



Full wwPDB NMR Structure Validation Report ⓘ

Mar 23, 2026 – 01:02 AM UTC

PDB ID : 6BA6 / pdb_00006ba6
BMRB ID : 30353
Title : Solution structure of Rap1b/talin complex
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Deposited on : 2017-10-12

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with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

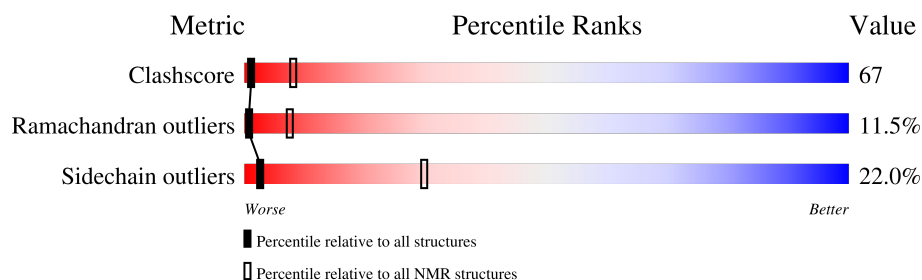
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 73%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	A	93	
2	B	168	

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:86, B:1-B:167 (252)	0.73	2

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 4 clusters and 6 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4045 atoms, of which 2022 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Talin-1.

Mol	Chain	Residues	Atoms						Trace
1	A	86	Total	C	H	N	O	S	0
			1384	437	696	117	127	7	

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP P26039
A	-5	ALA	-	expression tag	UNP P26039
A	-4	MET	-	expression tag	UNP P26039
A	-3	ASP	-	expression tag	UNP P26039
A	-2	PRO	-	expression tag	UNP P26039
A	-1	GLU	-	expression tag	UNP P26039
A	0	PHE	-	expression tag	UNP P26039

- Molecule 2 is a protein called Ras-related protein Rap-1b.

Mol	Chain	Residues	Atoms						Trace
2	B	167	Total	C	H	N	O	S	0
			2661	836	1326	228	263	8	

There are 2 discrepancies between the modelled and reference sequences:

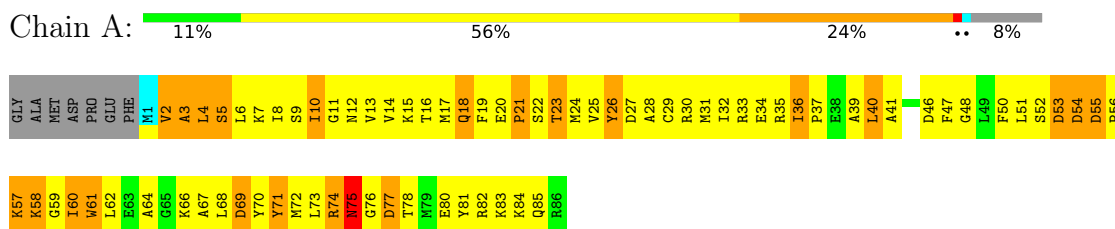
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP P61224
B	12	VAL	GLY	engineered mutation	UNP P61224

4 Residue-property plots [i](#)

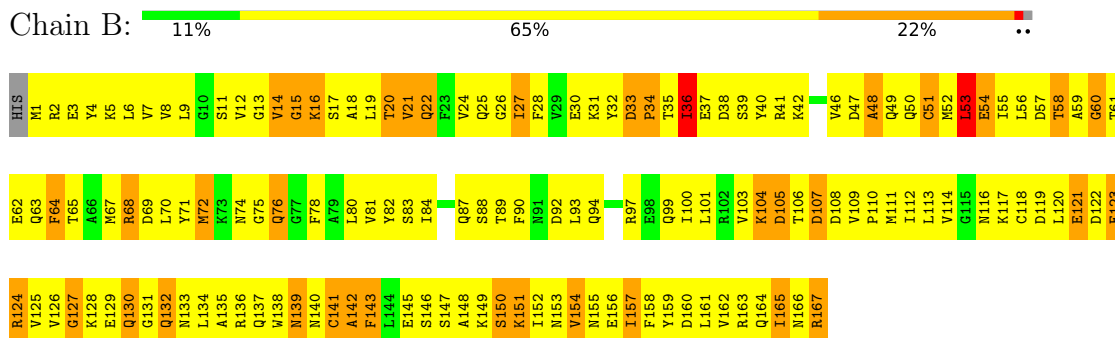
4.1 Average score per residue in the NMR ensemble

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: Talin-1



• Molecule 2: Ras-related protein Rap-1b

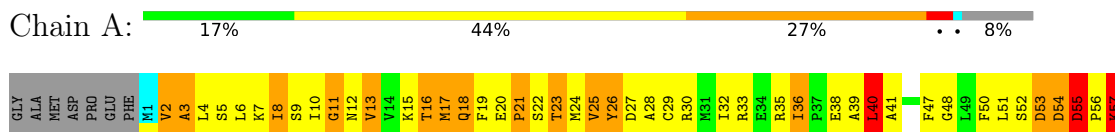


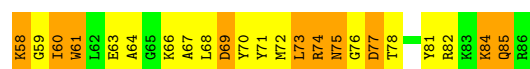
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

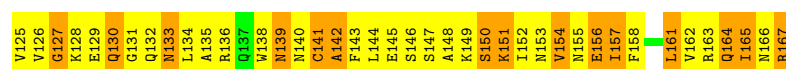
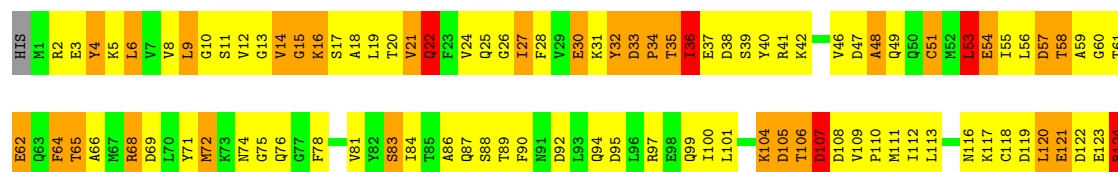
• Molecule 1: Talin-1





• Molecule 2: Ras-related protein Rap-1b

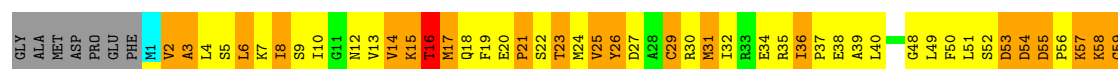
Chain B: 17% 53% 26% ..



