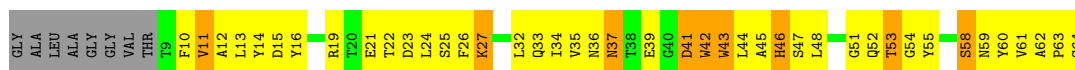
- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)



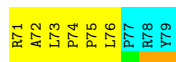
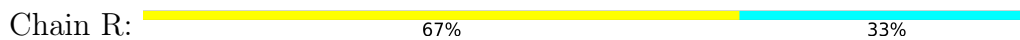
4.2.10 Score per residue for model 10

- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN



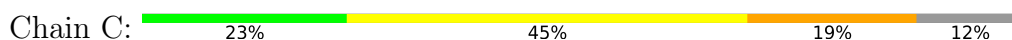


- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)



4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN

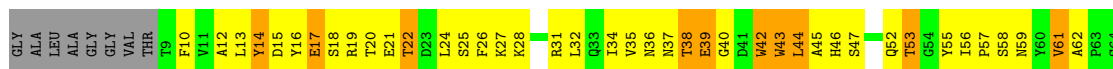


- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)



4.2.12 Score per residue for model 12

- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN

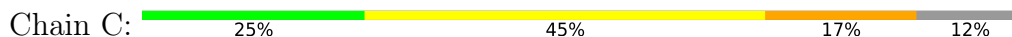


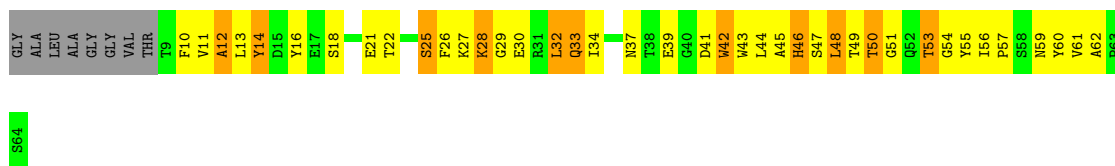
- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)



4.2.13 Score per residue for model 13

- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN





S64

- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)

Chain R: 33% 22% 11% 33%

R71
A72
L73
P77
R78
Y79

4.2.14 Score per residue for model 14

- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN

Chain C: 28% 50% 9% 12%

GLY
ALA
LEU
ALA
GLY
GLY
VAL
THR
T9
F10
V11
A12
L13
Y14
D15
Y16
E17
S18
R19
T20
E21
T22
D23
L24
S25
F26
K27
L32
Q33
I34
V35
D41
W42
W43
L44
A45
H46
T49
T53
G54
Y55
I56
P57
S58
N59
Y60
V61
A62
P63
S64

- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)

Chain R: 33% 11% 22% 33%

R71
A72
L73
P74
P77
R78
Y79

4.2.15 Score per residue for model 15

- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN

Chain C: 19% 52% 14% 12%

GLY
ALA
LEU
ALA
GLY
GLY
VAL
THR
T9
F10
V11
A12
L13
Y14
D15
Y16
E17
S18
R19
T20
E21
T22
D23
L24
S25
F26
K27
K28
L32
Q33
I34
V35
N36
N37
T38
D41
W42
W43
L44
A45
H46
S47
L48
T49
T50
G51
Q52
T53
G54
Y55
I56
P57
S58
N59
Y60
V61
A62
P63
S64

S64

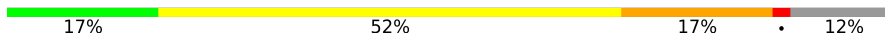
- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)

Chain R: 22% 44% 33%

R71
A72
L73
P74
L76
P77
R78
Y79

4.2.16 Score per residue for model 16

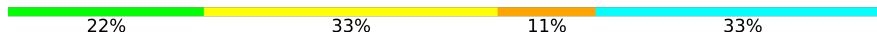
- Molecule 1: C-SRC TYROSINE KINASE SH3 DOMAIN

Chain C: 



A62
P63
S64

- Molecule 2: PROLINE-RICH LIGAND RLP2 (RALPPLPRY)

Chain R: 



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 16 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	C	1.12±0.00	3±0/464 (0.6± 0.0%)	1.24±0.00	8±0/632 (1.3± 0.0%)
2	R	0.94±0.01	0±0/48 (0.0± 0.0%)	0.99±0.01	0±0/68 (0.0± 0.0%)
All	All	1.11	48/8192 (0.6%)	1.22	129/11200 (1.2%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	43	TRP	CG-CD2	-6.08	1.33	1.43	4	16
1	C	42	TRP	CG-CD2	-6.03	1.33	1.43	6	16
1	C	46	HIS	CG-ND1	-5.44	1.26	1.38	16	16

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	42	TRP	NE1-CE2-CZ2	8.04	139.25	130.40	4	16
1	C	43	TRP	NE1-CE2-CZ2	8.04	139.25	130.40	9	16
1	C	43	TRP	CD1-NE1-CE2	6.92	115.23	109.00	7	16
1	C	42	TRP	CD1-NE1-CE2	6.86	115.17	109.00	12	16
1	C	43	TRP	CG-CD1-NE1	-6.61	103.49	110.10	7	16
1	C	42	TRP	CG-CD1-NE1	-6.60	103.50	110.10	12	16
1	C	43	TRP	NE1-CE2-CD2	-6.50	100.80	107.30	9	16
1	C	42	TRP	NE1-CE2-CD2	-6.46	100.84	107.30	9	16
1	C	43	TRP	CG-CD2-CE3	-5.00	129.40	133.90	12	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	C	452	421	421	53±12
2	R	46	56	53	6±3
All	All	7968	7632	7584	876

