

Full wwPDB NMR Structure Validation Report (i)

Apr 20, 2024 – 12:17 PM EDT

PDB ID : 2KBM

Title: Ca-S100A1 interacting with TRTK12

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Deposited on : 2008-12-02

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

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

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

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

MolProbity: 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

wwPDB-RCI : v 1n 11 5 13 A (Berjanski et al., 2005)

PANAV : Wang et al. (2010)

wwPDB-ShiftChecker : v1.2

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

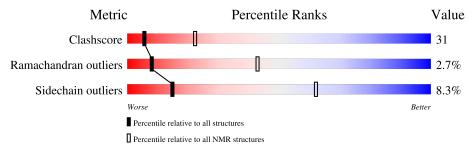
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive	NMR archive
Metric	$(\# \mathrm{Entries})$	$(\# \mathrm{Entries})$
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	X	12	8%	58%	33%				
1	Y	12	25%	42%	33%				
2	A	93		55%	40%	•••			
2	В	93		55%	39%	• •			



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 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	X:5-X:12, Y:5-Y:12, A:1-	0.77	1					
	A:90, B:2-B:90 (195)							

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 3 single-model clusters were found.

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



3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3322 atoms, of which 1644 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called F-actin-capping protein subunit alpha-2.

Mol	Chain	Residues		Atoms				
1	v	19	Total	С	Н	N	О	0
	12	217	66	113	19	19	0	
1	V	19	Total	С	Н	N	О	0
1 Y	12	217	66	113	19	19	U	

• Molecule 2 is a protein called Protein S100-A1.

Mol	Chain	Residues		Atoms					Trace	
2	Λ	93	Total	С	Н	N	О	S	0	
	\mathcal{L} A	90	1442	462	709	115	153	3	U	
9	D	93	Total	С	Н	N	О	S	0	
	Б	90	1442	462	709	115	153	3		

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms
2	Λ	9	Total Ca
3	Α		$2 \qquad 2$
2	D	9	Total Ca
3	Ъ	2	$2 \qquad 2$

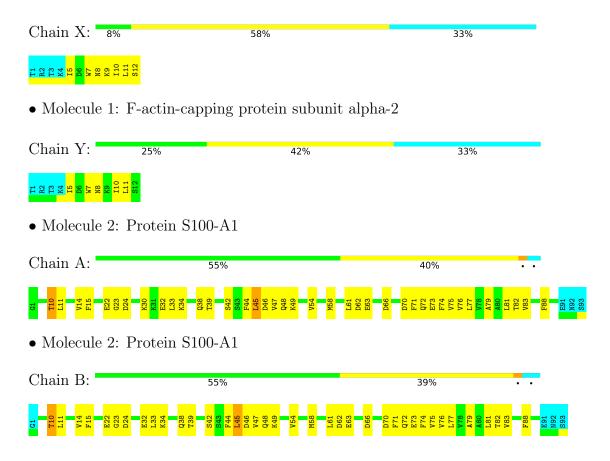


4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: F-actin-capping protein subunit alpha-2



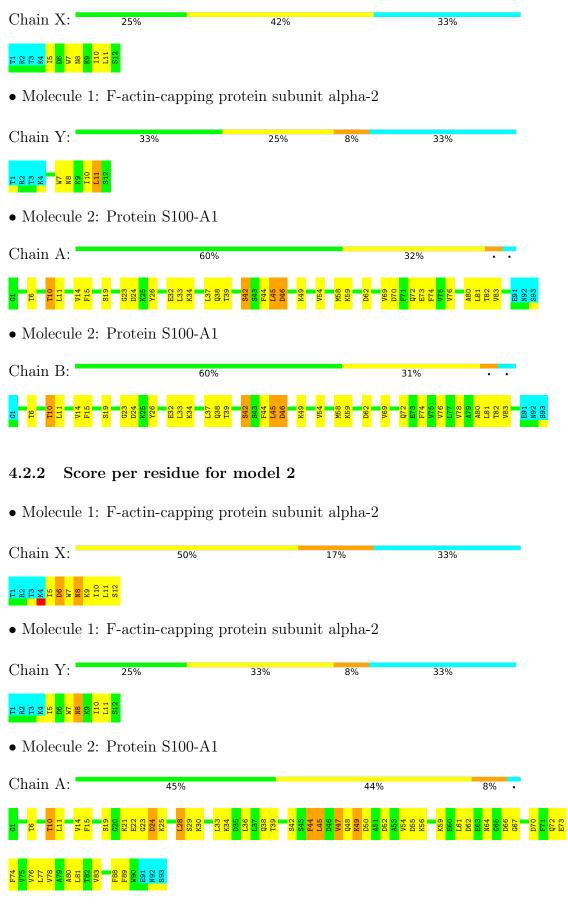
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

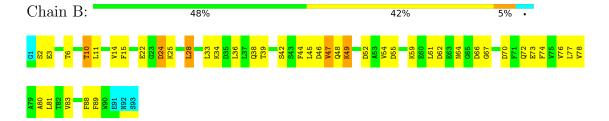
• Molecule 1: F-actin-capping protein subunit alpha-2





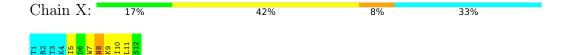






4.2.3 Score per residue for model 3

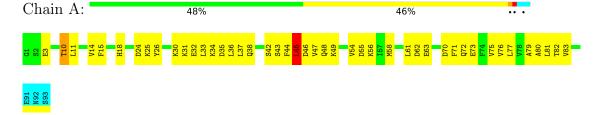
• Molecule 1: F-actin-capping protein subunit alpha-2



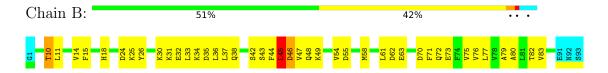
 \bullet Molecule 1: F-actin-capping protein subunit alpha-2



• Molecule 2: Protein S100-A1



• Molecule 2: Protein S100-A1

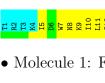


4.2.4 Score per residue for model 4

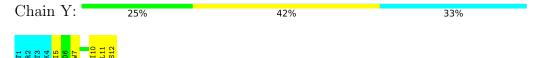
• Molecule 1: F-actin-capping protein subunit alpha-2



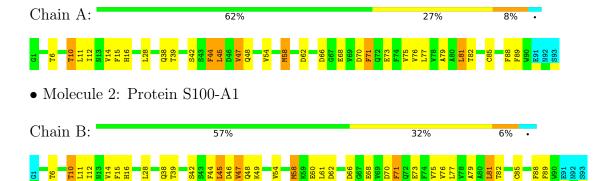




• Molecule 1: F-actin-capping protein subunit alpha-2

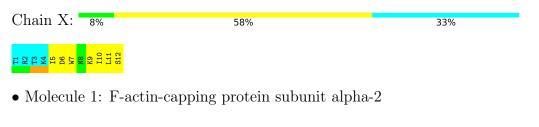


• Molecule 2: Protein S100-A1



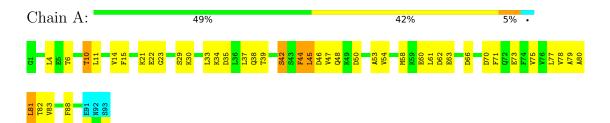
4.2.5 Score per residue for model 5

• Molecule 1: F-actin-capping protein subunit alpha-2



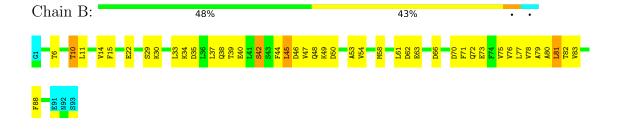






• Molecule 2: Protein S100-A1





4.2.6 Score per residue for model 6

• Molecule 1: F-actin-capping protein subunit alpha-2

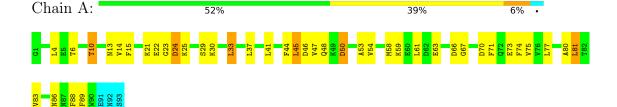
Chain X: 50% 17% 33%

• Molecule 1: F-actin-capping protein subunit alpha-2

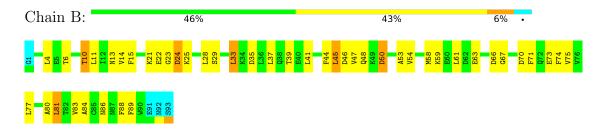
Chain Y: 33% 33% 33%

T1 R2 T3 K4 I5 N8 N8 K9 L110 L111 S12

• Molecule 2: Protein S100-A1

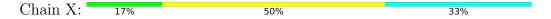


• Molecule 2: Protein S100-A1



4.2.7 Score per residue for model 7

• Molecule 1: F-actin-capping protein subunit alpha-2







• Molecule 1: F-actin-capping protein subunit alpha-2

Chain Y: 42% 25% 33%

T1 R2 T3 K4 I5 D6 W7 M7 L111

• Molecule 2: Protein S100-A1

Chain A: 48% 43% ...



• Molecule 2: Protein S100-A1

Chain B: 52% 39% 5% .

4.2.8 Score per residue for model 8

• Molecule 1: F-actin-capping protein subunit alpha-2

Chain X: 17% 50% 33%

T1 R2 R4 W7 N8 K9 I110 L111

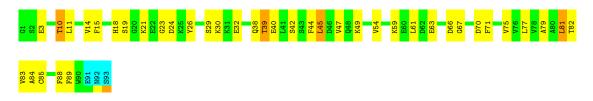
• Molecule 1: F-actin-capping protein subunit alpha-2

Chain Y: 17% 42% 8% 33%

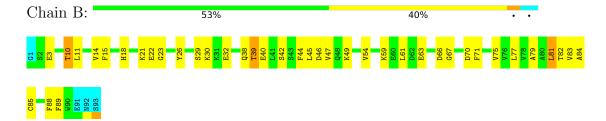
• Molecule 2: Protein S100-A1

Chain A: 54% 39% . .



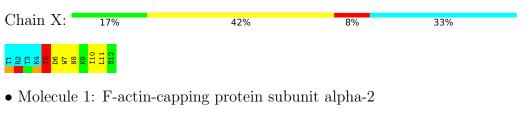


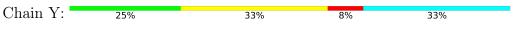
• Molecule 2: Protein S100-A1



4.2.9 Score per residue for model 9

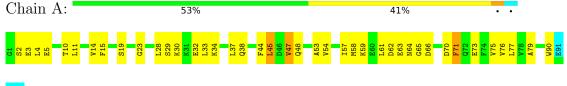
• Molecule 1: F-actin-capping protein subunit alpha-2





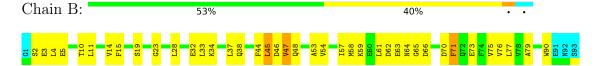


• Molecule 2: Protein S100-A1



N92 S93

• Molecule 2: Protein S100-A1





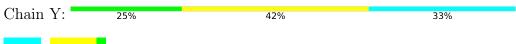
4.2.10 Score per residue for model 10

• Molecule 1: F-actin-capping protein subunit alpha-2



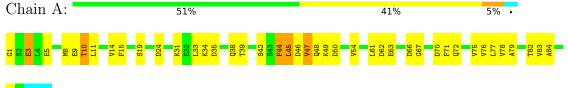
T11 T3 T43 K4 K4 N7 W7 N8 K9 L110 L110

• Molecule 1: F-actin-capping protein subunit alpha-2



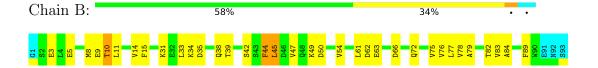


• Molecule 2: Protein S100-A1



F89 W90 N92 S93

• Molecule 2: Protein S100-A1



4.2.11 Score per residue for model 11

• Molecule 1: F-actin-capping protein subunit alpha-2



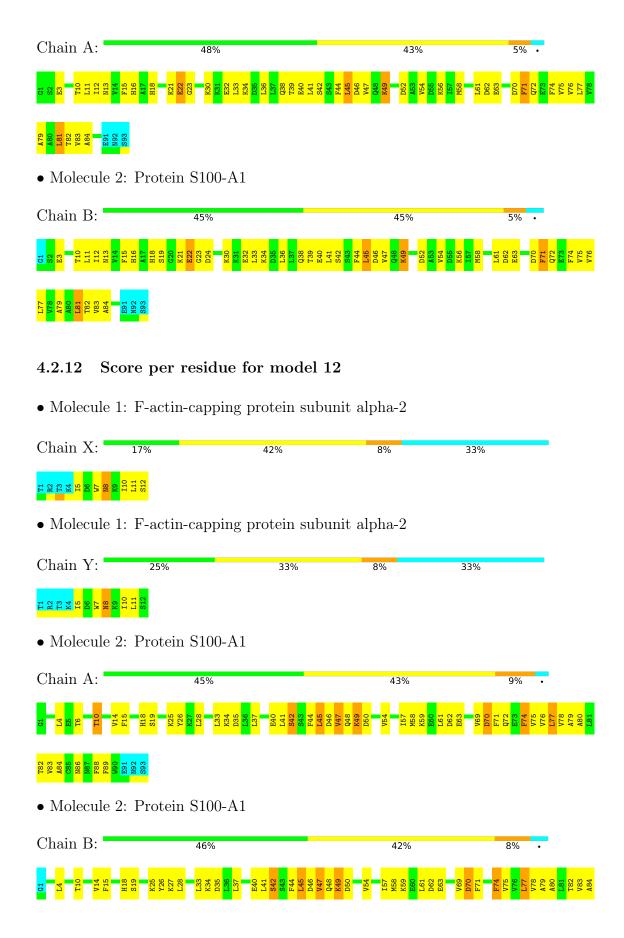
T1 T3 K4 I5 D6 W7 W8 K9 I110 L111

• Molecule 1: F-actin-capping protein subunit alpha-2



• Molecule 2: Protein S100-A1



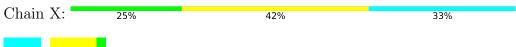






4.2.13 Score per residue for model 13

• Molecule 1: F-actin-capping protein subunit alpha-2

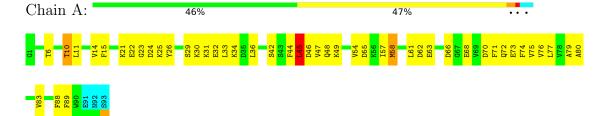


T11 R2 T3 K4 W7 N8 K9 I10 I110

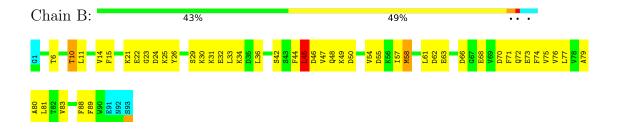
• Molecule 1: F-actin-capping protein subunit alpha-2