4.2.2 Score per residue for model 2 (medoid)

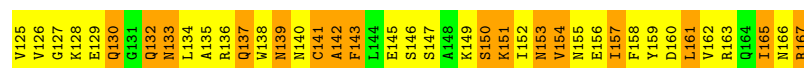
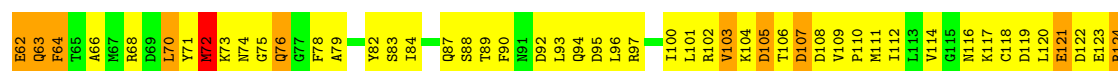
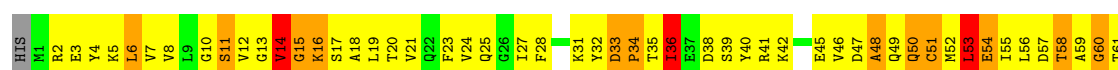
• Molecule 1: Talin-1

Chain A: 15% 45% 30% .. 8%



• Molecule 2: Ras-related protein Rap-1b

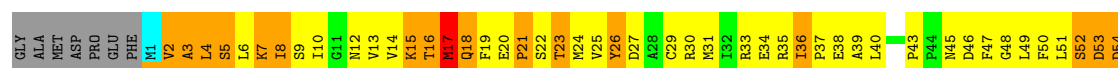
Chain B: 15% 59% 23% ..



4.2.3 Score per residue for model 3

• Molecule 1: Talin-1

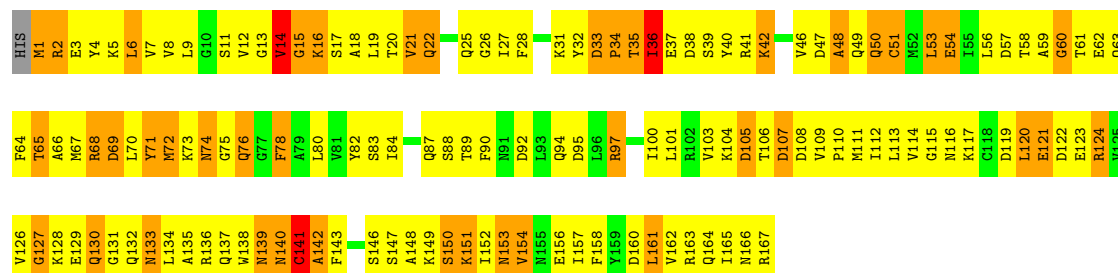
Chain A: 13% 47% 29% .. 8%





• Molecule 2: Ras-related protein Rap-1b

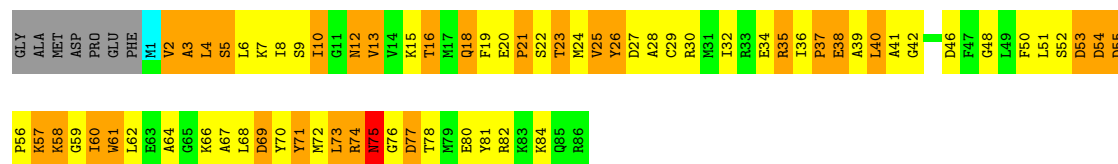
Chain B: 16% 57% 25% ..



4.2.4 Score per residue for model 4

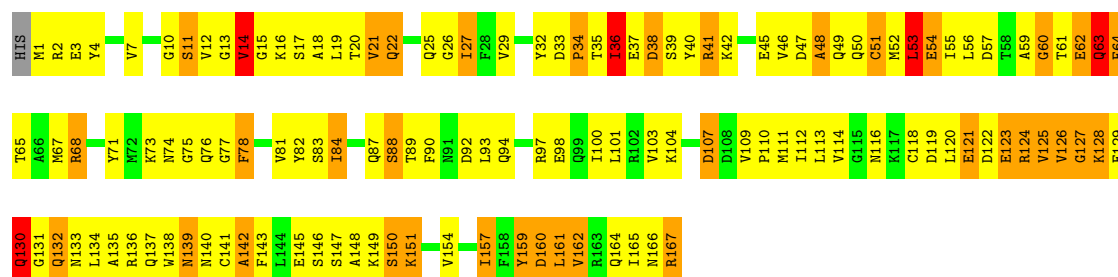
• Molecule 1: Talin-1

Chain A: 17% 42% 31% .. 8%



• Molecule 2: Ras-related protein Rap-1b

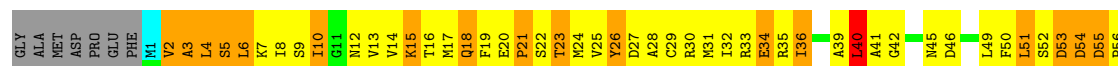
Chain B: 22% 53% 21% ..