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 56.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:13:LEU:HD11	1:C:62:ALA:HB2	1.00	1.28	3	8
1:C:32:LEU:HD13	1:C:56:ILE:HG21	0.95	1.37	8	1
1:C:44:LEU:HD21	1:C:53:THR:HG21	0.92	1.39	13	3
1:C:44:LEU:HD12	1:C:55:TYR:CD1	0.90	2.02	9	3
1:C:41:ASP:CB	2:R:73:LEU:HD11	0.89	1.97	10	4
1:C:32:LEU:HD22	1:C:56:ILE:HG21	0.88	1.45	7	5
1:C:41:ASP:HB3	2:R:73:LEU:HD11	0.88	1.45	10	4
1:C:56:ILE:HD13	1:C:61:VAL:HG11	0.88	1.43	15	4
1:C:33:GLN:OE1	1:C:48:LEU:HD21	0.88	1.69	2	1
1:C:13:LEU:HD11	1:C:62:ALA:CB	0.86	2.00	7	11
1:C:34:ILE:HD11	1:C:56:ILE:HD11	0.86	1.46	12	3
2:R:73:LEU:HD13	2:R:74:PRO:HD2	0.86	1.47	12	2
1:C:12:ALA:HB1	1:C:26:PHE:CE1	0.86	2.05	9	10
1:C:46:HIS:CD2	1:C:48:LEU:HD23	0.85	2.07	15	2
1:C:47:SER:O	1:C:48:LEU:HD23	0.85	1.71	16	1
1:C:35:VAL:HG21	1:C:44:LEU:CD2	0.83	2.03	11	4
1:C:56:ILE:CD1	1:C:61:VAL:HG11	0.82	2.05	9	5
1:C:13:LEU:HD21	1:C:62:ALA:HB3	0.81	1.48	8	1
1:C:24:LEU:HD22	1:C:53:THR:O	0.79	1.77	1	1
1:C:44:LEU:HD23	1:C:44:LEU:O	0.79	1.77	7	6
1:C:59:ASN:OD1	2:R:73:LEU:HD13	0.79	1.78	14	1
1:C:13:LEU:HD11	1:C:62:ALA:HB3	0.78	1.53	7	6
1:C:24:LEU:HD11	1:C:53:THR:O	0.78	1.78	9	7
1:C:33:GLN:O	1:C:45:ALA:HB1	0.77	1.79	16	1
1:C:59:ASN:ND2	2:R:73:LEU:HD13	0.77	1.94	9	1
1:C:44:LEU:HD13	1:C:55:TYR:CE1	0.76	2.14	13	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:41:ASP:HB3	2:R:73:LEU:HD21	0.75	1.58	13	7
1:C:54:GLY:O	1:C:56:ILE:HG23	0.75	1.82	2	3
1:C:24:LEU:HD23	1:C:24:LEU:N	0.75	1.96	7	3
1:C:44:LEU:HD13	1:C:55:TYR:CD1	0.73	2.18	13	3
1:C:50:THR:HG22	1:C:50:THR:O	0.72	1.82	16	1
1:C:48:LEU:HD13	1:C:48:LEU:N	0.72	2.00	8	1
1:C:24:LEU:HD12	1:C:53:THR:O	0.70	1.86	8	1
1:C:32:LEU:HD13	1:C:56:ILE:HD13	0.70	1.63	14	1
1:C:44:LEU:C	1:C:44:LEU:HD23	0.69	2.08	8	6
1:C:59:ASN:HB3	2:R:76:LEU:HD21	0.69	1.65	8	2
1:C:13:LEU:CD1	1:C:62:ALA:HB2	0.69	2.18	5	5
1:C:56:ILE:HD12	1:C:61:VAL:HG11	0.69	1.62	13	2
1:C:61:VAL:HG13	1:C:62:ALA:N	0.67	2.03	16	4
1:C:53:THR:HG21	1:C:55:TYR:CE1	0.67	2.25	7	1
1:C:41:ASP:CB	2:R:73:LEU:HD21	0.67	2.20	13	3
1:C:44:LEU:HD23	1:C:44:LEU:C	0.67	2.08	7	3
1:C:14:TYR:CD1	1:C:14:TYR:N	0.67	2.61	1	14
1:C:12:ALA:HB1	1:C:26:PHE:CD1	0.66	2.24	7	11
1:C:44:LEU:HD21	1:C:53:THR:HG23	0.66	1.65	4	2
1:C:12:ALA:CB	1:C:26:PHE:CD1	0.66	2.79	16	10
1:C:34:ILE:HD13	1:C:45:ALA:HB2	0.66	1.65	6	4
1:C:46:HIS:CE1	1:C:52:GLN:O	0.66	2.48	16	1
1:C:11:VAL:HG21	1:C:64:SER:C	0.66	2.11	10	1
1:C:56:ILE:H	1:C:56:ILE:HD13	0.66	1.50	11	2
1:C:16:TYR:CB	1:C:26:PHE:CZ	0.65	2.80	12	11
1:C:47:SER:C	1:C:48:LEU:HD23	0.65	2.11	16	1
1:C:44:LEU:HD12	1:C:55:TYR:CE1	0.65	2.27	11	4
1:C:32:LEU:HD13	1:C:56:ILE:CG2	0.65	2.20	8	1
1:C:44:LEU:HD23	1:C:45:ALA:N	0.64	2.06	8	3
1:C:53:THR:CG2	1:C:55:TYR:CE1	0.64	2.80	7	2
2:R:71:ARG:O	2:R:72:ALA:HB3	0.64	1.91	12	5
1:C:59:ASN:O	2:R:76:LEU:HD21	0.64	1.92	6	1
1:C:59:ASN:HD21	2:R:73:LEU:HD22	0.63	1.53	9	1
1:C:59:ASN:ND2	2:R:73:LEU:HD12	0.63	2.08	12	1
1:C:32:LEU:HD22	1:C:56:ILE:CG2	0.63	2.23	7	1
1:C:59:ASN:CG	2:R:73:LEU:HD12	0.63	2.13	12	1
1:C:10:PHE:CG	1:C:34:ILE:CG1	0.63	2.81	3	4
1:C:46:HIS:CE1	1:C:52:GLN:N	0.62	2.67	16	1
1:C:46:HIS:NE2	1:C:52:GLN:N	0.62	2.46	8	2
1:C:41:ASP:HB2	2:R:73:LEU:HD21	0.62	1.71	16	1