• Molecule 2: Protein S100-A1

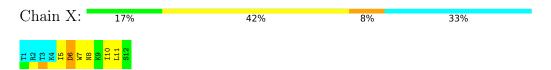


• Molecule 2: Protein S100-A1



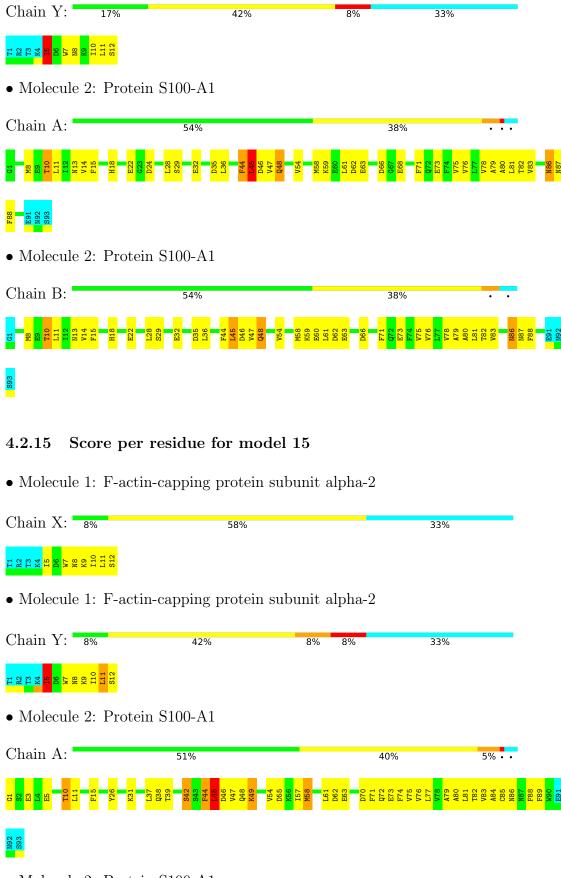
4.2.14 Score per residue for model 14

• Molecule 1: F-actin-capping protein subunit alpha-2



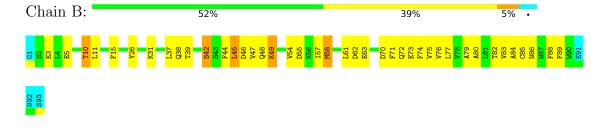
• Molecule 1: F-actin-capping protein subunit alpha-2





• Molecule 2: Protein S100-A1





4.2.16 Score per residue for model 16

• Molecule 1: F-actin-capping protein subunit alpha-2

Chain X: 8% 58% 33%

• Molecule 1: F-actin-capping protein subunit alpha-2

Chain Y: 17% 50% 33%

T1 T3 T3 K4 K4 W7 W7 N8 N8 L110 L111

• Molecule 2: Protein S100-A1

Chain A: 55% 38%

• Molecule 2: Protein S100-A1

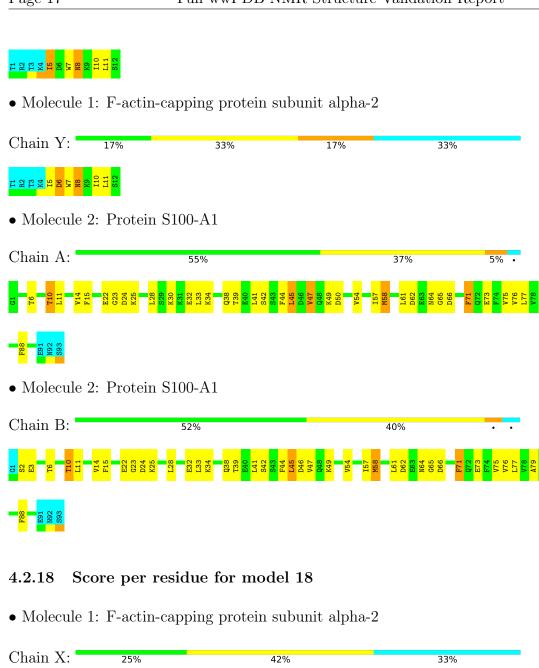
Chain B: 555% 38% . . .

4.2.17 Score per residue for model 17

• Molecule 1: F-actin-capping protein subunit alpha-2

Chain X: 25% 25% 17% 33%





• Molecule 1: F-actin-capping protein subunit alpha-2

Chain Y: 33% 42%

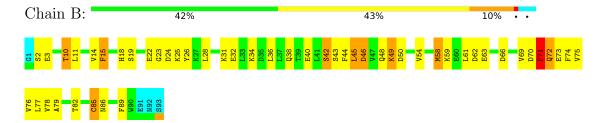
• Molecule 2: Protein S100-A1

Chain A: 46% 40% 10%



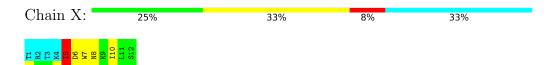


• Molecule 2: Protein S100-A1



4.2.19 Score per residue for model 19

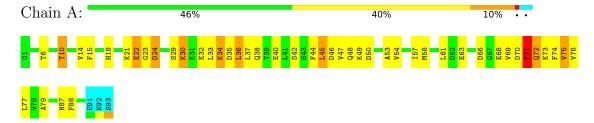
• Molecule 1: F-actin-capping protein subunit alpha-2



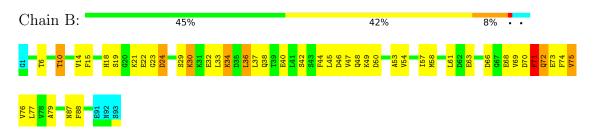
• Molecule 1: F-actin-capping protein subunit alpha-2



• Molecule 2: Protein S100-A1



• Molecule 2: Protein S100-A1





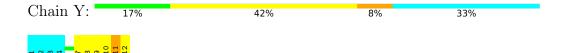
4.2.20 Score per residue for model 20

• Molecule 1: F-actin-capping protein subunit alpha-2





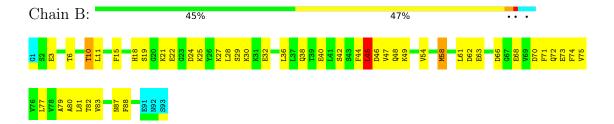
• Molecule 1: F-actin-capping protein subunit alpha-2



• Molecule 2: Protein S100-A1



• Molecule 2: Protein S100-A1





Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: simulated annealing, DGSA-distance geometry simulated annealing.

Of the 200 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
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

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

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		В	Sond lengths	Bond angles		
		RMSZ	#Z>5	RMSZ	#Z>5	
1	X	0.90 ± 0.01	$0\pm0/71~(~0.0\pm~0.0\%)$	1.08 ± 0.03	$0\pm0/94~(~0.0\pm~0.0\%)$	
1	Y	0.91 ± 0.02	$0\pm0/71~(~0.0\pm~0.0\%)$	1.09 ± 0.02	$0\pm0/94~(~0.0\pm~0.0\%)$	
2	A	1.15 ± 0.01	$0\pm0/720~(~0.0\pm~0.0\%)$	0.92 ± 0.01	$0\pm0/970~(~0.0\pm~0.0\%)$	
2	В	1.13 ± 0.01	$0\pm0/716~(~0.0\pm~0.0\%)$	0.91 ± 0.01	$0\pm0/965~(~0.0\pm~0.0\%)$	
All	All	1.12	1/31560~(~0.0%)	0.93	0/42460 (0.0%)	

All unique bond outliers are listed below.

1/4	ام1	Chain	Dec	Tune	Atoma	7	Observed (Å)	Ideal(Å)	Mod	dels			
101	101	Chain	Tes Type Atoms	Atoms	Atoms	Type Atoms		Observed(A)	Observed(Å) Ideal(Å	Observed(A)	ideal(A)	Worst	Total
6	2	A	1	GLY	N-CA	5.26	1.53	1.46	18	1			

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	X	70	71	71	11±4
1	Y	70	71	71	10±4
2	A	709	693	691	42±7
2	В	705	688	686	41±6
All	All	31160	30460	30372	1892



The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 31.