4.2.5 Score per residue for model 5

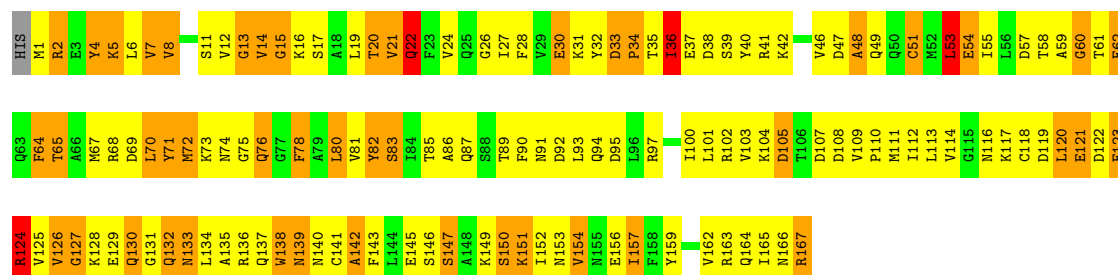
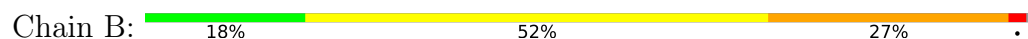
• Molecule 1: Talin-1

Chain A: 17% 42% 30% .. 8%



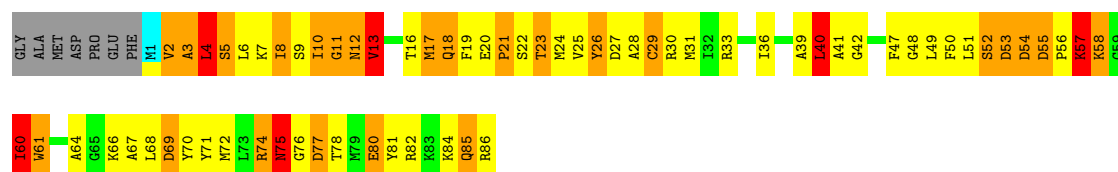
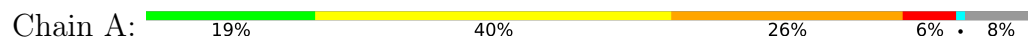


• Molecule 2: Ras-related protein Rap-1b

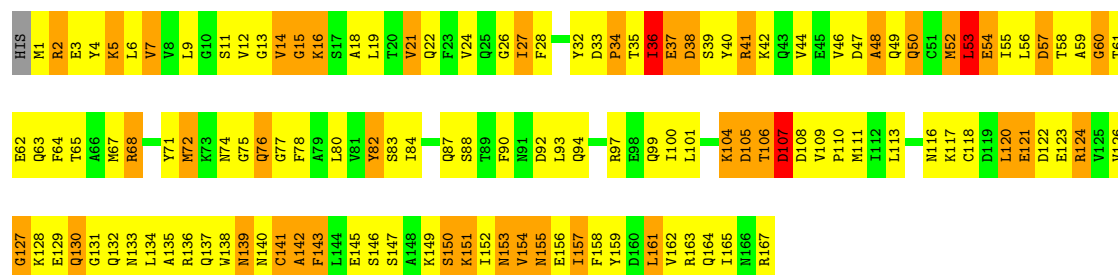


4.2.6 Score per residue for model 6

• Molecule 1: Talin-1

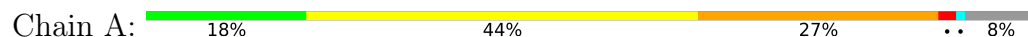


• Molecule 2: Ras-related protein Rap-1b



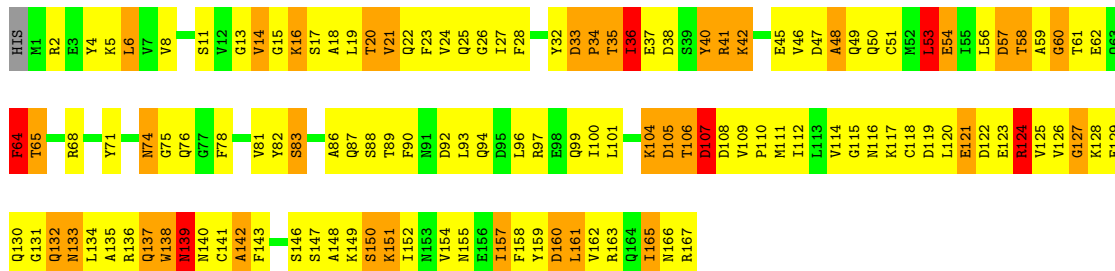
4.2.7 Score per residue for model 7

• Molecule 1: Talin-1



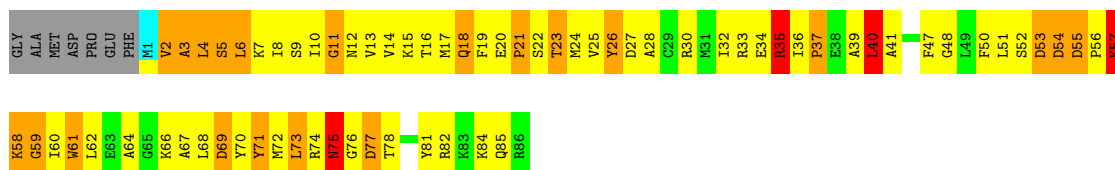
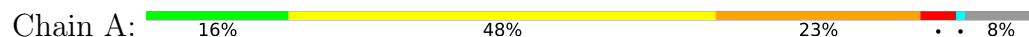