1:C:44:LEU:HD21	1:C:53:THR:CG2	0.62	2.21	13	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:38:THR:HG22	1:C:39:GLU:N	0.61	2.11	12	1
1:C:57:PRO:O	1:C:61:VAL:HG12	0.61	1.94	9	5
1:C:10:PHE:CD1	1:C:34:ILE:CG1	0.61	2.84	5	4
1:C:53:THR:HG23	1:C:54:GLY:N	0.61	2.11	6	4
1:C:35:VAL:HG21	1:C:44:LEU:HD22	0.61	1.73	16	2
1:C:12:ALA:CB	1:C:26:PHE:CE1	0.61	2.81	9	1
1:C:59:ASN:ND2	1:C:60:TYR:CE1	0.60	2.69	10	2
1:C:59:ASN:HB2	2:R:76:LEU:HD21	0.60	1.71	16	1
1:C:35:VAL:CG2	1:C:44:LEU:HD23	0.60	2.27	11	2
1:C:16:TYR:CB	1:C:26:PHE:CE2	0.60	2.85	4	4
1:C:35:VAL:HG21	1:C:44:LEU:HD23	0.60	1.71	11	1
1:C:14:TYR:CE2	2:R:76:LEU:HD22	0.59	2.32	2	2
1:C:49:THR:HG22	1:C:50:THR:N	0.59	2.12	13	3
1:C:38:THR:HG23	1:C:39:GLU:HG2	0.59	1.73	11	1
1:C:55:TYR:CD1	1:C:55:TYR:N	0.59	2.67	4	4
1:C:50:THR:HG23	1:C:52:GLN:HG2	0.59	1.74	7	1
1:C:48:LEU:HD23	1:C:52:GLN:O	0.59	1.98	8	1
1:C:23:ASP:OD1	1:C:55:TYR:CD2	0.58	2.57	4	2
1:C:16:TYR:HB2	1:C:26:PHE:CZ	0.58	2.34	16	16
1:C:14:TYR:CE2	1:C:59:ASN:O	0.58	2.57	13	4
1:C:40:GLY:O	1:C:43:TRP:CD1	0.58	2.57	1	1
1:C:37:ASN:O	1:C:43:TRP:CD1	0.58	2.57	2	3
1:C:45:ALA:HB2	1:C:56:ILE:HG12	0.58	1.75	13	3
1:C:60:TYR:CE1	2:R:76:LEU:CD2	0.58	2.86	11	1
1:C:44:LEU:CD1	1:C:55:TYR:CE1	0.58	2.87	9	3
1:C:32:LEU:HD22	1:C:45:ALA:HB3	0.58	1.75	8	1
1:C:61:VAL:CG2	1:C:62:ALA:N	0.58	2.67	13	11
1:C:61:VAL:HG22	1:C:62:ALA:N	0.58	2.13	2	12
1:C:16:TYR:CB	1:C:26:PHE:CE1	0.58	2.87	15	6
1:C:30:GLU:O	1:C:32:LEU:HD12	0.58	1.99	16	1
1:C:33:GLN:CD	1:C:48:LEU:HD21	0.58	2.19	2	1
1:C:46:HIS:CD2	1:C:52:GLN:O	0.58	2.57	8	1
1:C:37:ASN:O	1:C:38:THR:HG22	0.57	1.99	1	1
1:C:13:LEU:CD1	1:C:62:ALA:CB	0.57	2.81	2	4
1:C:40:GLY:O	1:C:41:ASP:CB	0.57	2.53	6	2
1:C:13:LEU:C	1:C:14:TYR:CD1	0.57	2.78	7	9
1:C:61:VAL:HG22	1:C:62:ALA:H	0.57	1.60	5	4
1:C:41:ASP:O	1:C:42:TRP:CG	0.57	2.57	7	7
1:C:13:LEU:HB3	1:C:14:TYR:CE1	0.56	2.35	6	1
1:C:46:HIS:O	1:C:46:HIS:CD2	0.56	2.58	2	1
1:C:10:PHE:CD1	1:C:34:ILE:HG13	0.56	2.36	5	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:13:LEU:CB	1:C:14:TYR:CE1	0.56	2.88	6	2
1:C:14:TYR:HB2	1:C:60:TYR:CD2	0.56	2.34	7	1
1:C:11:VAL:HG21	1:C:64:SER:OXT	0.56	2.00	10	1
1:C:59:ASN:OD1	1:C:60:TYR:CD1	0.56	2.58	13	1
1:C:37:ASN:HB3	1:C:43:TRP:CD1	0.56	2.36	6	1
1:C:56:ILE:HD12	1:C:56:ILE:O	0.56	1.99	15	2
1:C:53:THR:HG22	1:C:54:GLY:N	0.55	2.16	2	5
1:C:13:LEU:O	1:C:14:TYR:CD1	0.55	2.59	8	1
1:C:37:ASN:O	1:C:43:TRP:CG	0.55	2.59	10	1
1:C:24:LEU:CD1	1:C:53:THR:O	0.55	2.54	2	8
1:C:44:LEU:CD1	1:C:55:TYR:CD1	0.55	2.90	10	4
1:C:53:THR:CG2	1:C:54:GLY:N	0.55	2.69	2	8
1:C:37:ASN:O	1:C:43:TRP:NE1	0.55	2.40	6	2
1:C:16:TYR:HB3	1:C:26:PHE:CE2	0.55	2.37	1	4
1:C:61:VAL:O	1:C:62:ALA:HB2	0.55	2.02	6	3
1:C:38:THR:CG2	1:C:39:GLU:N	0.55	2.70	12	1
1:C:16:TYR:HB2	1:C:26:PHE:CE1	0.55	2.36	16	4
1:C:32:LEU:CD2	1:C:56:ILE:HG21	0.55	2.26	7	1
1:C:42:TRP:CE2	2:R:71:ARG:HG2	0.55	2.37	12	1
1:C:35:VAL:CG2	1:C:44:LEU:CD2	0.55	2.81	11	2
1:C:34:ILE:CD1	1:C:56:ILE:HD11	0.54	2.29	12	2
1:C:59:ASN:ND2	2:R:73:LEU:HD22	0.54	2.17	9	1
1:C:35:VAL:HG23	1:C:44:LEU:O	0.54	2.02	10	1
1:C:47:SER:O	1:C:48:LEU:C	0.54	2.44	13	2
1:C:10:PHE:CD2	1:C:34:ILE:HG13	0.54	2.38	8	3
1:C:10:PHE:CG	1:C:34:ILE:HG12	0.54	2.38	4	4
1:C:16:TYR:CD2	1:C:57:PRO:HD3	0.54	2.37	1	3
1:C:42:TRP:CD1	2:R:71:ARG:HG2	0.54	2.37	3	3
1:C:58:SER:HA	1:C:61:VAL:HG12	0.54	1.76	12	1