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

2:B:\$1:LEU:HD13	Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models		
2:A:81:LEU:HD13 2:A:82:THR:N 0.99 1.72 11 4 2:B:81:LEU:HD13 2:B:82:THR:H 0.90 1.27 5 4 2:B:81:LEU:HD12 2:B:82:THR:N 0.89 1.82 1 1 2:A:81:LEU:HD13 2:A:82:THR:N 0.89 1.28 5 4 2:A:81:LEU:HD12 2:A:82:THR:N 0.89 1.82 1 1 2:A:81:LEU:HD11 0.80 1.91 12 1 1:X:8:ASN:ND2 2:A:28:LEU:HD11 0.79 1.92 12 1 1:X:8:ASN:ND2 2:A:81:LEU:HD11 0.78 1.93 12 1 1:X:8:ASN:ND2 2:A:45:LEU:HD11 0.78 1.98 6 2 2:A:44:PHE:O 2:A:45:LEU:HD11 0.73 1.98 6 2 1:Y:8:ASN:ND2 2:A:46:ASP:H 0.71 1.82 18 1 1:Y:8:ASN:ND2 2:B:57:ILE:HD11 0.71 1.82 18 1 1:Y:8:ASN:ND2 2:B:33:LY:S:N 0.70	Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
2:B:81:LEU:HD13 2:B:82:THR:H 0.90 1.27 5 4 2:B:81:LEU:HD12 2:B:82:THR:N 0.89 1.82 1 1 2:A:81:LEU:HD13 2:A:82:THR:H 0.89 1.28 5 4 2:A:81:LEU:HD11 2:A:82:THR:N 0.88 1.82 1 1 2:B:18:HIS:NE2 2:B:28:LEU:HD11 0.80 1.91 12 1 2:A:18:HIS:NE2 2:A:28:LEU:HD11 0.79 1.92 12 1 1:X:8:ASN:ND2 2:A:57:ILE:HD11 0.78 1.93 12 1 1:X:8:ASN:ND2 2:A:45:LEU:HD11 0.78 1.38 17 1 1:X:8:ASN:ND2 2:A:45:LEU:HD11 0.73 1.98 6 2 2:A:44:PHE:O 2:A:45:LEU:HD11 0.73 1.98 6 2 1:X:8:ASN:ND2 2:A:46:ASP:H 0.71 1.85 16 3 1:X:8:ASN:ND2 2:B:57:ILE:HD11 0.71 1.82 18 1 1:Y:8:ASN:OD1 2:A:45:LEU:H		2:B:82:THR:N	1.00		11	4	
2:B:81:LEU:HD12 2:B:82:THR:N 0.89 1.82 1 1 2:A:81:LEU:HD13 2:A:82:THR:H 0.89 1.28 5 4 2:A:81:LEU:HD12 2:A:82:THR:N 0.88 1.82 1 1 2:B:18:HIS:NE2 2:B:28:LEU:HD11 0.80 1.91 12 1 2:A:18:HIS:NE2 2:A:28:LEU:HD11 0.79 1.92 12 1 1:X:8:ASN:ND2 2:A:57:ILE:HD11 0.78 1.93 12 1 1:Y:5:ILE:HG23 1:Y:6:ASP:H 0.78 1.38 17 1 1:X:8:ASN:ND2 2:A:45:LEU:HD11 0.73 1.98 6 2 2:A:44:PHE:O 2:A:45:LEU:HD11 0.73 2.05 20 20 1:Y:8:ASN:ND2 2:B:57:ILE:HD11 0.72 1.85 16 3 1:Y:8:ASN:ND2 2:B:57:ILE:HD11 0.71 1.82 18 1 1:Y:8:ASN:ND2 2:B:34:LYS:N 0.70 2.02 12 12 2:B:33:LEU:HD12 2:B:34:S	2:A:81:LEU:HD13	2:A:82:THR:N	0.99	1.72	11	4	
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1:X:7:TRP:O 1:X:10:ILE:N 0.61 2.33 20 19 2:B:34:LYS:NZ 2:B:48:GLN:NE2 0.60 2.49 3 1 2:A:15:PHE:CE1 2:A:74:PHE:CE2 0.60 2.88 11 3 2:A:41:LEU:N 2:A:41:LEU:HD12 0.60 2.10 12 1 2:B:86:ASN:ND2 2:B:87:ASN:N 0.60 2.49 14 1 1:X:11:LEU:C 1:X:11:LEU:HD23 0.60 2.16 20 1 2:A:71:PHE:CE2 2:B:86:ASN:ND2 0.60 2.69 6 1 2:A:34:LYS:NZ 2:A:48:GLN:NE2 0.60 2.50 3 1 2:B:10:THR:O 2:B:14:VAL:HG12 0.60 1.97 13 1 2:B:38:GLN:HE20 2:A:45:LEU:C 0.60 2.39 6 20 2:B:38:GLN:HE21 2:B:48:GLN:NE2 0.60 1.95 16 1 1:Y:7:TRP:CG 1:Y:8:ASN:N 0.60 2.69 20 5 2:B:21:LYS:O 2:B:23:GLY:N 0.59 2.35 13 5 2:A:38:GLN:HE21 2:A:4	2:A:86:ASN:ND2	2:A:87:ASN:N	0.61	2.49	14	1
2:B:34:LYS:NZ 2:B:48:GLN:NE2 0.60 2.49 3 1 2:A:15:PHE:CE1 2:A:74:PHE:CE2 0.60 2.88 11 3 2:A:41:LEU:N 2:A:41:LEU:HD12 0.60 2.10 12 1 2:B:86:ASN:ND2 2:B:87:ASN:N 0.60 2.49 14 1 1:X:11:LEU:C 1:X:11:LEU:HD23 0.60 2.16 20 1 2:A:71:PHE:CE2 2:B:86:ASN:ND2 0.60 2.69 6 1 2:A:34:LYS:NZ 2:A:48:GLN:NE2 0.60 2.50 3 1 2:B:10:THR:O 2:B:14:VAL:HG12 0.60 1.97 13 1 2:A:44:PHE:O 2:A:45:LEU:C 0.60 2.39 6 20 2:B:38:GLN:HE21 2:B:48:GLN:NE2 0.60 1.95 16 1 1:Y:7:TRP:CG 1:Y:8:ASN:N 0.60 2.69 20 5 2:B:21:LYS:O 2:B:23:GLY:N 0.59 2.35 13 5 2:A:38:GLN:HE21 2:A:48:GLN:NE2 0.59 1.74 14 2 2:A:45:LEU:HD11 2:A	2:B:15:PHE:CE1	2:B:74:PHE:CE2	0.61	2.88	11	3
2:A:15:PHE:CE1 2:A:74:PHE:CE2 0.60 2.88 11 3 2:A:41:LEU:N 2:A:41:LEU:HD12 0.60 2.10 12 1 2:B:86:ASN:ND2 2:B:87:ASN:N 0.60 2.49 14 1 1:X:11:LEU:C 1:X:11:LEU:HD23 0.60 2.16 20 1 2:A:71:PHE:CE2 2:B:86:ASN:ND2 0.60 2.69 6 1 2:A:34:LYS:NZ 2:A:48:GLN:NE2 0.60 2.50 3 1 2:B:10:THR:O 2:B:14:VAL:HG12 0.60 1.97 13 1 2:A:44:PHE:O 2:A:45:LEU:C 0.60 2.39 6 20 2:B:38:GLN:HE21 2:B:48:GLN:NE2 0.60 1.95 16 1 1:Y:7:TRP:CG 1:Y:8:ASN:N 0.60 2.69 20 5 2:B:21:LYS:O 2:B:23:GLY:N 0.59 2.35 13 5 2:A:45:LEU:HD11 2:A:48:GLN:NE2 0.59 1.74 14 2 2:A:71:PHE:O 2:A:73:GLU:N 0.59 2.35 19 2	1:X:7:TRP:O	1:X:10:ILE:N	0.61	2.33	20	19
2:A:41:LEU:N 2:A:41:LEU:HD12 0.60 2.10 12 1 2:B:86:ASN:ND2 2:B:87:ASN:N 0.60 2.49 14 1 1:X:11:LEU:C 1:X:11:LEU:HD23 0.60 2.16 20 1 2:A:71:PHE:CE2 2:B:86:ASN:ND2 0.60 2.69 6 1 2:A:34:LYS:NZ 2:A:48:GLN:NE2 0.60 2.50 3 1 2:B:10:THR:O 2:B:14:VAL:HG12 0.60 1.97 13 1 2:A:44:PHE:O 2:A:45:LEU:C 0.60 2.39 6 20 2:B:38:GLN:HE21 2:B:48:GLN:NE2 0.60 1.95 16 1 1:Y:7:TRP:CG 1:Y:8:ASN:N 0.60 2.69 20 5 2:B:21:LYS:O 2:B:23:GLY:N 0.59 2.35 13 5 2:A:38:GLN:HE21 2:A:48:GLN:NE2 0.59 1.74 14 2 2:A:71:PHE:O 2:A:73:GLU:N 0.59 2.35 19 2	2:B:34:LYS:NZ	2:B:48:GLN:NE2	0.60	2.49	3	1
2:B:86:ASN:ND2 2:B:87:ASN:N 0.60 2.49 14 1 1:X:11:LEU:C 1:X:11:LEU:HD23 0.60 2.16 20 1 2:A:71:PHE:CE2 2:B:86:ASN:ND2 0.60 2.69 6 1 2:A:34:LYS:NZ 2:A:48:GLN:NE2 0.60 2.50 3 1 2:B:10:THR:O 2:B:14:VAL:HG12 0.60 1.97 13 1 2:A:44:PHE:O 2:A:45:LEU:C 0.60 2.39 6 20 2:B:38:GLN:HE21 2:B:48:GLN:NE2 0.60 1.95 16 1 1:Y:7:TRP:CG 1:Y:8:ASN:N 0.60 2.69 20 5 2:B:21:LYS:O 2:B:23:GLY:N 0.59 2.35 13 5 2:A:38:GLN:HE21 2:A:48:GLN:NE2 0.59 1.74 14 2 2:A:45:LEU:HD11 2:A:81:LEU:HD22 0.59 1.74 14 2 2:A:71:PHE:O 2:A:73:GLU:N 0.59 2.35 19 2	2:A:15:PHE:CE1	2:A:74:PHE:CE2	0.60	2.88	11	3
1:X:11:LEU:C 1:X:11:LEU:HD23 0.60 2.16 20 1 2:A:71:PHE:CE2 2:B:86:ASN:ND2 0.60 2.69 6 1 2:A:34:LYS:NZ 2:A:48:GLN:NE2 0.60 2.50 3 1 2:B:10:THR:O 2:B:14:VAL:HG12 0.60 1.97 13 1 2:A:44:PHE:O 2:A:45:LEU:C 0.60 2.39 6 20 2:B:38:GLN:HE21 2:B:48:GLN:NE2 0.60 1.95 16 1 1:Y:7:TRP:CG 1:Y:8:ASN:N 0.60 2.69 20 5 2:B:21:LYS:O 2:B:23:GLY:N 0.59 2.35 13 5 2:A:38:GLN:HE21 2:A:48:GLN:NE2 0.59 1.95 16 1 2:A:45:LEU:HD11 2:A:81:LEU:HD22 0.59 1.74 14 2 2:A:71:PHE:O 2:A:73:GLU:N 0.59 2.35 19 2	2:A:41:LEU:N	2:A:41:LEU:HD12	0.60	2.10	12	1
2:A:71:PHE:CE2 2:B:86:ASN:ND2 0.60 2.69 6 1 2:A:34:LYS:NZ 2:A:48:GLN:NE2 0.60 2.50 3 1 2:B:10:THR:O 2:B:14:VAL:HG12 0.60 1.97 13 1 2:A:44:PHE:O 2:A:45:LEU:C 0.60 2.39 6 20 2:B:38:GLN:HE21 2:B:48:GLN:NE2 0.60 1.95 16 1 1:Y:7:TRP:CG 1:Y:8:ASN:N 0.60 2.69 20 5 2:B:21:LYS:O 2:B:23:GLY:N 0.59 2.35 13 5 2:A:38:GLN:HE21 2:A:48:GLN:NE2 0.59 1.95 16 1 2:A:45:LEU:HD11 2:A:81:LEU:HD22 0.59 1.74 14 2 2:A:71:PHE:O 2:A:73:GLU:N 0.59 2.35 19 2	2:B:86:ASN:ND2	2:B:87:ASN:N	0.60	2.49	14	1
2:A:34:LYS:NZ 2:A:48:GLN:NE2 0.60 2.50 3 1 2:B:10:THR:O 2:B:14:VAL:HG12 0.60 1.97 13 1 2:A:44:PHE:O 2:A:45:LEU:C 0.60 2.39 6 20 2:B:38:GLN:HE21 2:B:48:GLN:NE2 0.60 1.95 16 1 1:Y:7:TRP:CG 1:Y:8:ASN:N 0.60 2.69 20 5 2:B:21:LYS:O 2:B:23:GLY:N 0.59 2.35 13 5 2:A:38:GLN:HE21 2:A:48:GLN:NE2 0.59 1.95 16 1 2:A:45:LEU:HD11 2:A:81:LEU:HD22 0.59 1.74 14 2 2:A:71:PHE:O 2:A:73:GLU:N 0.59 2.35 19 2	1:X:11:LEU:C	1:X:11:LEU:HD23	0.60	2.16	20	1
2:B:10:THR:O 2:B:14:VAL:HG12 0.60 1.97 13 1 2:A:44:PHE:O 2:A:45:LEU:C 0.60 2.39 6 20 2:B:38:GLN:HE21 2:B:48:GLN:NE2 0.60 1.95 16 1 1:Y:7:TRP:CG 1:Y:8:ASN:N 0.60 2.69 20 5 2:B:21:LYS:O 2:B:23:GLY:N 0.59 2.35 13 5 2:A:38:GLN:HE21 2:A:48:GLN:NE2 0.59 1.95 16 1 2:A:45:LEU:HD11 2:A:81:LEU:HD22 0.59 1.74 14 2 2:A:71:PHE:O 2:A:73:GLU:N 0.59 2.35 19 2	2:A:71:PHE:CE2	2:B:86:ASN:ND2	0.60	2.69	6	1
2:B:10:THR:O 2:B:14:VAL:HG12 0.60 1.97 13 1 2:A:44:PHE:O 2:A:45:LEU:C 0.60 2.39 6 20 2:B:38:GLN:HE21 2:B:48:GLN:NE2 0.60 1.95 16 1 1:Y:7:TRP:CG 1:Y:8:ASN:N 0.60 2.69 20 5 2:B:21:LYS:O 2:B:23:GLY:N 0.59 2.35 13 5 2:A:38:GLN:HE21 2:A:48:GLN:NE2 0.59 1.95 16 1 2:A:45:LEU:HD11 2:A:81:LEU:HD22 0.59 1.74 14 2 2:A:71:PHE:O 2:A:73:GLU:N 0.59 2.35 19 2	2:A:34:LYS:NZ	2:A:48:GLN:NE2	0.60	2.50	3	1
2:A:44:PHE:O 2:A:45:LEU:C 0.60 2.39 6 20 2:B:38:GLN:HE21 2:B:48:GLN:NE2 0.60 1.95 16 1 1:Y:7:TRP:CG 1:Y:8:ASN:N 0.60 2.69 20 5 2:B:21:LYS:O 2:B:23:GLY:N 0.59 2.35 13 5 2:A:38:GLN:HE21 2:A:48:GLN:NE2 0.59 1.95 16 1 2:A:45:LEU:HD11 2:A:81:LEU:HD22 0.59 1.74 14 2 2:A:71:PHE:O 2:A:73:GLU:N 0.59 2.35 19 2	2:B:10:THR:O		0.60	1.97		
2:B:38:GLN:HE21 2:B:48:GLN:NE2 0.60 1.95 16 1 1:Y:7:TRP:CG 1:Y:8:ASN:N 0.60 2.69 20 5 2:B:21:LYS:O 2:B:23:GLY:N 0.59 2.35 13 5 2:A:38:GLN:HE21 2:A:48:GLN:NE2 0.59 1.95 16 1 2:A:45:LEU:HD11 2:A:81:LEU:HD22 0.59 1.74 14 2 2:A:71:PHE:O 2:A:73:GLU:N 0.59 2.35 19 2	2:A:44:PHE:O					20
1:Y:7:TRP:CG 1:Y:8:ASN:N 0.60 2.69 20 5 2:B:21:LYS:O 2:B:23:GLY:N 0.59 2.35 13 5 2:A:38:GLN:HE21 2:A:48:GLN:NE2 0.59 1.95 16 1 2:A:45:LEU:HD11 2:A:81:LEU:HD22 0.59 1.74 14 2 2:A:71:PHE:O 2:A:73:GLU:N 0.59 2.35 19 2		2:B:48:GLN:NE2				
2:B:21:LYS:O 2:B:23:GLY:N 0.59 2.35 13 5 2:A:38:GLN:HE21 2:A:48:GLN:NE2 0.59 1.95 16 1 2:A:45:LEU:HD11 2:A:81:LEU:HD22 0.59 1.74 14 2 2:A:71:PHE:O 2:A:73:GLU:N 0.59 2.35 19 2	1:Y:7:TRP:CG	1:Y:8:ASN:N	0.60		20	5
2:A:38:GLN:HE21 2:A:48:GLN:NE2 0.59 1.95 16 1 2:A:45:LEU:HD11 2:A:81:LEU:HD22 0.59 1.74 14 2 2:A:71:PHE:O 2:A:73:GLU:N 0.59 2.35 19 2	2:B:21:LYS:O					
2:A:45:LEU:HD11 2:A:81:LEU:HD22 0.59 1.74 14 2 2:A:71:PHE:O 2:A:73:GLU:N 0.59 2.35 19 2	2:A:38:GLN:HE21					
2:A:71:PHE:O 2:A:73:GLU:N 0.59 2.35 19 2						
		-				
	1:Y:7:TRP:CZ3	2:B:44:PHE:CE2	0.59	2.90	17	3



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Continued from pres	1 0	Clash (Å)	Distance (Å)	Models	
Atom-1	Atom-2	Clash(Å)	$\operatorname{Distance}(\operatorname{\AA})$	Worst	Total
2:B:11:LEU:O	2:B:15:PHE:CG	0.59	2.56	20	2
2:B:37:LEU:HD12	2:B:45:LEU:HD22	0.59	1.72	15	3
2:A:21:LYS:O	2:A:23:GLY:N	0.59	2.35	13	5
2:A:11:LEU:O	2:A:15:PHE:CG	0.59	2.56	20	2
2:B:71:PHE:O	2:B:73:GLU:N	0.59	2.35	19	2
2:A:61:LEU:O	2:A:63:GLU:N	0.59	2.36	14	15
2:A:38:GLN:O	2:A:42:SER:N	0.59	2.36	10	4
1:X:7:TRP:N	2:A:46:ASP:OD2	0.58	2.35	3	5
2:A:14:VAL:HG23	2:A:15:PHE:N	0.58	2.13	19	5
1:Y:5:ILE:O	1:Y:7:TRP:N	0.58	2.36	17	1
1:Y:8:ASN:N	2:B:46:ASP:OD2	0.58	2.34	18	2
2:B:58:MET:O	2:B:62:ASP:N	0.58	2.36	1	9
2:A:79:ALA:HB1	2:B:75:VAL:HG12	0.58	1.73	13	9
2:A:46:ASP:O	2:A:46:ASP:OD1	0.58	2.21	14	1
1:Y:8:ASN:ND2	1:Y:9:LYS:N	0.58	2.52	18	1
2:B:38:GLN:O	2:B:42:SER:N	0.58	2.36	10	4
2:B:14:VAL:HG23	2:B:15:PHE:N	0.58	2.14	19	5
1:X:7:TRP:CZ3	2:A:44:PHE:CZ	0.58	2.91	19	5
2:A:58:MET:O	2:A:62:ASP:N	0.58	2.36	1	9
1:Y:8:ASN:ND2	2:B:81:LEU:HD21	0.58	2.13	2	1
2:B:45:LEU:O	2:B:49:LYS:NZ	0.57	2.37	11	1
2:A:10:THR:O	2:A:14:VAL:HG12	0.57	1.98	13	1
2:B:44:PHE:O	2:B:45:LEU:C	0.57	2.42	6	20
1:Y:8:ASN:CG	2:B:57:ILE:HD11	0.57	2.20	15	4
1:X:8:ASN:N	2:A:46:ASP:OD2	0.57	2.38	13	4
2:A:75:VAL:HG12	2:B:79:ALA:HB1	0.57	1.75	13	9
2:A:15:PHE:CZ	2:A:74:PHE:CZ	0.57	2.92	15	2
2:B:61:LEU:O	2:B:63:GLU:N	0.57	2.36	8	16
2:B:15:PHE:CZ	2:B:74:PHE:CZ	0.57	2.92	15	2
1:X:8:ASN:ND2	2:A:46:ASP:N	0.57	2.53	18	1
2:A:29:SER:O	2:A:32:GLU:N	0.57	2.37	8	4
1:X:7:TRP:CZ3	2:A:81:LEU:HD22	0.57	2.34	2	1
2:A:86:ASN:ND2	2:B:71:PHE:CE2	0.57	2.72	6	1
2:B:23:GLY:N	2:B:32:GLU:OE2	0.57	2.38	18	6
1:X:11:LEU:C	1:X:11:LEU:HD13	0.56	2.20	18	1
2:A:23:GLY:N	2:A:32:GLU:OE2	0.56	2.38	18	6
2:B:14:VAL:HG13	2:B:15:PHE:CD1	0.56	2.35	13	1
2:A:26:TYR:O	2:A:26:TYR:CD2	0.56	2.58	1	6
2:A:21:LYS:C	2:A:23:GLY:H	0.56	2.04	13	6
2:B:79:ALA:O	2:B:83:VAL:HG13	0.56	1.99	11	2
2:B:46:ASP:N	2:B:46:ASP:OD1	0.56	2.38	1	7