- Molecule 2: Ras-related protein Rap-1b

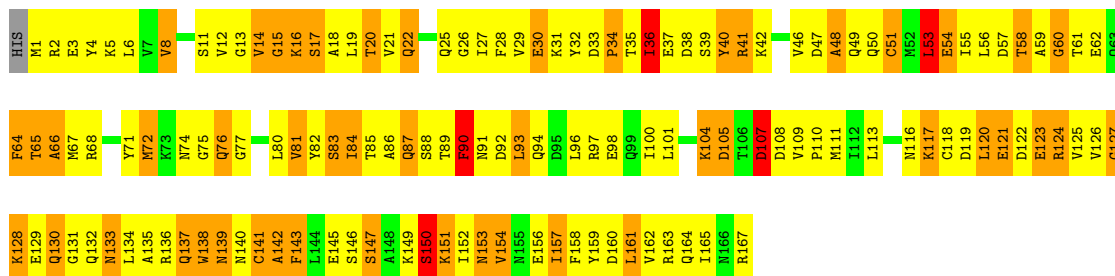
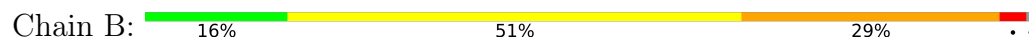


4.2.8 Score per residue for model 8

- Molecule 1: Talin-1

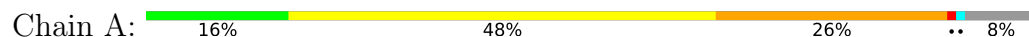


- Molecule 2: Ras-related protein Rap-1b



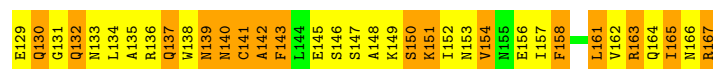
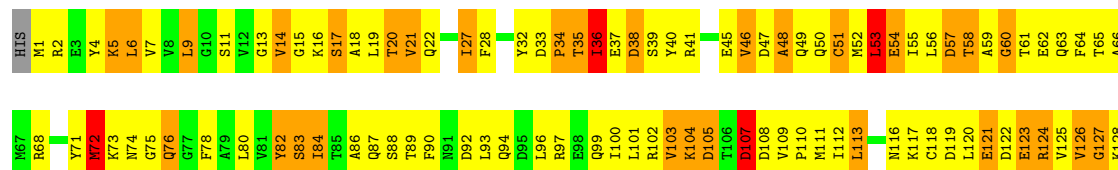
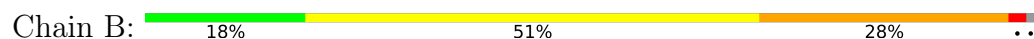
4.2.9 Score per residue for model 9

- Molecule 1: Talin-1



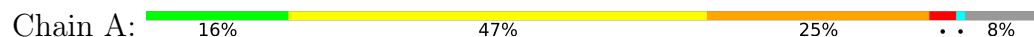


• Molecule 2: Ras-related protein Rap-1b

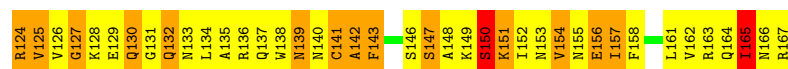
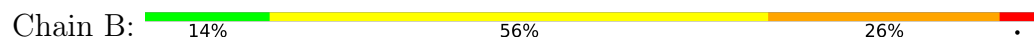


4.2.10 Score per residue for model 10

• Molecule 1: Talin-1

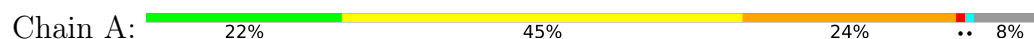


• Molecule 2: Ras-related protein Rap-1b



4.2.11 Score per residue for model 11

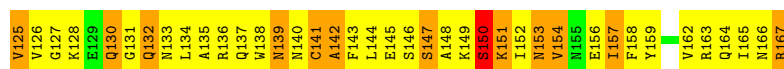
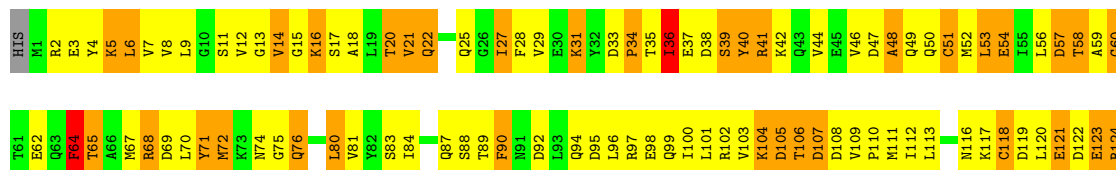
• Molecule 1: Talin-1





• Molecule 2: Ras-related protein Rap-1b

Chain B: 17% 52% 28% ..



4.2.12 Score per residue for model 12

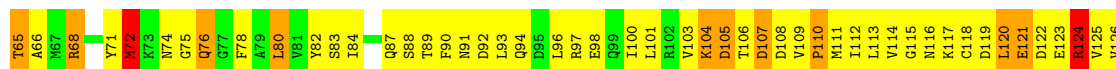
• Molecule 1: Talin-1

Chain A: 19% 41% 31% 8%



• Molecule 2: Ras-related protein Rap-1b

Chain B: 16% 55% 26% ..



4.2.13 Score per residue for model 13

• Molecule 1: Talin-1

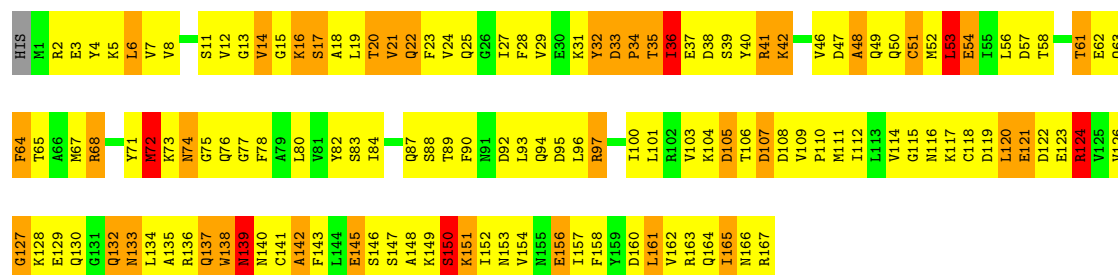
Chain A: 16% 44% 27% 8%





• Molecule 2: Ras-related protein Rap-1b

Chain B: 17% 58% 21% ..