1:C:34:ILE:HD11	1:C:56:ILE:CD1	0.54	2.26	12	1
1:C:46:HIS:ND1	1:C:49:THR:O	0.54	2.40	16	1
1:C:43:TRP:CE2	1:C:58:SER:HB2	0.54	2.38	6	1
1:C:45:ALA:O	1:C:54:GLY:N	0.54	2.41	2	2
1:C:16:TYR:CZ	1:C:18:SER:HB3	0.53	2.38	5	2
1:C:16:TYR:CE2	1:C:18:SER:HB3	0.53	2.38	16	4
1:C:55:TYR:O	1:C:56:ILE:CG2	0.53	2.57	15	1
1:C:11:VAL:HG22	1:C:31:ARG:HG3	0.53	1.80	2	1
1:C:37:ASN:O	1:C:38:THR:CG2	0.53	2.57	1	1
1:C:10:PHE:CG	1:C:34:ILE:HG13	0.53	2.39	12	9
1:C:53:THR:HG22	1:C:54:GLY:H	0.53	1.63	8	2
1:C:37:ASN:HB2	1:C:43:TRP:CD1	0.53	2.39	4	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:16:TYR:CZ	1:C:18:SER:OG	0.53	2.57	15	1
1:C:14:TYR:CE2	2:R:76:LEU:CD2	0.52	2.92	5	1
1:C:33:GLN:NE2	1:C:47:SER:CB	0.52	2.72	8	1
1:C:48:LEU:HD22	1:C:48:LEU:H	0.52	1.63	8	1
1:C:20:THR:CG2	1:C:22:THR:OG1	0.52	2.57	15	1
1:C:56:ILE:HD13	1:C:56:ILE:N	0.52	2.19	11	2
1:C:59:ASN:ND2	2:R:74:PRO:O	0.52	2.42	6	1
1:C:36:ASN:O	1:C:37:ASN:ND2	0.52	2.42	7	1
1:C:38:THR:O	1:C:38:THR:OG1	0.52	2.28	8	1
1:C:35:VAL:CG2	1:C:44:LEU:O	0.52	2.57	10	2
1:C:15:ASP:N	1:C:15:ASP:OD1	0.52	2.43	11	2
1:C:16:TYR:HB3	1:C:26:PHE:CZ	0.52	2.40	12	9
1:C:54:GLY:O	1:C:56:ILE:N	0.52	2.43	2	1
1:C:12:ALA:HB2	1:C:32:LEU:HD11	0.52	1.80	3	1
1:C:59:ASN:OD1	2:R:73:LEU:CD1	0.52	2.58	3	1
1:C:37:ASN:HA	1:C:43:TRP:CD1	0.52	2.40	7	1
1:C:21:GLU:O	1:C:22:THR:CB	0.52	2.57	14	1
1:C:44:LEU:CD2	1:C:53:THR:HG21	0.52	2.33	10	1
1:C:46:HIS:CE1	1:C:51:GLY:HA2	0.52	2.40	9	8
1:C:23:ASP:N	1:C:23:ASP:OD1	0.52	2.41	2	4
1:C:14:TYR:CD2	2:R:76:LEU:CD2	0.52	2.93	5	1
1:C:59:ASN:ND2	1:C:60:TYR:CD1	0.52	2.78	6	1
1:C:45:ALA:HB3	1:C:56:ILE:HG12	0.52	1.82	16	2
1:C:11:VAL:CG2	1:C:64:SER:O	0.51	2.58	6	1
1:C:44:LEU:HD13	1:C:55:TYR:CZ	0.51	2.39	10	1
1:C:33:GLN:O	1:C:45:ALA:CB	0.51	2.57	16	1
1:C:61:VAL:CG1	1:C:62:ALA:N	0.51	2.73	16	3
1:C:26:PHE:CB	1:C:30:GLU:OE1	0.51	2.58	11	1
1:C:14:TYR:CD2	2:R:76:LEU:HD23	0.51	2.40	5	1
1:C:14:TYR:CB	1:C:60:TYR:CD2	0.51	2.93	7	1
1:C:39:GLU:CB	1:C:42:TRP:O	0.51	2.58	5	1
1:C:24:LEU:O	1:C:25:SER:C	0.51	2.49	8	3
1:C:13:LEU:HD21	1:C:62:ALA:CB	0.51	2.28	8	1
1:C:44:LEU:HD12	1:C:55:TYR:HD1	0.51	1.54	9	1
2:R:71:ARG:O	2:R:72:ALA:CB	0.51	2.57	12	2
1:C:47:SER:O	1:C:49:THR:N	0.51	2.43	13	1
1:C:44:LEU:HD11	1:C:53:THR:HG23	0.51	1.83	12	3
1:C:44:LEU:HD12	1:C:55:TYR:HE1	0.51	1.65	6	1
1:C:15:ASP:O	1:C:60:TYR:CE2	0.51	2.64	1	1
1:C:41:ASP:CG	2:R:73:LEU:HD11	0.51	2.26	14	3
1:C:16:TYR:CZ	1:C:18:SER:HB2	0.51	2.41	7	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:24:LEU:N	1:C:24:LEU:CD2	0.51	2.65	8	3
1:C:23:ASP:OD2	1:C:55:TYR:CB	0.51	2.58	8	1
1:C:44:LEU:CD1	1:C:53:THR:HG23	0.50	2.37	2	1
1:C:55:TYR:O	1:C:56:ILE:HG23	0.50	2.06	15	1
1:C:23:ASP:OD1	1:C:23:ASP:N	0.50	2.42	4	3
1:C:10:PHE:CD2	1:C:34:ILE:HD11	0.50	2.42	7	1
1:C:37:ASN:C	1:C:38:THR:CG2	0.50	2.80	8	1
1:C:11:VAL:HG21	1:C:64:SER:O	0.50	2.07	6	2
1:C:16:TYR:CE1	1:C:57:PRO:HG3	0.50	2.41	6	1
1:C:26:PHE:CE2	1:C:56:ILE:HB	0.50	2.41	11	1
1:C:32:LEU:HD23	1:C:47:SER:OG	0.50	2.05	16	1
1:C:37:ASN:C	1:C:38:THR:HG23	0.50	2.27	8	1
1:C:19:ARG:O	1:C:20:THR:CB	0.50	2.58	14	1
1:C:46:HIS:CD2	1:C:47:SER:O	0.50	2.64	6	2
1:C:36:ASN:O	1:C:37:ASN:O	0.50	2.30	7	3
1:C:10:PHE:CD2	1:C:63:PRO:N	0.50	2.80	6	1
1:C:44:LEU:O	1:C:44:LEU:CD2	0.50	2.57	7	2
1:C:32:LEU:HD23	1:C:48:LEU:HD11	0.50	1.84	8	1