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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
		` ′	,	Worst	Total
2:A:42:SER:O	2:A:49:LYS:NZ	0.56	2.38	17	11
2:A:70:ASP:OD1	2:A:71:PHE:N	0.56	2.38	8	9
1:X:9:LYS:O	1:X:12:SER:N	0.56	2.39	5	7
2:A:49:LYS:H	2:A:49:LYS:CD	0.56	2.13	11	3
2:B:71:PHE:O	2:B:74:PHE:N	0.56	2.39	19	2
1:Y:10:ILE:CG2	1:Y:11:LEU:N	0.56	2.68	11	13
2:B:26:TYR:CD2	2:B:26:TYR:O	0.56	2.59	1	5
2:B:21:LYS:C	2:B:23:GLY:H	0.56	2.04	13	4
2:A:37:LEU:HD11	2:A:74:PHE:CZ	0.56	2.36	7	1
2:B:29:SER:O	2:B:32:GLU:N	0.56	2.37	8	4
2:A:79:ALA:O	2:A:83:VAL:HG13	0.56	2.00	11	2
1:Y:5:ILE:HG23	1:Y:6:ASP:N	0.56	2.11	17	1
1:X:5:ILE:O	1:X:7:TRP:N	0.56	2.39	9	5
2:B:85:CYS:SG	2:B:89:PHE:CE1	0.56	2.99	4	2
2:A:71:PHE:O	2:A:75:VAL:HG23	0.56	2.01	6	3
2:A:71:PHE:CD2	2:B:86:ASN:ND2	0.56	2.74	6	1
2:A:71:PHE:O	2:A:74:PHE:N	0.56	2.38	19	2
2:B:44:PHE:CG	2:B:45:LEU:N	0.55	2.73	12	3
2:B:70:ASP:OD1	2:B:71:PHE:N	0.55	2.38	8	8
1:X:7:TRP:CZ3	2:A:44:PHE:CE2	0.55	2.94	19	3
2:B:71:PHE:O	2:B:75:VAL:HG23	0.55	2.01	6	3
2:B:49:LYS:CD	2:B:49:LYS:H	0.55	2.14	12	2
2:B:37:LEU:HD22	2:B:37:LEU:N	0.55	2.16	12	1
2:A:85:CYS:SG	2:A:89:PHE:CE1	0.55	2.99	4	2
2:B:26:TYR:O	2:B:26:TYR:CG	0.55	2.60	15	3
2:A:46:ASP:N	2:A:46:ASP:OD1	0.55	2.37	1	7
2:A:10:THR:O	2:A:13:ASN:N	0.55	2.39	11	4
2:B:10:THR:O	2:B:13:ASN:N	0.55	2.40	7	4
2:B:37:LEU:HD11	2:B:74:PHE:CZ	0.55	2.36	7	1
2:A:26:TYR:O	2:A:26:TYR:CG	0.55	2.60	15	3
2:A:70:ASP:N	2:A:70:ASP:OD1	0.55	2.39	12	1
2:A:14:VAL:HG13	2:A:15:PHE:CD1	0.55	2.36	13	1
1:X:10:ILE:CG2	1:X:11:LEU:N	0.55	2.70	4	15
2:A:72:GLN:O	2:A:76:VAL:HG23	0.55	2.02	19	10
2:B:50:ASP:N	2:B:50:ASP:OD1	0.55	2.38	6	2
1:X:8:ASN:ND2	2:A:57:ILE:CD1	0.55	2.69	12	1
2:B:83:VAL:HG23	2:B:84:ALA:N	0.55	2.17	11	4
2:B:30:LYS:NZ	2:B:55:ASP:OD1	0.54	2.38	3	2
2:B:45:LEU:HD11	2:B:81:LEU:HD13	0.54	1.78	20	1
2:B:88:PHE:CD1	2:B:88:PHE:O	0.54	2.61	13	4
2:A:43:SER:O	2:A:49:LYS:NZ	0.54	2.40	3	1
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Atom 1		Clash (Å)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(Å)	,	Worst	Total
2:A:45:LEU:O	2:A:49:LYS:NZ	0.54	2.40	11	1
2:A:77:LEU:O	2:A:80:ALA:N	0.54	2.40	12	1
2:B:77:LEU:O	2:B:80:ALA:N	0.54	2.41	12	1
2:A:33:LEU:HD11	2:A:69:VAL:HG21	0.54	1.78	19	1
2:A:70:ASP:O	2:A:73:GLU:N	0.54	2.38	4	8
2:B:72:GLN:O	2:B:76:VAL:HG23	0.54	2.03	18	10
2:B:42:SER:O	2:B:49:LYS:NZ	0.54	2.39	11	12
2:B:39:THR:O	2:B:39:THR:HG22	0.54	2.03	8	1
2:B:77:LEU:CD1	2:B:81:LEU:HD12	0.54	2.32	20	1
1:X:8:ASN:OD1	2:A:81:LEU:HD11	0.54	2.02	2	2
2:A:24:ASP:OD1	2:A:25:LYS:N	0.54	2.41	3	8
2:A:50:ASP:N	2:A:50:ASP:OD1	0.54	2.39	6	2
2:B:46:ASP:O	2:B:46:ASP:OD1	0.54	2.26	14	1
2:B:33:LEU:HD11	2:B:69:VAL:HG21	0.54	1.79	19	1
2:A:83:VAL:HG23	2:A:84:ALA:N	0.54	2.16	11	4
2:A:37:LEU:HD22	2:A:37:LEU:N	0.54	2.18	12	1
1:X:8:ASN:OD1	2:A:81:LEU:HD22	0.54	2.02	15	1
2:B:24:ASP:OD1	2:B:25:LYS:N	0.54	2.41	6	8
1:Y:7:TRP:CZ2	2:B:44:PHE:CZ	0.54	2.95	13	2
1:Y:7:TRP:O	1:Y:10:ILE:CG2	0.54	2.55	1	20
2:A:18:HIS:NE2	2:A:35:ASP:OD2	0.54	2.41	3	1
1:X:7:TRP:CZ2	1:X:8:ASN:OD1	0.54	2.61	11	1
1:X:8:ASN:O	1:X:11:LEU:N	0.54	2.40	11	2
2:B:70:ASP:O	2:B:71:PHE:HB2	0.54	2.03	19	1
2:B:70:ASP:O	2:B:73:GLU:N	0.54	2.39	4	7
2:B:70:ASP:N	2:B:70:ASP:OD1	0.54	2.39	12	1
2:A:70:ASP:O	2:A:71:PHE:HB2	0.54	2.03	19	1
2:A:24:ASP:OD2	2:A:27:LYS:NZ	0.54	2.40	20	1
2:A:35:ASP:OD1	2:A:36:LEU:N	0.53	2.41	3	2
2:B:35:ASP:OD1	2:B:36:LEU:N	0.53	2.41	3	2
2:B:43:SER:O	2:B:49:LYS:NZ	0.53	2.41	3	1
1:Y:8:ASN:ND2	2:B:57:ILE:CD1	0.53	2.71	19	2
2:A:88:PHE:CD1	2:A:88:PHE:O	0.53	2.61	5	4
1:Y:5:ILE:CG1	1:Y:5:ILE:O	0.53	2.56	9	3
1:Y:11:LEU:O	1:Y:11:LEU:HD13	0.53	2.03	15	2
1:X:7:TRP:CD2	1:X:8:ASN:N	0.53	2.77	11	1
1:X:7:TRP:O	1:X:10:ILE:CG2	0.53	2.56	17	18
2:B:18:HIS:NE2	2:B:35:ASP:OD2	0.53	2.41	3	1
2:B:71:PHE:CE1	2:B:75:VAL:CG2	0.53	2.92	12	5
2:A:31:LYS:NZ	2:A:35:ASP:OD2	0.53	2.41	10	1
2:B:62:ASP:OD1	2:B:66:ASP:N	0.53	2.42	2	3
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Atom-1	Atom-2	$\operatorname{Clash}(\mathring{\mathbf{A}})$	$\operatorname{Distance}(\mathring{\mathrm{A}})$	Models	
			` ,	Worst	Total
2:A:38:GLN:NE2	2:A:48:GLN:NE2	0.53	2.55	5	2
2:A:39:THR:HG22	2:A:39:THR:O	0.53	2.04	8	1
2:B:44:PHE:O	2:B:45:LEU:O	0.53	2.27	20	10
2:A:42:SER:OG	2:A:48:GLN:NE2	0.53	2.42	13	1
2:B:26:TYR:O	2:B:26:TYR:CD2	0.53	2.62	15	1
2:A:88:PHE:O	2:A:88:PHE:CD2	0.53	2.62	7	5
1:X:5:ILE:HG23	1:X:5:ILE:O	0.53	2.04	17	2
2:B:31:LYS:NZ	2:B:35:ASP:OD2	0.53	2.41	10	1
2:A:62:ASP:OD1	2:A:66:ASP:N	0.53	2.42	2	3
2:B:33:LEU:CD1	2:B:34:LYS:N	0.53	2.72	12	9
2:B:88:PHE:O	2:B:88:PHE:CD2	0.52	2.62	8	4
2:B:64:ASN:OD1	2:B:65:GLY:N	0.52	2.42	17	2
2:B:14:VAL:HG13	2:B:15:PHE:N	0.52	2.20	17	10
1:Y:9:LYS:O	1:Y:12:SER:N	0.52	2.42	8	6
2:A:50:ASP:O	2:A:53:ALA:N	0.52	2.42	5	3
1:X:5:ILE:O	2:A:46:ASP:OD2	0.52	2.28	5	4
2:A:71:PHE:CE1	2:A:75:VAL:CG2	0.52	2.92	12	5
2:A:38:GLN:O	2:A:42:SER:CA	0.52	2.58	5	1
2:A:11:LEU:O	2:A:15:PHE:CD2	0.52	2.63	20	1
2:A:18:HIS:CE1	2:A:22:GLU:OE1	0.52	2.62	20	1
2:B:42:SER:O	2:B:49:LYS:CE	0.52	2.58	2	7
1:Y:7:TRP:CD2	1:Y:8:ASN:N	0.52	2.78	11	1
2:A:14:VAL:HG13	2:A:15:PHE:N	0.52	2.19	17	8
2:A:1:GLY:O	2:A:3:GLU:N	0.52	2.42	7	1
2:A:14:VAL:CG2	2:A:15:PHE:N	0.52	2.73	7	5
2:A:33:LEU:CD1	2:A:34:LYS:N	0.52	2.73	12	8
2:B:18:HIS:CE1	2:B:22:GLU:OE1	0.52	2.63	20	1
2:A:33:LEU:CD2	2:A:58:MET:SD	0.52	2.98	1	1
1:X:7:TRP:CZ2	1:X:8:ASN:ND2	0.52	2.77	11	1
2:A:77:LEU:CD1	2:A:81:LEU:HD12	0.51	2.34	20	1
2:A:81:LEU:CD1	2:A:82:THR:N	0.51	2.69	1	3
2:A:89:PHE:CD1	2:A:89:PHE:O	0.51	2.63	6	3
2:B:3:GLU:OE1	2:B:3:GLU:N	0.51	2.42	20	4
2:A:82:THR:O	2:A:85:CYS:SG	0.51	2.67	15	2
2:B:11:LEU:O	2:B:15:PHE:CD2	0.51	2.63	20	1
2:B:37:LEU:N	2:B:37:LEU:CD2	0.51	2.74	5	4
2:B:38:GLN:CG	2:B:39:THR:N	0.51	2.74	11	10
2:A:33:LEU:HD12	2:A:33:LEU:C	0.51	2.26	5	8
2:B:38:GLN:O	2:B:42:SER:CA	0.51	2.58	5	1
2:B:89:PHE:CD1	2:B:89:PHE:O	0.51	2.64	6	3
2:A:64:ASN:OD1	2:A:65:GLY:N	0.51	2.42	17	2
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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
		` ′	,	Worst	Total
2:B:36:LEU:HD23	2:B:74:PHE:CZ	0.51	2.40	13	2
1:X:8:ASN:OD1	2:A:57:ILE:CD1	0.51	2.58	16	1
2:A:22:GLU:OE1	2:A:31:LYS:CE	0.51	2.59	18	1
1:Y:5:ILE:O	2:B:46:ASP:OD2	0.51	2.28	2	7
2:B:14:VAL:CG2	2:B:15:PHE:N	0.51	2.73	7	5
2:A:3:GLU:H	2:A:3:GLU:CD	0.51	2.08	10	3
2:A:42:SER:O	2:A:49:LYS:CE	0.51	2.58	2	7
2:B:33:LEU:CD2	2:B:58:MET:SD	0.51	2.99	1	1
2:B:47:VAL:CG2	2:B:48:GLN:N	0.51	2.74	4	6
1:Y:11:LEU:HD23	1:Y:11:LEU:O	0.51	2.06	12	1
2:A:36:LEU:HD23	2:A:74:PHE:CZ	0.51	2.40	13	2
2:B:82:THR:O	2:B:85:CYS:SG	0.51	2.67	18	2
1:X:8:ASN:C	1:X:8:ASN:HD22	0.51	2.09	3	2
2:B:82:THR:HG23	2:B:83:VAL:N	0.51	2.21	7	6
2:A:86:ASN:ND2	2:B:71:PHE:CD2	0.51	2.79	6	1
2:A:12:ILE:O	2:A:16:HIS:CD2	0.51	2.64	11	1
1:X:7:TRP:CD1	1:X:8:ASN:N	0.51	2.79	20	1
2:B:38:GLN:O	2:B:42:SER:CB	0.50	2.58	18	2
1:Y:5:ILE:HD11	2:B:46:ASP:OD1	0.50	2.06	17	1
2:A:3:GLU:OE1	2:A:3:GLU:N	0.50	2.42	20	4
2:B:3:GLU:CD	2:B:3:GLU:H	0.50	2.08	10	1
2:A:82:THR:HG23	2:A:83:VAL:N	0.50	2.22	7	5
2:A:15:PHE:CD2	2:A:74:PHE:CE2	0.50	2.99	15	1
1:Y:5:ILE:O	1:Y:5:ILE:CG1	0.50	2.59	14	2
2:B:42:SER:OG	2:B:48:GLN:NE2	0.50	2.43	13	1
1:Y:7:TRP:CZ3	2:B:81:LEU:HD12	0.50	2.41	17	1
2:A:58:MET:SD	2:A:62:ASP:OD2	0.50	2.70	4	4
2:B:58:MET:SD	2:B:62:ASP:OD2	0.50	2.70	4	3
2:A:23:GLY:O	2:A:24:ASP:O	0.50	2.29	19	2
2:B:6:THR:O	2:B:10:THR:OG1	0.50	2.29	19	9
2:A:30:LYS:NZ	2:A:55:ASP:OD1	0.50	2.39	3	2
2:A:47:VAL:CG2	2:A:48:GLN:N	0.50	2.74	4	7
2:A:19:SER:OG	2:A:28:LEU:CD1	0.50	2.60	20	2
2:B:12:ILE:O	2:B:16:HIS:CD2	0.50	2.64	11	1
2:A:37:LEU:N	2:A:37:LEU:CD2	0.50	2.74	12	4
1:Y:7:TRP:CZ2	2:B:44:PHE:CE2	0.50	2.99	13	3
2:B:45:LEU:HD13	2:B:81:LEU:CD2	0.50	2.37	6	1
2:B:19:SER:OG	2:B:28:LEU:CD1	0.50	2.59	20	2
2:A:29:SER:N	2:A:32:GLU:OE1	0.50	2.41	20	2
2:A:89:PHE:O	2:A:89:PHE:CD2	0.50	2.65	15	1
2:B:15:PHE:CD2	2:B:74:PHE:CE2	0.50	3.00	15	1