4.2.14 Score per residue for model 14

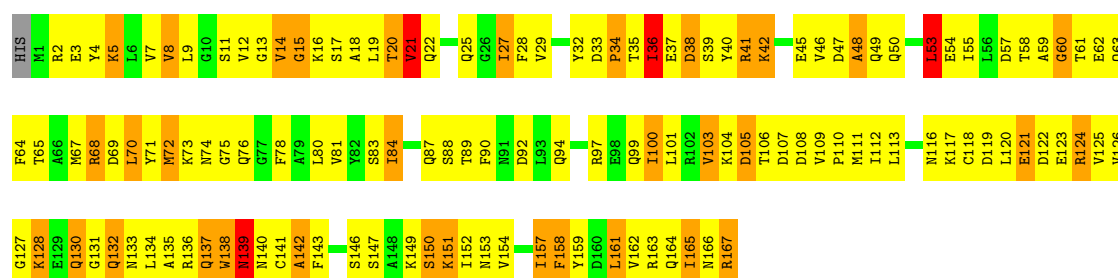
• Molecule 1: Talin-1

Chain A: 14% 51% 26% .. 8%



• Molecule 2: Ras-related protein Rap-1b

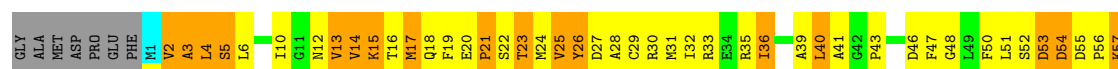
Chain B: 20% 57% 20% ..



4.2.15 Score per residue for model 15

• Molecule 1: Talin-1

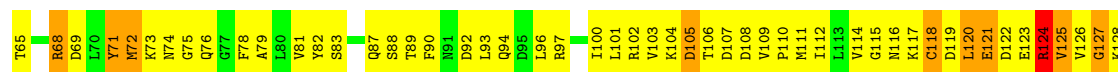
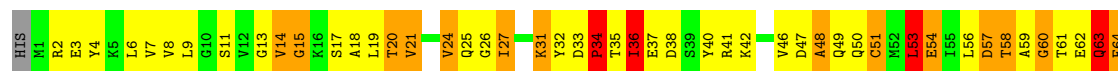
Chain A: 16% 47% 27% .. 8%





• Molecule 2: Ras-related protein Rap-1b

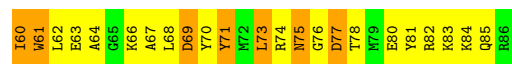
Chain B: 18% 58% 19% ..



4.2.16 Score per residue for model 16

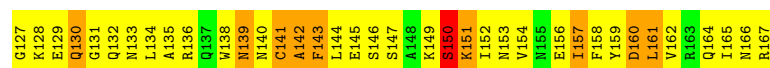
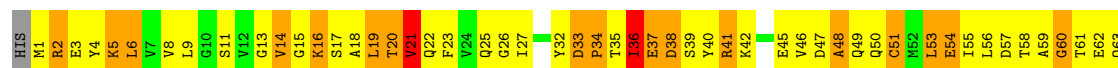
• Molecule 1: Talin-1

Chain A: 19% 46% 25% .. 8%



• Molecule 2: Ras-related protein Rap-1b

Chain B: 15% 58% 24% ..



4.2.17 Score per residue for model 17

• Molecule 1: Talin-1

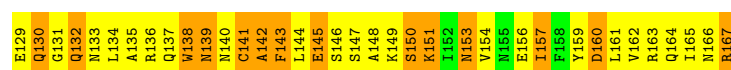
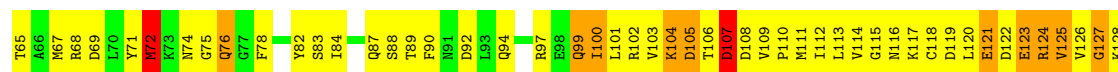
Chain A: 17% 38% 31% 5% .. 8%





• Molecule 2: Ras-related protein Rap-1b

Chain B: 19% 55% 23% ..



4.2.18 Score per residue for model 18

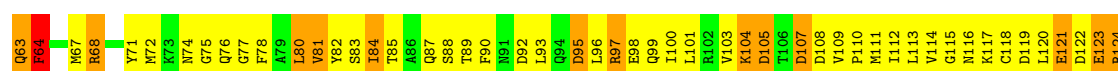
• Molecule 1: Talin-1

Chain A: 14% 46% 28% .. 8%



• Molecule 2: Ras-related protein Rap-1b

Chain B: 15% 56% 26% ..