1:C:16:TYR:CE2	1:C:57:PRO:HD3	0.50	2.41	14	4
1:C:34:ILE:HG22	1:C:35:VAL:N	0.49	2.22	15	1
1:C:40:GLY:O	1:C:43:TRP:NE1	0.49	2.44	1	1
1:C:16:TYR:CZ	1:C:18:SER:CB	0.49	2.94	5	4
1:C:56:ILE:HD12	1:C:61:VAL:CG1	0.49	2.37	13	1
1:C:46:HIS:CD2	1:C:46:HIS:C	0.49	2.84	2	2
1:C:44:LEU:C	1:C:44:LEU:CD2	0.49	2.79	8	7
1:C:43:TRP:CZ2	1:C:58:SER:HB2	0.49	2.42	7	5
1:C:16:TYR:CE2	1:C:18:SER:OG	0.49	2.62	11	2
1:C:60:TYR:CD1	2:R:76:LEU:HD21	0.49	2.42	11	1
1:C:24:LEU:N	1:C:24:LEU:HD12	0.49	2.22	1	1
1:C:36:ASN:O	1:C:37:ASN:CB	0.49	2.61	2	3
1:C:35:VAL:HB	1:C:44:LEU:O	0.49	2.08	7	8
1:C:11:VAL:CG2	1:C:64:SER:C	0.49	2.81	10	1
1:C:46:HIS:NE2	1:C:48:LEU:HD11	0.49	2.22	16	1
1:C:60:TYR:CE1	2:R:74:PRO:HB2	0.48	2.43	8	1
1:C:26:PHE:CE2	1:C:56:ILE:HG22	0.48	2.43	1	3
1:C:56:ILE:HD12	1:C:56:ILE:C	0.48	2.29	2	1
1:C:42:TRP:CE2	2:R:71:ARG:CG	0.48	2.96	12	1
1:C:21:GLU:O	1:C:21:GLU:CG	0.48	2.61	8	1
1:C:46:HIS:NE2	1:C:51:GLY:C	0.48	2.67	8	1
1:C:42:TRP:NE1	2:R:73:LEU:HD23	0.48	2.24	16	1
1:C:46:HIS:HA	1:C:48:LEU:CD2	0.48	2.38	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:10:PHE:HB3	1:C:61:VAL:HG22	0.48	1.85	6	1
1:C:37:ASN:O	1:C:37:ASN:OD1	0.48	2.32	7	1
1:C:46:HIS:O	1:C:47:SER:CB	0.48	2.62	8	1
1:C:11:VAL:HG23	1:C:64:SER:O	0.48	2.08	3	1
1:C:16:TYR:CZ	1:C:42:TRP:CZ3	0.48	3.01	8	1
1:C:59:ASN:HB2	2:R:73:LEU:CD1	0.48	2.39	12	1
1:C:43:TRP:CH2	1:C:58:SER:HB2	0.47	2.44	9	2
1:C:46:HIS:HD2	1:C:48:LEU:HD23	0.47	1.59	10	1
1:C:50:THR:O	1:C:50:THR:CG2	0.47	2.55	16	1
1:C:10:PHE:HB3	1:C:61:VAL:CG2	0.47	2.39	10	7
1:C:44:LEU:HB2	1:C:55:TYR:CE1	0.47	2.44	10	2
1:C:16:TYR:O	1:C:25:SER:CB	0.47	2.62	9	3
1:C:46:HIS:NE2	1:C:52:GLN:O	0.47	2.48	8	1
1:C:60:TYR:CZ	2:R:74:PRO:HB2	0.47	2.44	14	2
1:C:60:TYR:CE1	2:R:74:PRO:HG2	0.47	2.43	3	3
1:C:22:THR:O	1:C:23:ASP:O	0.47	2.33	9	1
2:R:71:ARG:CG	2:R:71:ARG:O	0.47	2.62	9	1
2:R:73:LEU:HD23	2:R:74:PRO:HD2	0.47	1.86	10	1
1:C:10:PHE:CD2	1:C:62:ALA:C	0.47	2.89	16	3
1:C:59:ASN:OD1	2:R:73:LEU:HD12	0.46	2.10	3	1
1:C:22:THR:O	1:C:24:LEU:HD23	0.46	2.10	7	1
1:C:17:GLU:O	1:C:18:SER:O	0.46	2.33	14	4
1:C:24:LEU:O	1:C:25:SER:O	0.46	2.33	8	1
1:C:33:GLN:CG	1:C:47:SER:HB2	0.46	2.40	8	1
1:C:9:THR:HG22	1:C:9:THR:O	0.46	2.10	2	1
1:C:42:TRP:NE1	2:R:73:LEU:CD2	0.46	2.78	12	1
1:C:12:ALA:HB3	1:C:27:LYS:O	0.46	2.10	7	2
1:C:42:TRP:CZ2	2:R:74:PRO:HD3	0.46	2.45	1	2
1:C:33:GLN:NE2	1:C:47:SER:HB2	0.46	2.26	8	1
1:C:42:TRP:NE1	2:R:71:ARG:HG2	0.46	2.25	12	5
1:C:23:ASP:C	1:C:24:LEU:HD23	0.46	2.29	8	1
1:C:22:THR:HG22	1:C:23:ASP:N	0.46	2.25	7	1
1:C:35:VAL:CB	1:C:44:LEU:O	0.46	2.64	10	1
1:C:30:GLU:OE2	1:C:31:ARG:O	0.46	2.34	4	1
1:C:23:ASP:OD2	1:C:55:TYR:HB2	0.46	2.11	8	1
1:C:46:HIS:O	1:C:47:SER:HB2	0.46	2.11	8	1
1:C:15:ASP:OD1	1:C:28:LYS:N	0.46	2.49	12	1
1:C:15:ASP:OD1	1:C:26:PHE:O	0.45	2.34	3	2
2:R:71:ARG:O	2:R:72:ALA:O	0.45	2.34	16	2
1:C:24:LEU:HD21	1:C:52:GLN:HB2	0.45	1.87	10	1
1:C:24:LEU:HD23	1:C:54:GLY:CA	0.45	2.41	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:56:ILE:CD1	1:C:61:VAL:CG1	0.45	2.92	3	1
1:C:13:LEU:N	1:C:60:TYR:O	0.45	2.50	6	2
1:C:44:LEU:HD11	1:C:53:THR:CG2	0.45	2.40	15	3
1:C:16:TYR:HB3	1:C:26:PHE:CE1	0.45	2.47	15	3
1:C:12:ALA:HB2	1:C:26:PHE:CD1	0.45	2.45	5	2
1:C:35:VAL:CG2	1:C:44:LEU:HD22	0.45	2.41	16	1
1:C:37:ASN:O	1:C:37:ASN:CG	0.45	2.55	7	1