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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
2:B:23:GLY:O	2:B:24:ASP:O	0.50	2.29	19	1
2:B:24:ASP:OD2	2:B:27:LYS:NZ	0.50	2.40	20	1
2:B:44:PHE:C	2:B:44:PHE:CD1	0.50	2.85	12	2
2:B:72:GLN:OE1	2:B:72:GLN:N	0.50	2.45	3	1
1:X:7:TRP:CZ2	2:A:44:PHE:CE2	0.50	3.00	17	1
2:A:6:THR:O	2:A:10:THR:OG1	0.49	2.28	19	10
2:A:38:GLN:CG	2:A:39:THR:N	0.49	2.74	11	10
2:A:10:THR:CG2	2:A:11:LEU:N	0.49	2.75	9	10
2:B:18:HIS:NE2	2:B:35:ASP:CG	0.49	2.66	3	1
1:Y:10:ILE:HG23	1:Y:11:LEU:N	0.49	2.21	11	3
2:B:41:LEU:N	2:B:41:LEU:CD1	0.49	2.74	12	1
2:B:38:GLN:NE2	2:B:48:GLN:CD	0.49	2.66	18	1
2:B:33:LEU:HD12	2:B:33:LEU:C	0.49	2.27	12	8
2:A:18:HIS:NE2	2:A:35:ASP:CG	0.49	2.66	3	1
2:B:10:THR:CG2	2:B:11:LEU:N	0.49	2.75	9	10
2:B:38:GLN:NE2	2:B:48:GLN:NE2	0.49	2.59	16	2
2:B:22:GLU:OE1	2:B:31:LYS:NZ	0.49	2.45	18	1
2:A:14:VAL:CG1	2:A:15:PHE:N	0.49	2.76	14	10
1:Y:7:TRP:CD1	1:Y:8:ASN:N	0.49	2.81	20	2
2:B:71:PHE:O	2:B:75:VAL:CG2	0.49	2.61	6	3
2:A:78:VAL:HG23	2:A:79:ALA:N	0.49	2.23	18	1
2:A:38:GLN:CD	2:A:39:THR:N	0.49	2.66	17	3
2:A:41:LEU:N	2:A:41:LEU:CD1	0.49	2.74	12	1
2:B:15:PHE:CD2	2:B:74:PHE:CD2	0.49	3.00	15	1
2:A:71:PHE:O	2:A:75:VAL:CG2	0.49	2.60	6	3
2:B:89:PHE:CD2	2:B:89:PHE:O	0.49	2.65	15	1
2:A:1:GLY:N	2:A:5:GLU:OE1	0.49	2.42	15	2
2:A:15:PHE:CD2	2:A:74:PHE:CD2	0.49	2.99	15	1
2:A:22:GLU:OE1	2:A:31:LYS:NZ	0.49	2.44	18	1
2:A:42:SER:OG	2:A:43:SER:N	0.49	2.45	18	1
2:B:50:ASP:O	2:B:53:ALA:N	0.49	2.45	5	3
1:X:11:LEU:HD13	1:X:11:LEU:O	0.49	2.08	11	2
2:B:37:LEU:CD1	2:B:37:LEU:N	0.49	2.76	3	2
2:B:38:GLN:CD	2:B:39:THR:N	0.49	2.66	17	3
1:Y:5:ILE:C	1:Y:7:TRP:N	0.49	2.66	17	1
2:A:70:ASP:O	2:A:71:PHE:CB	0.49	2.60	18	2
2:B:45:LEU:CD1	2:B:81:LEU:HD13	0.49	2.37	20	1
2:A:19:SER:O	2:A:24:ASP:O	0.49	2.31	2	6
2:B:58:MET:SD	2:B:62:ASP:OD1	0.49	2.71	4	3
2:B:83:VAL:CG2	2:B:84:ALA:N	0.49	2.76	11	1
1:Y:8:ASN:ND2	1:Y:9:LYS:H	0.49	2.06	18	1



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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
2:B:64:ASN:ND2	2:B:66:ASP:CG	0.48	2.66	2	1
2:A:58:MET:SD	2:A:62:ASP:OD1	0.48	2.71	4	3
2:A:83:VAL:CG2	2:A:84:ALA:N	0.48	2.75	11	2
2:A:37:LEU:CD1	2:A:37:LEU:N	0.48	2.76	3	2
2:A:72:GLN:N	2:A:72:GLN:OE1	0.48	2.46	3	1
2:A:38:GLN:O	2:A:42:SER:CB	0.48	2.61	18	2
2:B:85:CYS:SG	2:B:86:ASN:N	0.48	2.86	15	2
2:A:38:GLN:NE2	2:A:48:GLN:CD	0.48	2.67	18	1
2:B:14:VAL:CG1	2:B:15:PHE:N	0.48	2.76	14	10
2:A:40:GLU:OE1	2:B:4:LEU:N	0.48	2.46	12	1
2:B:10:THR:HG23	2:B:11:LEU:N	0.48	2.22	9	3
2:B:37:LEU:HD22	2:B:37:LEU:H	0.48	1.69	19	1
1:X:7:TRP:O	1:X:10:ILE:CB	0.48	2.61	17	11
2:A:77:LEU:C	2:A:77:LEU:CD1	0.48	2.82	2	14
2:B:11:LEU:CD1	2:B:11:LEU:N	0.48	2.77	17	5
2:B:61:LEU:CD1	2:B:73:GLU:O	0.48	2.61	2	1
2:A:4:LEU:N	2:B:40:GLU:OE1	0.48	2.46	12	2
2:B:46:ASP:OD2	2:B:50:ASP:OD2	0.48	2.31	19	3
2:A:10:THR:HG23	2:A:11:LEU:N	0.48	2.22	9	3
2:A:52:ASP:CG	2:A:56:LYS:NZ	0.48	2.66	11	1
2:B:70:ASP:O	2:B:71:PHE:CB	0.48	2.62	19	2
2:B:81:LEU:CD1	2:B:82:THR:N	0.48	2.69	1	1
1:X:9:LYS:NZ	2:A:56:LYS:HZ2	0.48	2.05	2	1
2:B:22:GLU:N	2:B:22:GLU:OE1	0.48	2.47	17	1
2:B:38:GLN:HE22	2:B:48:GLN:HE21	0.48	1.51	20	1
2:B:48:GLN:O	2:B:49:LYS:C	0.48	2.52	7	1
2:B:52:ASP:CG	2:B:56:LYS:NZ	0.48	2.67	11	1
2:A:16:HIS:CD2	2:A:16:HIS:C	0.48	2.87	16	1
2:A:64:ASN:ND2	2:A:66:ASP:CG	0.48	2.66	2	2
2:B:15:PHE:C	2:B:15:PHE:CD1	0.48	2.87	6	5
1:X:8:ASN:HD21	2:A:81:LEU:CD1	0.48	2.22	15	1
2:A:85:CYS:SG	2:A:86:ASN:N	0.48	2.86	15	2
1:X:8:ASN:H	2:A:46:ASP:CG	0.48	2.12	3	2
2:A:46:ASP:OD2	2:A:50:ASP:OD2	0.48	2.32	19	3
1:X:7:TRP:CH2	2:A:44:PHE:CZ	0.48	3.02	7	1
2:A:48:GLN:O	2:A:49:LYS:C	0.48	2.52	7	1
2:B:16:HIS:CD2	2:B:16:HIS:C	0.48	2.88	16	1
2:B:66:ASP:CG	2:B:67:GLY:N	0.48	2.67	2	3
2:A:61:LEU:HD22	2:A:73:GLU:O	0.48	2.09	19	2
2:B:22:GLU:OE1	2:B:31:LYS:CE	0.48	2.61	18	1
2:A:79:ALA:HB1	2:B:75:VAL:HB	0.48	1.86	19	1



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At am 1		Cleab (Å)	Distance (Å)	Models	
Atom-1	Atom-2	Clash(Å)	$\operatorname{Distance}(\operatorname{\AA})$	Worst	Total
2:A:38:GLN:NE2	2:A:48:GLN:HE21	0.48	2.06	20	1
2:B:38:GLN:O	2:B:42:SER:OG	0.47	2.31	5	2
2:B:38:GLN:OE1	2:B:48:GLN:NE2	0.47	2.47	9	1
1:X:8:ASN:HD21	2:A:81:LEU:HD13	0.47	1.68	15	1
2:A:11:LEU:N	2:A:11:LEU:CD1	0.47	2.77	4	6
2:A:15:PHE:C	2:A:15:PHE:CD1	0.47	2.87	6	4
2:A:37:LEU:N	2:A:37:LEU:HD12	0.47	2.23	6	1
2:B:61:LEU:HD22	2:B:73:GLU:O	0.47	2.09	19	2
2:B:78:VAL:HG23	2:B:79:ALA:N	0.47	2.24	18	1
2:B:38:GLN:NE2	2:B:48:GLN:HE21	0.47	2.06	20	1
2:A:15:PHE:CD1	2:A:15:PHE:C	0.47	2.87	17	2
2:A:66:ASP:CG	2:A:67:GLY:N	0.47	2.67	2	3
2:B:21:LYS:C	2:B:23:GLY:N	0.47	2.68	13	2
2:A:81:LEU:HD13	2:A:81:LEU:C	0.47	2.29	11	1
2:B:37:LEU:HD21	2:B:74:PHE:CE1	0.47	2.45	1	1
2:B:15:PHE:CZ	2:B:28:LEU:HD13	0.47	2.44	12	1
2:B:18:HIS:CE1	2:B:28:LEU:HD11	0.47	2.45	12	1
1:Y:8:ASN:OD1	2:B:46:ASP:OD2	0.47	2.33	20	1
2:B:37:LEU:HD12	2:B:37:LEU:N	0.47	2.24	6	1
2:A:11:LEU:N	2:A:11:LEU:HD12	0.47	2.25	4	5
1:X:5:ILE:C	1:X:7:TRP:N	0.47	2.68	9	3
2:A:64:ASN:HD21	2:A:66:ASP:CG	0.47	2.13	2	3
2:B:77:LEU:C	2:B:77:LEU:CD1	0.47	2.83	7	14
2:A:38:GLN:O	2:A:42:SER:OG	0.47	2.33	5	3
2:A:21:LYS:C	2:A:23:GLY:N	0.47	2.67	13	2
2:B:59:LYS:NZ	2:B:62:ASP:OD2	0.47	2.42	9	1
1:X:7:TRP:CZ2	1:X:8:ASN:CG	0.47	2.87	11	1
2:A:86:ASN:HD22	2:A:87:ASN:N	0.47	2.07	14	1
2:A:75:VAL:HB	2:B:79:ALA:HB1	0.47	1.85	19	1
2:A:66:ASP:N	2:A:66:ASP:OD1	0.47	2.48	13	4
2:B:58:MET:SD	2:B:62:ASP:CG	0.47	2.93	17	3
2:B:31:LYS:CE	2:B:35:ASP:OD2	0.47	2.63	10	1
2:B:36:LEU:O	2:B:40:GLU:OE1	0.47	2.33	11	2
2:B:29:SER:N	2:B:32:GLU:OE2	0.47	2.41	13	1
2:A:58:MET:SD	2:A:62:ASP:CG	0.47	2.93	17	3
1:Y:8:ASN:CB	2:B:46:ASP:CG	0.47	2.83	20	1
2:A:47:VAL:HG23	2:A:48:GLN:N	0.47	2.25	15	5
1:Y:7:TRP:CH2	2:B:44:PHE:CZ	0.47	3.03	17	2
1:Y:8:ASN:HD21	2:B:57:ILE:CG1	0.47	2.23	12	1
1:X:8:ASN:CB	2:A:46:ASP:CG	0.46	2.83	20	2
2:B:71:PHE:C	2:B:73:GLU:N	0.46	2.69	18	2