4.2.19 Score per residue for model 19

• Molecule 1: Talin-1

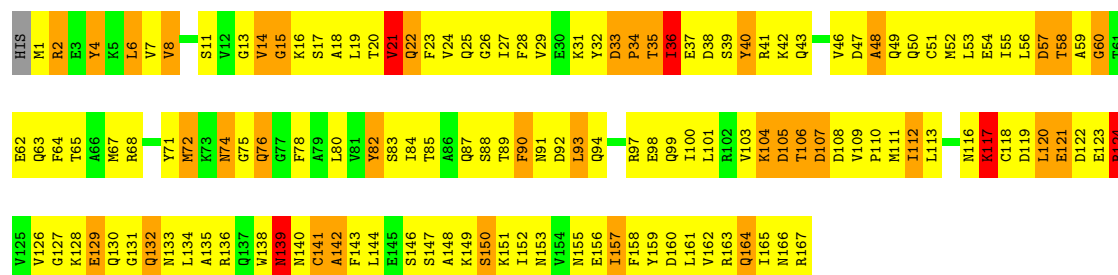
Chain A: 19% 43% 25% .. 8%





• Molecule 2: Ras-related protein Rap-1b

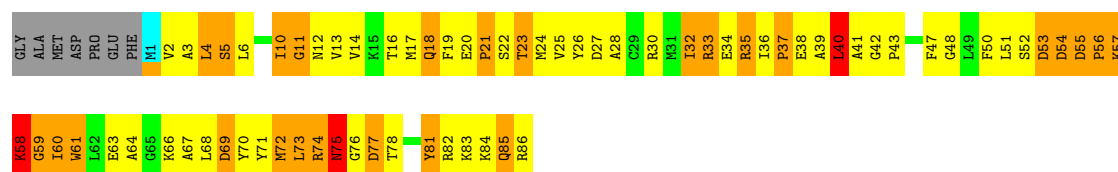
Chain B: 15% 60% 21% ..



4.2.20 Score per residue for model 20

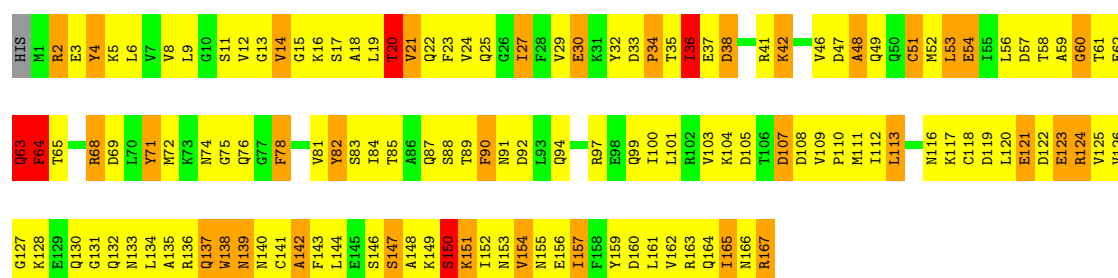
• Molecule 1: Talin-1

Chain A: 15% 45% 28% .. 8%



• Molecule 2: Ras-related protein Rap-1b

Chain B: 19% 57% 20% ..



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *20 structures for lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	
X-PLOR NIH	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	3
Total number of shifts	4180
Number of shifts mapped to atoms	4180
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	73%

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	A	1.52±0.02	0±1/693 (0.1± 0.1%)	1.33±0.03	5±1/930 (0.6± 0.1%)
2	B	1.57±0.02	2±1/1351 (0.2± 0.1%)	1.45±0.02	11±2/1819 (0.6± 0.1%)
All	All	1.55	57/40880 (0.1%)	1.41	319/54980 (0.6%)

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
2	B	54	GLU	N-CA	7.51	1.55	1.46	8	18
2	B	127	GLY	N-CA	6.79	1.50	1.44	7	14
2	B	36	ILE	C-N	-5.81	1.25	1.33	12	1
2	B	64	PHE	C-N	-5.67	1.27	1.33	18	2
2	B	77	GLY	N-CA	5.61	1.50	1.45	8	1
2	B	126	VAL	C-N	-5.50	1.28	1.33	9	2
2	B	41	ARG	C-N	-5.45	1.27	1.33	14	1
1	A	48	GLY	N-CA	5.41	1.50	1.45	19	2
2	B	111	MET	C-N	-5.33	1.28	1.33	16	1
1	A	63	GLU	N-CA	5.31	1.49	1.46	1	2
2	B	66	ALA	C-N	-5.31	1.26	1.33	8	4
1	A	4	LEU	C-N	-5.30	1.27	1.33	19	1
1	A	30	ARG	C-N	-5.20	1.26	1.34	12	1
2	B	2	ARG	C-N	-5.19	1.26	1.33	6	1
2	B	95	ASP	C-N	-5.13	1.27	1.34	18	1
2	B	124	ARG	N-CA	5.06	1.52	1.46	15	3
1	A	55	ASP	C-O	-5.00	1.19	1.24	1	1
2	B	46	VAL	C-N	-5.00	1.26	1.33	9	1