2:R:73:LEU:CD2	2:R:74:PRO:HD2	0.45	2.42	10	1
1:C:11:VAL:O	1:C:12:ALA:O	0.45	2.35	13	1
1:C:16:TYR:O	1:C:25:SER:HB3	0.45	2.12	9	6
1:C:37:ASN:O	1:C:38:THR:HG23	0.45	2.11	8	1
1:C:46:HIS:NE2	1:C:52:GLN:C	0.45	2.70	16	2
1:C:24:LEU:HG	1:C:54:GLY:CA	0.45	2.42	9	1
1:C:46:HIS:CE1	1:C:49:THR:O	0.45	2.70	16	1
1:C:41:ASP:OD1	1:C:41:ASP:N	0.45	2.50	4	2
1:C:39:GLU:HB2	1:C:42:TRP:O	0.45	2.11	5	1
1:C:32:LEU:HB3	1:C:45:ALA:HB1	0.45	1.88	15	2
1:C:42:TRP:NE1	2:R:71:ARG:CG	0.45	2.79	9	1
1:C:10:PHE:CZ	1:C:63:PRO:HG3	0.45	2.47	10	1
1:C:55:TYR:C	1:C:56:ILE:HG23	0.45	2.33	15	1
1:C:23:ASP:CB	1:C:55:TYR:HB2	0.44	2.42	8	1
1:C:57:PRO:HG2	1:C:60:TYR:CD2	0.44	2.47	13	1
1:C:34:ILE:HD13	1:C:45:ALA:CB	0.44	2.42	16	1
1:C:24:LEU:HG	1:C:54:GLY:HA3	0.44	1.89	9	1
1:C:37:ASN:O	1:C:38:THR:C	0.44	2.55	6	2
2:R:75:PRO:O	2:R:76:LEU:C	0.44	2.56	10	3
1:C:36:ASN:O	1:C:37:ASN:CG	0.44	2.56	7	2
1:C:23:ASP:OD2	2:R:71:ARG:NH1	0.44	2.51	11	1
1:C:33:GLN:CG	1:C:48:LEU:HD11	0.44	2.42	15	1
1:C:10:PHE:CD1	1:C:63:PRO:HA	0.44	2.48	2	1
1:C:16:TYR:HB3	1:C:26:PHE:CD2	0.44	2.48	4	1
1:C:16:TYR:HA	1:C:60:TYR:CD2	0.44	2.47	4	1
1:C:41:ASP:O	1:C:42:TRP:CD1	0.44	2.71	5	3
1:C:32:LEU:CD1	1:C:56:ILE:HG21	0.44	2.26	8	1
1:C:10:PHE:HB2	1:C:34:ILE:HD11	0.44	1.89	2	1
1:C:16:TYR:CE1	1:C:18:SER:HB2	0.44	2.47	7	1
1:C:16:TYR:CZ	1:C:42:TRP:CH2	0.44	3.06	1	2
1:C:46:HIS:CD2	1:C:46:HIS:O	0.44	2.71	4	1
1:C:41:ASP:HB3	2:R:73:LEU:CD1	0.44	2.43	6	1
1:C:43:TRP:CD1	1:C:43:TRP:N	0.44	2.83	6	1
1:C:11:VAL:HG23	1:C:64:SER:OG	0.44	2.12	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:21:GLU:O	1:C:21:GLU:HG2	0.44	2.12	8	1
1:C:33:GLN:HB2	1:C:48:LEU:CD1	0.44	2.42	11	1
1:C:47:SER:O	1:C:48:LEU:CD2	0.44	2.56	16	1
2:R:71:ARG:O	2:R:72:ALA:C	0.43	2.57	2	1
1:C:46:HIS:HA	1:C:52:GLN:O	0.43	2.13	2	1
1:C:24:LEU:CG	1:C:53:THR:O	0.43	2.66	8	1
1:C:36:ASN:O	1:C:37:ASN:OD1	0.43	2.37	6	1
1:C:18:SER:OG	1:C:24:LEU:C	0.43	2.57	2	1
1:C:17:GLU:O	1:C:18:SER:C	0.43	2.57	16	6
1:C:16:TYR:CZ	1:C:57:PRO:HG3	0.43	2.48	6	2
1:C:47:SER:C	1:C:48:LEU:CD2	0.43	2.84	16	1
1:C:56:ILE:HD12	1:C:57:PRO:O	0.43	2.14	3	1
1:C:41:ASP:HB3	2:R:73:LEU:CD2	0.43	2.43	2	1
1:C:24:LEU:CD2	1:C:53:THR:O	0.43	2.67	3	1
1:C:40:GLY:O	1:C:41:ASP:HB2	0.43	2.14	6	2
1:C:13:LEU:C	1:C:14:TYR:CG	0.43	2.92	8	1
1:C:28:LYS:HG3	1:C:29:GLY:N	0.43	2.29	13	1
1:C:42:TRP:HE1	2:R:73:LEU:HD23	0.43	1.73	16	1
1:C:60:TYR:OH	2:R:75:PRO:O	0.43	2.33	2	1
1:C:61:VAL:O	1:C:62:ALA:CB	0.43	2.66	6	1
1:C:11:VAL:CG2	1:C:64:SER:HB2	0.43	2.44	9	1
1:C:38:THR:OG1	1:C:39:GLU:N	0.43	2.51	16	1
1:C:58:SER:HA	1:C:61:VAL:CG1	0.43	2.43	2	1
1:C:22:THR:HG22	1:C:55:TYR:HE2	0.43	1.74	3	1
1:C:16:TYR:HB2	1:C:26:PHE:CE2	0.43	2.48	4	1
1:C:12:ALA:O	1:C:13:LEU:C	0.43	2.56	8	1
1:C:12:ALA:O	1:C:13:LEU:HD23	0.43	2.14	13	1
1:C:24:LEU:CG	1:C:54:GLY:HA3	0.43	2.44	14	1
1:C:15:ASP:OD1	1:C:15:ASP:C	0.42	2.57	15	1
1:C:24:LEU:HD23	1:C:54:GLY:HA3	0.42	1.89	3	1
1:C:24:LEU:HD11	1:C:52:GLN:O	0.42	2.13	12	1
1:C:10:PHE:CD2	1:C:34:ILE:CG1	0.42	3.01	15	1
1:C:16:TYR:CE2	1:C:18:SER:CB	0.42	3.02	16	1
1:C:36:ASN:O	1:C:37:ASN:HB2	0.42	2.14	2	2
1:C:33:GLN:CD	1:C:47:SER:OG	0.42	2.57	8	1
1:C:45:ALA:CB	1:C:56:ILE:HG12	0.42	2.44	14	2
1:C:43:TRP:O	1:C:55:TYR:HA	0.42	2.15	3	2
1:C:12:ALA:HB2	1:C:32:LEU:CD1	0.42	2.45	13	1