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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
		` ′	, ,	Worst	Total
2:B:66:ASP:CG	2:B:67:GLY:H	0.46	2.14	2	1
1:Y:7:TRP:CZ2	2:B:84:ALA:HB3	0.46	2.46	15	1
2:A:22:GLU:N	2:A:22:GLU:OE1	0.46	2.47	17	1
2:A:66:ASP:CG	2:A:67:GLY:H	0.46	2.14	2	1
2:A:37:LEU:H	2:A:37:LEU:HD22	0.46	1.69	19	1
2:A:45:LEU:HD13	2:A:81:LEU:CD2	0.46	2.41	6	1
2:A:59:LYS:NZ	2:A:62:ASP:OD2	0.46	2.41	9	1
1:Y:7:TRP:O	1:Y:10:ILE:CB	0.46	2.63	11	12
2:B:19:SER:O	2:B:24:ASP:O	0.46	2.33	11	4
1:X:8:ASN:O	1:X:8:ASN:ND2	0.46	2.47	3	1
2:A:22:GLU:O	2:A:32:GLU:CG	0.46	2.64	14	2
2:B:86:ASN:HD22	2:B:87:ASN:N	0.46	2.09	14	1
2:B:18:HIS:CD2	2:B:35:ASP:OD1	0.46	2.69	3	1
2:A:8:MET:SD	2:A:8:MET:C	0.46	2.94	10	2
2:A:31:LYS:CE	2:A:35:ASP:OD2	0.46	2.64	10	1
2:A:18:HIS:CE1	2:A:28:LEU:HD11	0.46	2.45	12	1
2:B:24:ASP:O	2:B:26:TYR:N	0.46	2.49	13	1
2:B:42:SER:OG	2:B:43:SER:N	0.46	2.49	18	1
2:A:1:GLY:C	2:A:3:GLU:H	0.46	2.14	7	1
2:A:80:ALA:O	2:A:83:VAL:CG2	0.46	2.64	1	9
2:B:47:VAL:HG23	2:B:48:GLN:N	0.46	2.25	15	5
2:B:64:ASN:HD21	2:B:66:ASP:CG	0.46	2.14	2	3
1:X:7:TRP:CH2	1:X:8:ASN:OD1	0.46	2.69	11	1
2:B:22:GLU:O	2:B:32:GLU:CG	0.46	2.64	14	2
2:A:18:HIS:CG	2:A:19:SER:N	0.46	2.84	12	1
2:B:8:MET:SD	2:B:8:MET:C	0.46	2.94	10	2
2:A:36:LEU:O	2:A:40:GLU:OE1	0.46	2.33	11	2
2:B:18:HIS:CG	2:B:19:SER:N	0.46	2.84	12	1
2:A:29:SER:H	2:A:32:GLU:CD	0.46	2.15	13	1
1:Y:8:ASN:OD1	2:B:57:ILE:CD1	0.46	2.60	16	2
2:B:90:TRP:CD2	2:B:90:TRP:O	0.46	2.69	16	1
2:B:80:ALA:O	2:B:83:VAL:CG2	0.46	2.64	1	9
2:A:61:LEU:CD1	2:A:73:GLU:O	0.46	2.61	2	1
1:X:5:ILE:O	1:X:6:ASP:OD1	0.46	2.33	14	3
1:X:7:TRP:CZ2	2:A:84:ALA:HB3	0.46	2.46	15	1
1:Y:11:LEU:O	1:Y:12:SER:CB	0.45	2.62	4	1
2:B:64:ASN:OD1	2:B:66:ASP:N	0.45	2.46	9	1
2:A:24:ASP:O	2:A:26:TYR:N	0.45	2.49	13	1
2:A:71:PHE:C	2:A:73:GLU:N	0.45	2.68	18	2
2:B:46:ASP:OD1	2:B:50:ASP:OD1	0.45	2.34	19	1
2:A:38:GLN:HE22	2:A:48:GLN:HE21	0.45	1.52	20	1



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Atom 1		Clash (Å)	Distance (Å)	Models	
Atom-1	Atom-2	$\operatorname{Clash}(ext{Å})$	$\operatorname{Distance}(\operatorname{\check{A}})$	Worst	Total
2:B:38:GLN:NE2	2:B:39:THR:OG1	0.45	2.49	17	2
2:B:15:PHE:CD1	2:B:15:PHE:C	0.45	2.90	1	2
2:B:58:MET:SD	2:B:69:VAL:CG2	0.45	3.05	1	1
1:Y:12:SER:O	2:B:60:GLU:OE1	0.45	2.35	14	2
2:B:47:VAL:HG22	2:B:48:GLN:N	0.45	2.27	4	1
2:A:46:ASP:OD1	2:A:50:ASP:OD1	0.45	2.34	19	1
2:A:58:MET:SD	2:A:69:VAL:CG2	0.45	3.05	1	1
2:A:18:HIS:CD2	2:A:35:ASP:OD1	0.45	2.70	3	1
2:B:11:LEU:N	2:B:11:LEU:HD12	0.45	2.25	4	3
2:A:71:PHE:CD2	2:B:83:VAL:HG12	0.45	2.47	6	1
2:A:18:HIS:O	2:A:32:GLU:OE2	0.45	2.34	8	3
1:Y:7:TRP:CD1	2:B:46:ASP:OD1	0.45	2.69	13	1
2:A:66:ASP:O	2:A:68:GLU:OE1	0.45	2.35	20	3
2:B:82:THR:HG23	2:B:83:VAL:H	0.45	1.71	16	1
2:A:32:GLU:O	2:A:35:ASP:OD1	0.45	2.35	3	1
2:B:77:LEU:HD13	2:B:77:LEU:O	0.45	2.12	17	3
2:A:90:TRP:O	2:A:90:TRP:CD2	0.45	2.69	16	1
2:A:47:VAL:HG22	2:A:48:GLN:N	0.45	2.27	4	1
1:X:10:ILE:HG23	1:X:11:LEU:N	0.45	2.26	11	3
1:X:11:LEU:O	1:X:12:SER:O	0.45	2.35	12	1
2:B:29:SER:H	2:B:32:GLU:CD	0.45	2.14	13	1
1:X:8:ASN:HD21	2:A:45:LEU:HG	0.45	1.71	18	1
2:A:53:ALA:O	2:A:57:ILE:HD13	0.45	2.11	9	1
2:A:15:PHE:CZ	2:A:28:LEU:HD13	0.45	2.47	12	1
2:A:62:ASP:OD1	2:A:64:ASN:OD1	0.45	2.35	2	1
2:A:31:LYS:CB	2:A:31:LYS:NZ	0.45	2.80	15	1
2:A:38:GLN:NE2	2:A:39:THR:OG1	0.45	2.50	17	1
2:A:45:LEU:HD11	2:A:81:LEU:CD2	0.45	2.42	1	1
1:Y:11:LEU:HD21	2:B:80:ALA:HB1	0.45	1.89	15	2
2:B:32:GLU:O	2:B:35:ASP:OD1	0.45	2.35	3	1
2:A:37:LEU:N	2:A:37:LEU:CD1	0.45	2.79	6	1
2:B:37:LEU:N	2:B:37:LEU:CD1	0.45	2.80	6	1
2:A:10:THR:O	2:A:11:LEU:C	0.45	2.55	7	1
2:B:18:HIS:O	2:B:32:GLU:OE2	0.45	2.35	8	3
2:B:15:PHE:CD1	2:B:71:PHE:CE2	0.45	3.05	17	1
2:B:66:ASP:N	2:B:66:ASP:OD1	0.44	2.49	13	4
2:A:38:GLN:OE1	2:A:48:GLN:NE2	0.44	2.47	9	1
2:B:66:ASP:O	2:B:68:GLU:OE1	0.44	2.35	20	3
2:B:83:VAL:O	2:B:86:ASN:OD1	0.44	2.35	14	1
2:A:78:VAL:CG2	2:A:79:ALA:N	0.44	2.80	18	1
1:X:6:ASP:OD1	2:A:50:ASP:OD2	0.44	2.35	2	1



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	At 2	Clasta (Å)	Distance (Å)	Models	
Atom-1	Atom-2	$\operatorname{Clash}(ext{Å})$	$\operatorname{Distance}(\operatorname{\AA})$	Worst	Total
2:A:33:LEU:CG	2:A:34:LYS:N	0.44	2.80	9	7
2:B:88:PHE:O	2:B:88:PHE:CG	0.44	2.70	12	4
1:Y:11:LEU:O	1:Y:12:SER:OXT	0.44	2.34	14	1
2:A:26:TYR:OH	2:B:86:ASN:O	0.44	2.35	18	1
2:A:45:LEU:HD11	2:A:81:LEU:HD13	0.44	1.89	20	1
2:B:33:LEU:CG	2:B:34:LYS:N	0.44	2.80	9	7
2:B:37:LEU:N	2:B:37:LEU:HD22	0.44	2.28	15	2
2:A:77:LEU:HD13	2:A:77:LEU:O	0.44	2.12	17	2
1:Y:8:ASN:ND2	2:B:57:ILE:CG1	0.44	2.81	12	1
2:A:75:VAL:CG1	2:B:79:ALA:HB1	0.44	2.42	13	1
1:Y:5:ILE:O	1:Y:6:ASP:OD1	0.44	2.35	17	1
1:X:8:ASN:CG	2:A:81:LEU:HD11	0.44	2.33	2	1
2:A:62:ASP:OD1	2:A:66:ASP:OD1	0.44	2.35	13	2
2:A:64:ASN:OD1	2:A:66:ASP:N	0.44	2.46	9	1
2:A:86:ASN:ND2	2:B:26:TYR:OH	0.44	2.50	12	1
2:B:62:ASP:OD1	2:B:66:ASP:OD1	0.44	2.36	13	1
1:X:5:ILE:O	2:A:50:ASP:OD2	0.44	2.36	18	1
2:B:11:LEU:N	2:B:11:LEU:CD1	0.44	2.81	20	2
2:B:61:LEU:O	2:B:73:GLU:OE2	0.44	2.36	2	4
2:B:35:ASP:O	2:B:35:ASP:OD1	0.44	2.36	7	2
2:B:8:MET:SD	2:B:9:GLU:N	0.44	2.91	10	1
2:A:88:PHE:CG	2:A:88:PHE:O	0.44	2.70	12	1
2:A:1:GLY:O	2:B:40:GLU:OE1	0.44	2.35	20	1
2:B:11:LEU:HD12	2:B:11:LEU:N	0.44	2.27	1	1
2:B:62:ASP:OD1	2:B:64:ASN:OD1	0.44	2.35	2	1
2:B:29:SER:N	2:B:32:GLU:OE1	0.44	2.51	14	2
2:B:72:GLN:O	2:B:76:VAL:CG2	0.44	2.65	18	1
2:A:15:PHE:CG	2:A:71:PHE:CE2	0.44	3.06	4	1
1:X:8:ASN:HD22	2:A:57:ILE:CD1	0.44	2.25	15	1
2:B:71:PHE:O	2:B:72:GLN:C	0.44	2.56	19	2
2:B:10:THR:O	2:B:11:LEU:C	0.44	2.55	7	4
2:B:61:LEU:O	2:B:73:GLU:OE1	0.44	2.35	4	1
2:A:4:LEU:O	2:A:4:LEU:HD23	0.44	2.13	6	1
2:A:35:ASP:O	2:A:35:ASP:OD1	0.44	2.35	7	2
1:X:8:ASN:ND2	2:A:57:ILE:CG1	0.44	2.81	12	1
2:A:79:ALA:HB1	2:B:75:VAL:CG1	0.44	2.42	13	1
2:A:45:LEU:CD1	2:A:81:LEU:HD13	0.44	2.43	20	1
2:A:37:LEU:N	2:A:37:LEU:HD22	0.43	2.28	15	2
2:B:62:ASP:OD2	2:B:66:ASP:O	0.43	2.35	2	2
1:X:9:LYS:O	1:X:10:ILE:C	0.43	2.56	4	1
2:B:66:ASP:O	2:B:68:GLU:OE2	0.43	2.37	4	1