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
2	B	21	VAL	N-CA-C	-8.38	104.58	112.96	15	15
2	B	125	VAL	N-CA-C	-7.60	105.74	111.90	20	14
1	A	54	ASP	N-CA-C	-7.53	103.92	113.72	15	20
2	B	121	GLU	N-CA-C	-7.22	103.57	112.38	20	20
1	A	63	GLU	CA-C-O	7.00	122.00	117.94	7	3
1	A	71	TYR	N-CA-C	-6.90	104.74	113.02	16	20
2	B	133	ASN	N-CA-C	-6.83	104.42	112.89	15	20
1	A	58	LYS	N-CA-C	-6.79	105.12	113.41	19	20
1	A	57	LYS	N-CA-C	-6.49	104.84	112.89	18	20
2	B	22	GLN	N-CA-C	-6.42	105.27	113.23	6	8
2	B	72	MET	N-CA-C	-6.41	104.37	111.36	6	9
2	B	78	PHE	CA-CB-CG	-6.35	107.45	113.80	20	5
1	A	19	PHE	CA-CB-CG	-6.12	107.68	113.80	17	1
2	B	64	PHE	CA-CB-CG	6.07	119.87	113.80	18	4
2	B	143	PHE	CA-CB-CG	-5.99	107.81	113.80	2	10
2	B	107	ASP	N-CA-C	-5.98	105.64	113.17	5	20
2	B	130	GLN	N-CA-C	-5.88	104.95	111.36	5	15
2	B	150	SER	N-CA-C	-5.81	106.42	112.93	20	20
2	B	87	GLN	N-CA-C	-5.80	105.46	112.54	8	1
2	B	16	LYS	N-CA-C	-5.75	104.98	112.23	8	1
1	A	31	MET	N-CA-C	-5.75	105.76	112.89	13	1
2	B	63	GLN	N-CA-C	-5.74	105.16	111.82	15	5
2	B	17	SER	N-CA-C	-5.70	106.03	112.87	8	1
2	B	123	GLU	N-CA-C	-5.69	106.47	113.41	20	8
2	B	138	TRP	N-CA-C	-5.67	106.34	113.20	5	1
2	B	13	GLY	N-CA-C	-5.58	107.61	113.58	5	1
1	A	85	GLN	CA-C-O	5.58	121.84	118.33	7	2
1	A	12	ASN	N-CA-C	-5.57	107.03	113.88	4	1
2	B	85	THR	N-CA-C	-5.56	106.54	113.38	8	4
1	A	25	VAL	N-CA-C	-5.46	104.22	111.05	17	7
2	B	138	TRP	CA-CB-CG	-5.44	103.26	113.60	8	7
2	B	2	ARG	N-CA-C	-5.43	102.49	110.52	3	1
1	A	63	GLU	CB-CA-C	-5.38	109.33	117.07	7	3
1	A	28	ALA	N-CA-C	-5.36	105.84	112.38	13	1
1	A	84	LYS	N-CA-C	-5.33	107.15	113.97	17	1
1	A	29	CYS	N-CA-C	-5.32	106.79	113.28	6	3
2	B	158	PHE	CA-CB-CG	-5.30	108.50	113.80	14	2
2	B	120	LEU	N-CA-C	-5.29	105.48	112.94	15	8
2	B	154	VAL	N-CA-C	-5.24	106.02	111.58	15	1
2	B	19	LEU	N-CA-C	-5.22	105.48	111.07	16	1
1	A	46	ASP	N-CA-C	-5.21	105.63	112.41	10	2
2	B	117	LYS	N-CA-C	-5.16	106.29	112.58	19	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	162	VAL	N-CA-C	-5.15	105.36	110.62	4	1
2	B	53	LEU	CA-C-N	-5.12	115.93	123.00	1	2
2	B	53	LEU	C-N-CA	-5.12	115.93	123.00	1	2
2	B	53	LEU	N-CA-C	5.11	121.67	110.80	10	3
2	B	100	ILE	N-CA-C	-5.10	106.10	110.74	17	1
2	B	129	GLU	N-CA-C	-5.01	105.73	111.14	19	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	A	680	687	687	95±8
2	B	1335	1326	1328	189±14
All	All	40300	40260	40300	5374