1:C:10:PHE:CE2	1:C:63:PRO:CA	0.42	3.02	16	1
1:C:33:GLN:O	1:C:45:ALA:HA	0.42	2.14	8	1
1:C:49:THR:O	1:C:50:THR:C	0.42	2.57	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:17:GLU:O	1:C:17:GLU:HG3	0.42	2.15	1	2
1:C:21:GLU:HG3	1:C:22:THR:N	0.42	2.29	3	1
1:C:16:TYR:OH	1:C:18:SER:HB2	0.42	2.14	5	1
1:C:20:THR:OG1	1:C:23:ASP:OD2	0.42	2.34	5	1
1:C:38:THR:HG23	1:C:39:GLU:H	0.42	1.74	6	1
1:C:11:VAL:HG23	1:C:64:SER:CB	0.42	2.44	7	1
1:C:16:TYR:CE1	1:C:18:SER:CB	0.42	3.03	7	1
2:R:71:ARG:O	2:R:71:ARG:CD	0.42	2.67	9	1
2:R:72:ALA:O	2:R:73:LEU:C	0.42	2.57	9	1
1:C:40:GLY:O	1:C:41:ASP:C	0.42	2.58	1	1
1:C:12:ALA:HA	1:C:61:VAL:HG23	0.42	1.92	14	1
1:C:63:PRO:O	1:C:64:SER:HB2	0.42	2.14	6	1
1:C:30:GLU:HG3	1:C:31:ARG:N	0.42	2.30	7	1
1:C:37:ASN:O	1:C:38:THR:HB	0.42	2.14	7	1
1:C:11:VAL:O	1:C:61:VAL:HA	0.42	2.15	16	1
1:C:47:SER:C	1:C:48:LEU:CG	0.42	2.87	16	1
1:C:46:HIS:CE1	1:C:47:SER:O	0.42	2.72	2	1
2:R:75:PRO:O	2:R:76:LEU:O	0.42	2.37	10	2
1:C:13:LEU:O	1:C:28:LYS:HG3	0.41	2.15	1	1
1:C:20:THR:HG23	1:C:22:THR:H	0.41	1.75	12	1
1:C:33:GLN:O	1:C:34:ILE:C	0.41	2.57	14	2
1:C:46:HIS:CE1	1:C:52:GLN:H	0.41	2.30	16	1
1:C:17:GLU:O	1:C:17:GLU:CG	0.41	2.67	11	2
1:C:41:ASP:HB3	2:R:73:LEU:CG	0.41	2.45	6	1
1:C:44:LEU:HG	1:C:55:TYR:CE1	0.41	2.50	8	1
1:C:45:ALA:HB3	1:C:56:ILE:HD12	0.41	1.92	11	1
1:C:46:HIS:CD2	1:C:47:SER:H	0.41	2.34	8	1
1:C:15:ASP:OD1	1:C:15:ASP:N	0.41	2.53	12	1
1:C:13:LEU:HB2	1:C:14:TYR:CE1	0.41	2.51	15	1
1:C:37:ASN:HA	1:C:43:TRP:NE1	0.41	2.30	12	1
1:C:42:TRP:CH2	1:C:57:PRO:HB3	0.41	2.50	12	1
1:C:46:HIS:NE2	1:C:47:SER:O	0.41	2.54	4	1
1:C:33:GLN:HB2	1:C:46:HIS:O	0.41	2.15	8	2
1:C:44:LEU:CD2	1:C:53:THR:CG2	0.41	2.99	8	1
1:C:16:TYR:OH	1:C:42:TRP:CH2	0.41	2.72	1	1
1:C:26:PHE:CE2	1:C:56:ILE:CG2	0.41	3.03	2	1
1:C:45:ALA:O	1:C:54:GLY:CA	0.41	2.69	2	1
1:C:59:ASN:OD1	1:C:59:ASN:C	0.41	2.59	13	1
1:C:10:PHE:CE1	1:C:63:PRO:HA	0.41	2.51	7	1
1:C:22:THR:O	1:C:23:ASP:C	0.41	2.58	10	2
1:C:49:THR:CG2	1:C:50:THR:N	0.41	2.79	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:38:THR:O	1:C:38:THR:HG23	0.41	2.15	1	1
1:C:40:GLY:O	1:C:41:ASP:CG	0.41	2.59	11	1
1:C:11:VAL:O	1:C:61:VAL:CG2	0.41	2.69	16	1
1:C:32:LEU:CD2	1:C:48:LEU:HD11	0.40	2.46	8	1
1:C:36:ASN:O	1:C:43:TRP:CG	0.40	2.75	12	1
1:C:55:TYR:N	1:C:55:TYR:CD1	0.40	2.88	14	1
1:C:41:ASP:O	1:C:58:SER:HB3	0.40	2.16	1	1
1:C:13:LEU:HD23	1:C:13:LEU:HA	0.40	1.81	10	1
1:C:60:TYR:CE1	2:R:76:LEU:HD21	0.40	2.51	11	1
1:C:24:LEU:HD12	1:C:53:THR:C	0.40	2.36	15	1
1:C:42:TRP:CZ3	1:C:57:PRO:N	0.40	2.90	5	1
1:C:63:PRO:O	1:C:64:SER:CB	0.40	2.70	6	1
1:C:59:ASN:ND2	2:R:73:LEU:CD1	0.40	2.77	9	1
1:C:37:ASN:C	1:C:38:THR:HG22	0.40	2.36	1	1
1:C:23:ASP:HA	1:C:55:TYR:HB2	0.40	1.92	2	1
1:C:42:TRP:CZ3	1:C:57:PRO:CA	0.40	3.04	5	1
1:C:16:TYR:C	1:C:16:TYR:CD1	0.40	2.93	7	1
1:C:28:LYS:HG2	1:C:28:LYS:O	0.40	2.16	7	1
1:C:46:HIS:O	1:C:48:LEU:N	0.40	2.54	11	1
1:C:47:SER:O	1:C:48:LEU:HB2	0.40	2.16	11	1
1:C:16:TYR:CE2	1:C:18:SER:HB2	0.40	2.52	4	1
1:C:34:ILE:CG2	1:C:35:VAL:N	0.40	2.84	15	1
1:C:33:GLN:N	1:C:46:HIS:O	0.40	2.54	16	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	C	54/64 (84%)	41±3 (76±6%)	11±3 (20±5%)	2±2 (4±3%)	5	31
2	R	5/9 (56%)	4±1 (75±17%)	1±1 (18±12%)	0±0 (8±10%)	2	15
All	All	944/1168 (81%)	713 (76%)	190 (20%)	41 (4%)	5	29