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Atom-1 2:B:44:PHE:CD1 2:A:8:MET:SD 1:X:8:ASN:C 2:A:83:VAL:O 1:X:9:LYS:O 2:B:15:PHE:CG	2:B:44:PHE:C 2:A:9:GLU:N 1:X:8:ASN:ND2 2:A:86:ASN:OD1 1:X:12:SER:OXT	0.43 0.43 0.43	2.91 2.91	Worst 5	Total 2
2:A:8:MET:SD 1:X:8:ASN:C 2:A:83:VAL:O 1:X:9:LYS:O 2:B:15:PHE:CG	2:A:9:GLU:N 1:X:8:ASN:ND2 2:A:86:ASN:OD1	0.43 0.43	2.91		2
1:X:8:ASN:C 2:A:83:VAL:O 1:X:9:LYS:O 2:B:15:PHE:CG	1:X:8:ASN:ND2 2:A:86:ASN:OD1	0.43		10	
2:A:83:VAL:O 1:X:9:LYS:O 2:B:15:PHE:CG	2:A:86:ASN:OD1			10	1
1:X:9:LYS:O 2:B:15:PHE:CG			2.71	17	2
2:B:15:PHE:CG	1:X:12:SER:OXT	0.43	2.35	14	1
	· · · · · · · · · · · · · · · · · · ·	0.43	2.36	6	3
1.V.F.H D.O	2:B:71:PHE:CE2	0.43	3.06	4	1
1:X:5:ILE:O	1:X:5:ILE:CG1	0.43	2.66	15	3
2:A:55:ASP:O	2:A:55:ASP:OD1	0.43	2.37	7	3
2:B:55:ASP:O	2:B:55:ASP:OD1	0.43	2.37	7	3
2:A:66:ASP:O	2:A:68:GLU:OE2	0.43	2.36	4	1
1:Y:5:ILE:O	1:Y:5:ILE:HG23	0.43	2.13	7	1
2:A:1:GLY:O	2:B:40:GLU:OE2	0.43	2.36	7	1
2:A:40:GLU:OE1	2:A:40:GLU:N	0.43	2.51	11	1
2:A:82:THR:HG23	2:A:83:VAL:H	0.43	1.71	16	1
2:A:44:PHE:C	2:A:44:PHE:CD1	0.43	2.90	12	2
2:B:45:LEU:HD11	2:B:81:LEU:CD2	0.43	2.43	1	1
2:A:61:LEU:O	2:A:73:GLU:OE2	0.43	2.36	9	4
2:A:61:LEU:C	2:A:63:GLU:H	0.43	2.16	3	8
2:A:87:ASN:HD21	2:B:72:GLN:NE2	0.43	2.12	20	1
2:A:62:ASP:OD2	2:A:66:ASP:O	0.43	2.36	2	2
2:B:61:LEU:C	2:B:63:GLU:H	0.43	2.16	3	9
1:X:5:ILE:O	1:X:8:ASN:ND2	0.43	2.51	7	1
2:A:81:LEU:C	2:A:81:LEU:HD22	0.43	2.34	8	1
1:Y:5:ILE:O	2:B:50:ASP:OD2	0.43	2.36	13	2
1:X:5:ILE:O	1:X:6:ASP:C	0.43	2.57	14	1
1:Y:9:LYS:O	1:Y:12:SER:O	0.43	2.37	15	1
2:A:68:GLU:N	2:A:68:GLU:CD	0.43	2.72	19	1
1:X:11:LEU:C	1:X:11:LEU:CD2	0.43	2.87	20	1
2:A:18:HIS:NE2	2:A:22:GLU:OE1	0.43	2.51	20	1
2:B:90:TRP:O	2:B:90:TRP:CG	0.43	2.72	16	2
1:X:5:ILE:O	2:A:46:ASP:CG	0.43	2.57	10	2
2:A:1:GLY:N	2:A:5:GLU:CD	0.43	2.72	10	1
2:A:15:PHE:CD1	2:A:71:PHE:CE2	0.43	3.06	17	1
2:A:36:LEU:HD23	2:A:74:PHE:CE1	0.43	2.49	2	1
2:B:12:ILE:O	2:B:16:HIS:ND1	0.43	2.52	4	1
2:B:61:LEU:C	2:B:63:GLU:N	0.43	2.72	13	6
2:A:52:ASP:OD1	2:A:56:LYS:NZ	0.43	2.52	11	1
2:B:15:PHE:CZ	2:B:74:PHE:CD2	0.43	3.06	11	1
1:Y:5:ILE:CG2	1:Y:6:ASP:H	0.43	2.19	17	1
2:A:37:LEU:HD21	2:A:74:PHE:CE1	0.43	2.49	1	1
2:A:12:ILE:O	2:A:16:HIS:ND1	0.43	2.52	4	1



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2.B.4:LEU:HD23	Atom-1	Atom-2	Clash(Å)	$\operatorname{Distance}(\mathring{\mathrm{A}})$	Models	
2:A:61:LEU:C 2:A:63:GLU:N 0.43 2.72 13 5 2:A:49:LYS:O 2:A:50:ASP:ODI 0.43 2.36 10 1 2:B:49:LYS:O 2:B:50:ASP:ODI 0.43 2.36 10 1 2:A:15:PHE:CZ 2:A:74:PHE:CD2 0.43 2.36 10 1 2:A:71:PHE:O 2:A:74:PHE:CD2 0.43 2.56 19 2 1:X:8:ASN:ODI 2:A:46:ASP:OD2 0.43 2.36 20 1 2:B:18:HIS:NE2 2:B:22:GLU:OEI 0.43 2.57 13 8 2:A:29:SER:O 2:A:30:LYS:C 0.43 2.57 13 8 2:A:73:GLU:O 2:A:76:VAL:CG2 0.43 2.67 14 1 2:B:15:PHE:CEI 2:B:74:PHE:CZ 0.43 3.07 16 2 2:B:31:LYS:NZ 2:B:31:LYS:CB 0.43 2.81 15 1 2:A:26:TYR:OH 2:B:36:ASN:NDD 0.42 2.52 12 1 1:Y:8:ASN;CCG 1:Y:9:LYS:N			` ′	,	Worst	Total
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2:B:71:PHE:O 2:B:75:VAL:HG22 0.42 2.14 19 1 1:Y:10:ILE:HD12 2:B:88:PHE:CE1 0.42 2.48 20 1 2:B:40:GLU:OE1 2:B:40:GLU:N 0.42 2.52 11 1 1:X:9:LYS:HZ2 2:A:56:LYS:NZ 0.42 2.11 2 1 1:Y:7:TRP:CZ3 2:B:81:LEU:HD22 0.42 2.49 2 1 2:B:33:ASP:OD2 0.42 2.38 3 1 2:B:35:ASP:OD1 2:B:39:THR:OG1 0.42 2.38 5 1 2:A:45:LEU:H 2:A:45:LEU:HD12 0.42 1.74 10 1 2:A:88:PHE:O 2:A:88:PHE:CG 0.42 2.72 17 2 1:X:7:TRP:O 1:X:8:ASN:C 0.42 2.57 4 4 2:B:29:SER:O 2:B:30:LYS:C 0.42 2.57 13 4 2:B:2:SER:OG 2:B:5:GLU:OE1 0.42 2.37 9 1 1:X:12:SER:C 2:A:60:GLU:OE2 0.42 2.58 5 1 2:B:44:PHE:CD2 2:B:45:LEU:CD1 0.42	2:B:18:HIS:ND1	2:B:36:LEU:HD21	0.42	2.29	18	1
1:Y:10:ILE:HD12 2:B:88:PHE:CE1 0.42 2.48 20 1 2:B:40:GLU:OE1 2:B:40:GLU:N 0.42 2.52 11 1 1:X:9:LYS:HZ2 2:A:56:LYS:NZ 0.42 2.11 2 1 1:Y:7:TRP:CZ3 2:B:81:LEU:HD22 0.42 2.49 2 1 2:B:31:LYS:O 2:B:35:ASP:OD2 0.42 2.38 3 1 2:B:35:ASP:OD1 2:B:39:THR:OG1 0.42 2.38 5 1 2:A:45:LEU:H 2:A:45:LEU:HD12 0.42 1.74 10 1 2:A:88:PHE:O 2:A:88:PHE:CG 0.42 2.72 17 2 1:X:7:TRP:O 1:X:8:ASN:C 0.42 2.57 4 4 2:B:29:SER:O 2:B:30:LYS:C 0.42 2.57 13 4 2:B:2:SER:OG 2:B:5:GLU:OE1 0.42 2.37 9 1 1:X:12:SER:C 2:A:60:GLU:OE2 0.42 2.58 5 1 2:B:44:PHE:CD2 2:B:45:LEU:CD1 0.42 2.58 5 1 2:A:35:ASP:OD1 2:A:35:ASP:C <td>2:B:68:GLU:CD</td> <td>2:B:68:GLU:N</td> <td>0.42</td> <td>2.72</td> <td>19</td> <td>1</td>	2:B:68:GLU:CD	2:B:68:GLU:N	0.42	2.72	19	1
2:B:40:GLU:OE1 2:B:40:GLU:N 0.42 2.52 11 1 1:X:9:LYS:HZ2 2:A:56:LYS:NZ 0.42 2.11 2 1 1:Y:7:TRP:CZ3 2:B:81:LEU:HD22 0.42 2.49 2 1 2:B:31:LYS:O 2:B:35:ASP:OD2 0.42 2.38 3 1 2:B:35:ASP:OD1 2:B:39:THR:OG1 0.42 2.38 5 1 2:A:45:LEU:H 2:A:45:LEU:HD12 0.42 1.74 10 1 2:A:88:PHE:O 2:A:88:PHE:CG 0.42 2.72 17 2 1:X:7:TRP:O 1:X:8:ASN:C 0.42 2.57 4 4 2:B:29:SER:O 2:B:30:LYS:C 0.42 2.57 13 4 2:B:2:SER:OG 2:B:5:GLU:OE1 0.42 2.37 9 1 1:X:12:SER:C 2:A:60:GLU:OE2 0.42 2.58 5 1 2:B:44:PHE:CD2 2:B:45:LEU:CD1 0.42 2.58 12 1 2:A:35:ASP:OD1 2:A:35:ASP:C 0.42 2.58 12 1	2:B:71:PHE:O	2:B:75:VAL:HG22	0.42	2.14	19	1
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1:Y:7:TRP:CZ3 2:B:81:LEU:HD22 0.42 2.49 2 1 2:B:31:LYS:O 2:B:35:ASP:OD2 0.42 2.38 3 1 2:B:35:ASP:OD1 2:B:39:THR:OG1 0.42 2.38 5 1 2:A:45:LEU:H 2:A:45:LEU:HD12 0.42 1.74 10 1 2:A:88:PHE:O 2:A:88:PHE:CG 0.42 2.72 17 2 1:X:7:TRP:O 1:X:8:ASN:C 0.42 2.57 4 4 2:B:29:SER:O 2:B:30:LYS:C 0.42 2.57 13 4 2:B:2:SER:OG 2:B:5:GLU:OE1 0.42 2.37 9 1 1:X:12:SER:C 2:A:60:GLU:OE2 0.42 2.58 5 1 2:B:44:PHE:CD2 2:B:45:LEU:CD1 0.42 3.03 10 1 2:A:35:ASP:OD1 2:A:35:ASP:C 0.42 2.58 12 1	2:B:40:GLU:OE1	2:B:40:GLU:N	0.42	2.52	11	1
2:B:31:LYS:O 2:B:35:ASP:OD2 0.42 2.38 3 1 2:B:35:ASP:OD1 2:B:39:THR:OG1 0.42 2.38 5 1 2:A:45:LEU:H 2:A:45:LEU:HD12 0.42 1.74 10 1 2:A:88:PHE:O 2:A:88:PHE:CG 0.42 2.72 17 2 1:X:7:TRP:O 1:X:8:ASN:C 0.42 2.57 4 4 2:B:29:SER:O 2:B:30:LYS:C 0.42 2.57 13 4 2:B:2:SER:OG 2:B:5:GLU:OE1 0.42 2.37 9 1 1:X:12:SER:C 2:A:60:GLU:OE2 0.42 2.58 5 1 2:B:44:PHE:CD2 2:B:45:LEU:CD1 0.42 3.03 10 1 2:A:35:ASP:OD1 2:A:35:ASP:C 0.42 2.58 12 1	1:X:9:LYS:HZ2	2:A:56:LYS:NZ	0.42	2.11	2	1
2:B:35:ASP:OD1 2:B:39:THR:OG1 0.42 2.38 5 1 2:A:45:LEU:H 2:A:45:LEU:HD12 0.42 1.74 10 1 2:A:88:PHE:O 2:A:88:PHE:CG 0.42 2.72 17 2 1:X:7:TRP:O 1:X:8:ASN:C 0.42 2.57 4 4 2:B:29:SER:O 2:B:30:LYS:C 0.42 2.57 13 4 2:B:2:SER:OG 2:B:5:GLU:OE1 0.42 2.37 9 1 1:X:12:SER:C 2:A:60:GLU:OE2 0.42 2.58 5 1 2:B:44:PHE:CD2 2:B:45:LEU:CD1 0.42 3.03 10 1 2:A:35:ASP:OD1 2:A:35:ASP:C 0.42 2.58 12 1	1:Y:7:TRP:CZ3	2:B:81:LEU:HD22	0.42	2.49	2	1
2:A:45:LEU:H 2:A:45:LEU:HD12 0.42 1.74 10 1 2:A:88:PHE:O 2:A:88:PHE:CG 0.42 2.72 17 2 1:X:7:TRP:O 1:X:8:ASN:C 0.42 2.57 4 4 2:B:29:SER:O 2:B:30:LYS:C 0.42 2.57 13 4 2:B:2:SER:OG 2:B:5:GLU:OE1 0.42 2.37 9 1 1:X:12:SER:C 2:A:60:GLU:OE2 0.42 2.58 5 1 2:B:44:PHE:CD2 2:B:45:LEU:CD1 0.42 3.03 10 1 2:A:35:ASP:OD1 2:A:35:ASP:C 0.42 2.58 12 1	2:B:31:LYS:O	2:B:35:ASP:OD2	0.42	2.38	3	1
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1:X:7:TRP:O 1:X:8:ASN:C 0.42 2.57 4 4 2:B:29:SER:O 2:B:30:LYS:C 0.42 2.57 13 4 2:B:2:SER:OG 2:B:5:GLU:OE1 0.42 2.37 9 1 1:X:12:SER:C 2:A:60:GLU:OE2 0.42 2.58 5 1 2:B:44:PHE:CD2 2:B:45:LEU:CD1 0.42 3.03 10 1 2:A:35:ASP:OD1 2:A:35:ASP:C 0.42 2.58 12 1	2:A:45:LEU:H	2:A:45:LEU:HD12	0.42	1.74	10	1
2:B:29:SER:O 2:B:30:LYS:C 0.42 2.57 13 4 2:B:2:SER:OG 2:B:5:GLU:OE1 0.42 2.37 9 1 1:X:12:SER:C 2:A:60:GLU:OE2 0.42 2.58 5 1 2:B:44:PHE:CD2 2:B:45:LEU:CD1 0.42 3.03 10 1 2:A:35:ASP:OD1 2:A:35:ASP:C 0.42 2.58 12 1	2:A:88:PHE:O	2:A:88:PHE:CG	0.42	2.72	17	2
2:B:2:SER:OG 2:B:5:GLU:OE1 0.42 2.37 9 1 1:X:12:SER:C 2:A:60:GLU:OE2 0.42 2.58 5 1 2:B:44:PHE:CD2 2:B:45:LEU:CD1 0.42 3.03 10 1 2:A:35:ASP:OD1 2:A:35:ASP:C 0.42 2.58 12 1	1:X:7:TRP:O	1:X:8:ASN:C	0.42	2.57	4	4
1:X:12:SER:C 2:A:60:GLU:OE2 0.42 2.58 5 1 2:B:44:PHE:CD2 2:B:45:LEU:CD1 0.42 3.03 10 1 2:A:35:ASP:OD1 2:A:35:ASP:C 0.42 2.58 12 1	2:B:29:SER:O	2:B:30:LYS:C	0.42	2.57	13	4
2:B:44:PHE:CD2 2:B:45:LEU:CD1 0.42 3.03 10 1 2:A:35:ASP:OD1 2:A:35:ASP:C 0.42 2.58 12 1	2:B:2:SER:OG	2:B:5:GLU:OE1	0.42	2.37	9	1
2:A:35:ASP:OD1 2:A:35:ASP:C 0.42 2.58 12 1	1:X:12:SER:C	2:A:60:GLU:OE2	0.42	2.58	5	1
	2:B:44:PHE:CD2	2:B:45:LEU:CD1	0.42	3.03	10	1
1:X:11:LEU:HD23	2:A:35:ASP:OD1	2:A:35:ASP:C	0.42	2.58	12	1
	1:X:11:LEU:HD23	1:X:11:LEU:O	0.42	2.13	20	1



 $Continued\ from\ previous\ page...$

Atom-1	Atom-2	Clash(Å)	$\operatorname{Distance}(\mathring{\mathrm{A}})$	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
2:B:72:GLN:N	2:B:72:GLN:CD	0.42	2.73	3	1
2:B:3:GLU:H	2:B:3:GLU:CD	0.42	2.17	8	2
2:A:90:TRP:O	2:A:90:TRP:CG	0.42	2.72	16	2
2:A:29:SER:N	2:A:32:GLU:OE2	0.42	2.41	13	1
1:X:8:ASN:CB	2:A:46:ASP:OD1	0.42	2.68	14	1
1:X:8:ASN:HD22	2:A:57:ILE:HD11	0.42	1.74	15	1
2:B:66:ASP:OD1	2:B:66:ASP:N	0.42	2.52	18	1
2:B:45:LEU:HD21	2:B:81:LEU:CD2	0.42	2.45	13	2
1:Y:11:LEU:HD23	1:Y:11:LEU:C	0.42	2.35	12	1
1:X:8:ASN:HD21	2:A:57:ILE:CG1	0.42	2.28	12	1
2:B:28:LEU:CB	2:B:69:VAL:O	0.42	2.67	18	2
2:A:72:GLN:N	2:A:72:GLN:CD	0.41	2.73	3	1
1:Y:5:ILE:CD1	2:B:46:ASP:OD1	0.41	2.68	17	1
2:B:49:LYS:CD	2:B:49:LYS:N	0.41	2.83	11	1
1:X:10:ILE:HD12	2:A:88:PHE:CE1	0.41	2.50	20	1
2:A:70:ASP:O	2:A:71:PHE:C	0.41	2.59	4	1
2:A:39:THR:O	2:A:40:GLU:CG	0.41	2.68	8	1
2:B:39:THR:O	2:B:40:GLU:CG	0.41	2.69	8	1
2:B:3:GLU:CG	2:B:4:LEU:N	0.41	2.83	9	1
2:B:73:GLU:O	2:B:76:VAL:CG2	0.41	2.68	14	1
2:A:86:ASN:OD1	2:B:26:TYR:OH	0.41	2.37	18	1
2:B:36:LEU:HD23	2:B:74:PHE:CE1	0.41	2.51	2	1
2:B:38:GLN:NE2	2:B:42:SER:OG	0.41	2.52	3	1
2:B:77:LEU:HD11	2:B:81:LEU:CD1	0.41	2.45	7	1
2:A:3:GLU:CG	2:A:4:LEU:N	0.41	2.84	9	1
2:A:2:SER:OG	2:A:5:GLU:OE1	0.41	2.37	9	1
2:A:26:TYR:OH	2:B:86:ASN:OD1	0.41	2.38	18	1
2:A:40:GLU:CD	2:B:2:SER:OG	0.41	2.59	18	1
2:A:71:PHE:O	2:A:75:VAL:HG22	0.41	2.15	19	1
2:B:87:ASN:O	2:B:87:ASN:OD1	0.41	2.39	19	1
1:X:9:LYS:NZ	2:A:56:LYS:HZ3	0.41	2.14	2	1
2:A:52:ASP:OD1	2:A:52:ASP:O	0.41	2.38	2	1
2:A:77:LEU:HD13	2:A:78:VAL:N	0.41	2.31	2	1
2:B:64:ASN:OD1	2:B:64:ASN:N	0.41	2.52	2	1
2:A:31:LYS:O	2:A:35:ASP:OD2	0.41	2.37	3	1
2:A:23:GLY:O	2:A:24:ASP:C	0.41	2.59	6	3
2:B:23:GLY:O	2:B:24:ASP:C	0.41	2.59	6	2
2:A:74:PHE:O	2:A:77:LEU:N	0.41	2.53	12	1
2:A:2:SER:OG	2:B:40:GLU:CD	0.41	2.59	18	1
2:B:78:VAL:CG2	2:B:79:ALA:N	0.41	2.83	18	1
2:A:87:ASN:OD1	2:A:87:ASN:O	0.41	2.38	19	1



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Atom-1	Atom-2	Clash(Å)	$Distance(\mathring{A})$	Models	
		Clasii(A)	Distance(A)	Worst	Total
2:B:77:LEU:HD13	2:B:78:VAL:N	0.41	2.30	2	1
2:B:34:LYS:O	2:B:38:GLN:CB	0.41	2.69	18	3
2:B:46:ASP:O	2:B:47:VAL:CG1	0.41	2.68	7	1
2:A:62:ASP:CG	2:A:67:GLY:H	0.41	2.19	10	1
2:B:75:VAL:CG1	2:B:76:VAL:N	0.41	2.84	14	1
1:Y:8:ASN:H	2:B:46:ASP:CG	0.41	2.18	17	1
2:B:38:GLN:OE1	2:B:48:GLN:OE1	0.41	2.39	18	1
2:A:82:THR:CG2	2:A:83:VAL:N	0.41	2.84	3	1
2:A:77:LEU:HD11	2:A:81:LEU:CD1	0.41	2.45	7	1
2:B:75:VAL:HG13	2:B:76:VAL:N	0.41	2.31	14	1
2:A:22:GLU:CD	2:A:22:GLU:N	0.41	2.74	16	1
1:Y:5:ILE:CG2	1:Y:6:ASP:N	0.41	2.81	17	1
1:Y:9:LYS:O	1:Y:12:SER:OXT	0.41	2.39	19	1
2:B:70:ASP:O	2:B:71:PHE:C	0.41	2.59	4	1
2:A:29:SER:O	2:A:33:LEU:CD2	0.41	2.69	6	1
2:B:35:ASP:O	2:B:39:THR:OG1	0.41	2.33	6	1
1:X:6:ASP:O	1:X:9:LYS:N	0.41	2.51	11	1
2:B:42:SER:OG	2:B:48:GLN:OE1	0.41	2.39	12	1
2:A:79:ALA:HB1	2:B:75:VAL:CG2	0.41	2.43	14	1
2:A:15:PHE:CE1	2:A:74:PHE:CZ	0.41	3.08	15	2
2:A:37:LEU:HD21	2:A:74:PHE:CZ	0.41	2.51	15	1
2:A:30:LYS:CG	2:A:58:MET:SD	0.41	3.09	19	1
2:B:30:LYS:CG	2:B:58:MET:SD	0.41	3.09	19	1
1:Y:8:ASN:CG	2:B:46:ASP:OD2	0.41	2.59	20	1
2:A:72:GLN:NE2	2:B:87:ASN:HD21	0.41	2.13	20	1
2:B:52:ASP:O	2:B:52:ASP:OD1	0.41	2.39	2	1
2:B:29:SER:O	2:B:33:LEU:CD2	0.41	2.69	6	1
2:B:64:ASN:ND2	2:B:66:ASP:OD2	0.41	2.50	9	1
2:A:18:HIS:CE1	2:A:19:SER:OG	0.41	2.74	12	1
2:A:64:ASN:OD1	2:A:66:ASP:OD1	0.40	2.38	2	1
2:B:82:THR:CG2	2:B:83:VAL:N	0.40	2.84	3	1
2:B:35:ASP:OD1	2:B:35:ASP:C	0.40	2.58	12	1
2:A:35:ASP:O	2:A:39:THR:OG1	0.40	2.39	16	1
2:A:33:LEU:HD11	2:A:69:VAL:CG2	0.40	2.46	19	1
2:B:2:SER:O	2:B:3:GLU:C	0.40	2.60	2	2
2:A:34:LYS:O	2:A:38:GLN:CB	0.40	2.69	18	3
2:A:35:ASP:OD1	2:A:39:THR:OG1	0.40	2.39	5	1
2:A:35:ASP:O	2:A:39:THR:HG22	0.40	2.17	10	1
2:A:22:GLU:OE1	2:A:35:ASP:OD2	0.40	2.39	19	1
1:Y:5:ILE:HD13	2:B:49:LYS:NZ	0.40	2.32	4	1
2:A:38:GLN:C	2:A:40:GLU:H	0.40	2.20	8	1



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Atom-1	Atom-2	Clash(Å)	$Distance(\mathring{A})$	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
2:B:81:LEU:HD13	2:B:81:LEU:C	0.40	2.29	11	1
2:B:18:HIS:CE1	2:B:19:SER:OG	0.40	2.74	12	1
2:B:22:GLU:N	2:B:22:GLU:CD	0.40	2.75	16	1
2:A:47:VAL:O	2:A:50:ASP:C	0.40	2.60	17	1
2:A:38:GLN:OE1	2:A:48:GLN:OE1	0.40	2.40	18	1
1:Y:8:ASN:OD1	2:B:81:LEU:HD11	0.40	2.16	2	1
2:B:22:GLU:C	2:B:32:GLU:OE2	0.40	2.59	8	2
2:B:53:ALA:O	2:B:57:ILE:HD13	0.40	2.15	9	1
2:A:42:SER:OG	2:A:48:GLN:OE1	0.40	2.38	12	1
1:Y:7:TRP:O	1:Y:8:ASN:C	0.40	2.59	1	2
2:A:38:GLN:NE2	2:A:42:SER:OG	0.40	2.55	3	1
1:Y:6:ASP:O	1:Y:6:ASP:OD1	0.40	2.39	11	1
1:Y:11:LEU:O	1:Y:12:SER:OG	0.40	2.35	14	1
2:A:24:ASP:OD2	2:A:68:GLU:OE2	0.40	2.40	14	1
2:B:37:LEU:HD21	2:B:74:PHE:CZ	0.40	2.52	15	1
1:X:7:TRP:O	1:X:10:ILE:HB	0.40	2.16	17	1
2:A:22:GLU:C	2:A:32:GLU:OE2	0.40	2.60	17	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	X	7/12 (58%)	6±1 (89±12%)	0±1 (6±11%)	$0\pm1~(5\pm8\%)$	4 25
1	Y	7/12 (58%)	6±1 (93±10%)	0±1 (4±8%)	0±0 (4±6%)	6 34
2	A	89/93 (96%)	81±2 (91±3%)	5±2 (6±2%)	3±1 (3±1%)	7 40
2	В	89/93 (96%)	81±2 (91±3%)	6±2 (7±2%)	2±1 (2±1%)	10 49
All	All	3840/4200 (91%)	3499 (91%)	236 (6%)	105 (3%)	8 43

All 22 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	A	45	LEU	20



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Mol	Chain	Res	Type	Models (Total)
2	В	45	LEU	13
2	A	44	PHE	9
2	A	47	VAL	9
2	В	47	VAL	9
2	A	22	GLU	7
2	В	22	GLU	7
1	X	6	ASP	4
1	Y	5	ILE	4
2	A	24	ASP	3
2	В	24	ASP	3
1	X	5	ILE	3
2	A	71	PHE	2
2	A	72	GLN	2
2	В	71	PHE	2
2	В	72	GLN	2
2	A	2	SER	1
2	В	2	SER	1
2	A	39	THR	1
2	В	39	THR	1
2	В	44	PHE	1
1	Y	6	ASP	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	X	8/12 (67%)	7±1 (91±8%)	1±1 (9±8%)	12	58
1	Y	8/12 (67%)	7±1 (88±8%)	1±1 (12±8%)	8	50
2	A	78/81 (96%)	72±2 (92±3%)	6±2 (8±3%)	16	63
2	В	78/81 (96%)	72±2 (92±3%)	6±2 (8±3%)	16	63
All	All	3440/3720 (92%)	3156 (92%)	284 (8%)	15	62

All 74 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)
2	A	54	VAL	20
2	В	54	VAL	20
2	A	10	THR	17
2	В	10	THR	17
2	A	58	MET	9
2	В	58	MET	9
2	A	59	LYS	8
2	В	59	LYS	8
2	A	71	PHE	8
2	В	71	PHE	8
1	Y	8	ASN	7
2	A	45	LEU	7
2	В	45	LEU	7
1	X	8	ASN	6
2	A	49	LYS	6
2	В	49	LYS	6
1	Y	5	ILE	6
1	X	5	ILE	5
1	Y	11	LEU	5
2	A	42	SER	5
2	В	42	SER	5
2	A	81	LEU	5
2	В	81	LEU	5
2	A	76	VAL	4
2	В	76	VAL	4
2	A	30	LYS	4
2	A	77	LEU	4
2	В	77	LEU	4
2	В	46	ASP	3
2	A	74	PHE	3
2	В	74	PHE	3
2	В	30	LYS	3
2	A	47	VAL	3
2	В	47	VAL	3
2	A	46	ASP	2
2	A	28	LEU	2
2	В	28	LEU	2
1	Y	9	LYS	2
1	X	11	LEU	2
2	A	75	VAL	2
2	В	75	VAL	2
2	A	33	LEU	1
2	A	50	ASP	1



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Mol	Chain	$\overline{\mathrm{Res}}$	Type	Models (Total)
2	A	88	PHE	1
2	В	33	LEU	1
2	В	50	ASP	1
2	В	88	PHE	1
1	X	12	SER	1
2	A	3	GLU	1
2	A	25	LYS	1
2	A	70	ASP	1
2	В	25	LYS	1
2	В	27	LYS	1
2	В	70	ASP	1
1	X	9	LYS	1
2	A	31	LYS	1
2	В	31	LYS	1
2	A	48	GLN	1
2	A	86	ASN	1
2	В	48	GLN	1
2	В	86	ASN	1
2	A	38	GLN	1
2	В	38	GLN	1
2	A	82	THR	1
2	В	82	THR	1
2	A	15	PHE	1
2	В	15	PHE	1
2	В	85	CYS	1
2	A	34	LYS	1
2	A	36	LEU	1
2	В	34	LYS	1
2	В	36	LEU	1
2	A	21	LYS	1
2	В	21	LYS	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.



6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



7 Chemical shift validation (i)

No chemical shift data were provided