All 19 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	18	SER	7
1	C	37	ASN	7
2	R	72	ALA	5
1	C	55	TYR	4
1	C	22	THR	2
1	C	40	GLY	2
1	C	48	LEU	2
1	C	54	GLY	1
1	C	63	PRO	1
1	C	62	ALA	1
1	C	38	THR	1
1	C	39	GLU	1
1	C	49	THR	1
1	C	25	SER	1
1	C	23	ASP	1
2	R	75	PRO	1
1	C	12	ALA	1
1	C	33	GLN	1
1	C	34	ILE	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	C	49/52 (94%)	36±3 (73±6%)	13±3 (27±6%)	2 21
2	R	5/8 (62%)	4±1 (80±17%)	1±1 (20±17%)	4 34
All	All	864/960 (90%)	633 (73%)	231 (27%)	2 22

All 42 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	C	25	SER	16
1	C	19	ARG	12
1	C	22	THR	11
1	C	27	LYS	11
2	R	71	ARG	11
1	C	14	TYR	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	C	58	SER	9
1	C	39	GLU	8
1	C	38	THR	8
1	C	20	THR	8
1	C	18	SER	7
1	C	49	THR	7
1	C	23	ASP	7
1	C	47	SER	7
1	C	21	GLU	7
1	C	53	THR	7
1	C	17	GLU	7
1	C	28	LYS	6
1	C	41	ASP	5
1	C	15	ASP	5
1	C	32	LEU	5
1	C	33	GLN	5
1	C	9	THR	4
1	C	31	ARG	4
1	C	36	ASN	4
1	C	50	THR	4
1	C	59	ASN	3
1	C	64	SER	3
1	C	24	LEU	3
1	C	55	TYR	3
1	C	52	GLN	3
1	C	37	ASN	3
1	C	61	VAL	3
2	R	74	PRO	3
1	C	44	LEU	2
1	C	30	GLU	2
1	C	48	LEU	2
1	C	56	ILE	2
2	R	73	LEU	2
1	C	46	HIS	1
1	C	57	PRO	1
1	C	11	VAL	1

6.3.3 RNA

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

No chemical shift data were provided