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 67.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:161:LEU:HD23	2:B:161:LEU:H	0.95	1.16	6	9
2:B:20:THR:O	2:B:22:GLN:N	0.91	2.04	16	3
1:A:3:ALA:HB1	1:A:19:PHE:O	0.86	1.71	17	15
1:A:35:ARG:NE	1:A:36:ILE:H	0.85	1.70	13	1
2:B:64:PHE:O	2:B:68:ARG:N	0.84	2.10	18	17
2:B:70:LEU:O	2:B:70:LEU:HD22	0.82	1.75	5	1
2:B:90:PHE:CD1	2:B:126:VAL:HG21	0.81	2.10	9	5
2:B:112:ILE:HD12	2:B:142:ALA:O	0.81	1.76	17	6
1:A:16:THR:HG22	2:B:36:ILE:HD12	0.81	1.52	15	8
2:B:59:ALA:O	2:B:61:THR:N	0.81	2.14	6	7
2:B:53:LEU:HD13	2:B:53:LEU:H	0.81	1.33	2	4
1:A:39:ALA:C	1:A:40:LEU:HD12	0.81	2.00	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:90:PHE:CD2	2:B:126:VAL:HG21	0.81	2.11	10	6
2:B:68:ARG:O	2:B:71:TYR:CD2	0.80	2.35	3	2
2:B:111:MET:SD	2:B:112:ILE:N	0.80	2.55	15	5
2:B:161:LEU:N	2:B:161:LEU:HD23	0.80	1.92	16	4
1:A:16:THR:HG22	2:B:36:ILE:HD11	0.80	1.53	19	2
2:B:80:LEU:HD12	2:B:80:LEU:H	0.79	1.37	12	5
2:B:90:PHE:CG	2:B:126:VAL:HG21	0.79	2.12	5	10
2:B:20:THR:HG21	2:B:40:TYR:CE2	0.77	2.14	7	1
2:B:11:SER:O	2:B:14:VAL:HG22	0.77	1.79	13	16
2:B:141:CYS:O	2:B:142:ALA:O	0.77	2.03	6	14
2:B:22:GLN:HE21	2:B:148:ALA:HB1	0.77	1.40	1	2
2:B:119:ASP:O	2:B:120:LEU:HD23	0.77	1.80	18	12
2:B:93:LEU:H	2:B:93:LEU:HD23	0.77	1.40	8	1
2:B:37:GLU:CD	2:B:59:ALA:HB3	0.76	2.06	12	1
2:B:4:TYR:CE2	2:B:162:VAL:HG23	0.76	2.15	4	2
1:A:35:ARG:NE	1:A:35:ARG:H	0.75	1.78	13	1
2:B:58:THR:HG22	2:B:59:ALA:H	0.75	1.41	16	2
1:A:55:ASP:O	1:A:57:LYS:N	0.74	2.20	20	20
2:B:93:LEU:HD23	2:B:93:LEU:N	0.74	1.97	8	1
2:B:154:VAL:O	2:B:157:ILE:HD11	0.74	1.82	20	13
2:B:70:LEU:C	2:B:70:LEU:HD13	0.74	2.06	5	4
1:A:55:ASP:O	1:A:58:LYS:N	0.74	2.17	6	20
2:B:90:PHE:CE2	2:B:134:LEU:HD23	0.74	2.17	7	1
1:A:18:GLN:N	2:B:36:ILE:HD11	0.73	1.97	7	18
2:B:82:TYR:CZ	2:B:93:LEU:HD22	0.73	2.19	8	1
1:A:6:LEU:HD23	1:A:77:ASP:H	0.73	1.41	3	5
2:B:70:LEU:HD12	2:B:71:TYR:N	0.73	1.98	11	1
1:A:14:VAL:HG12	2:B:38:ASP:OD1	0.72	1.83	9	1
2:B:90:PHE:CE1	2:B:134:LEU:HD23	0.72	2.19	13	3
2:B:56:LEU:HD23	2:B:71:TYR:CD2	0.72	2.18	4	1
1:A:9:SER:O	1:A:10:ILE:HD13	0.72	1.83	12	7
2:B:40:TYR:CE1	2:B:55:ILE:HG21	0.72	2.19	6	2
2:B:161:LEU:HD23	2:B:161:LEU:N	0.72	1.98	6	6
2:B:82:TYR:CD1	2:B:90:PHE:CE2	0.72	2.77	20	2
2:B:17:SER:O	2:B:21:VAL:HG23	0.71	1.85	11	10
1:A:15:LYS:NZ	1:A:36:ILE:HD13	0.71	1.99	13	1
2:B:82:TYR:N	2:B:82:TYR:CD2	0.71	2.59	16	4
2:B:112:ILE:HD13	2:B:142:ALA:O	0.71	1.85	19	2
1:A:61:TRP:CD1	1:A:61:TRP:N	0.71	2.58	2	20
2:B:56:LEU:HD23	2:B:71:TYR:CE2	0.71	2.20	4	1
1:A:15:LYS:NZ	2:B:25:GLN:HE22	0.71	1.83	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:76:GLN:O	2:B:165:ILE:HD11	0.71	1.85	3	8
2:B:71:TYR:CD2	2:B:72:MET:N	0.71	2.58	3	2
2:B:7:VAL:HG13	2:B:71:TYR:CZ	0.70	2.21	4	1
2:B:72:MET:O	2:B:104:LYS:NZ	0.70	2.25	10	8
2:B:58:THR:HG21	2:B:64:PHE:CD2	0.70	2.21	14	1
2:B:78:PHE:CD1	2:B:111:MET:SD	0.70	2.84	14	1
2:B:4:TYR:O	2:B:54:GLU:O	0.69	2.10	18	19
2:B:143:PHE:CD2	2:B:144:LEU:N	0.69	2.60	20	1
1:A:17:MET:C	2:B:36:ILE:HD11	0.69	2.12	13	11
2:B:7:VAL:HG21	2:B:78:PHE:CZ	0.69	2.23	6	1
2:B:82:TYR:CZ	2:B:90:PHE:CE1	0.69	2.80	7	1
2:B:7:VAL:HG13	2:B:71:TYR:CE2	0.69	2.23	4	1
2:B:155:ASN:HD22	2:B:155:ASN:H	0.69	1.29	6	1
2:B:58:THR:HG21	2:B:64:PHE:CD1	0.69	2.22	16	1
1:A:5:SER:N	1:A:75:ASN:HD22	0.69	1.86	2	2
2:B:54:GLU:C	2:B:55:ILE:HD12	0.68	2.13	19	3
2:B:82:TYR:CD2	2:B:90:PHE:CD2	0.68	2.81	17	1
2:B:82:TYR:CE1	2:B:90:PHE:CE2	0.68	2.81	15	2
2:B:140:ASN:O	2:B:142:ALA:N	0.68	2.26	18	14
1:A:5:SER:O	1:A:76:GLY:N	0.68	2.26	2	20
2:B:2:ARG:NE	2:B:3:GLU:H	0.68	1.87	6	10
1:A:15:LYS:HZ1	2:B:25:GLN:HE22	0.68	1.31	4	1
2:B:82:TYR:CE2	2:B:90:PHE:CZ	0.68	2.82	6	5
2:B:82:TYR:CZ	2:B:90:PHE:CE2	0.68	2.82	15	3
2:B:56:LEU:HD22	2:B:71:TYR:CG	0.68	2.24	2	4
2:B:22:GLN:NE2	2:B:148:ALA:HB1	0.68	2.04	4	3
2:B:141:CYS:SG	2:B:141:CYS:O	0.68	2.52	17	3
1:A:12:ASN:HD21	2:B:41:ARG:C	0.68	1.97	13	18
2:B:82:TYR:CE1	2:B:90:PHE:CZ	0.67	2.82	20	1
2:B:134:LEU:HD11	2:B:138:TRP:HE1	0.67	1.49	5	20
2:B:141:CYS:O	2:B:141:CYS:SG	0.67	2.52	2	9
2:B:111:MET:CG	2:B:141:CYS:HG	0.67	2.02	18	5
2:B:82:TYR:CD1	2:B:90:PHE:CD2	0.67	2.82	13	2
2:B:134:LEU:HD11	2:B:138:TRP:NE1	0.67	2.04	10	11
2:B:4:TYR:CE2	2:B:52:MET:O	0.67	2.47	2	4
2:B:82:TYR:CE2	2:B:90:PHE:CE1	0.67	2.83	7	2
1:A:20:GLU:O	1:A:23:THR:N	0.66	2.26	8	20
2:B:57:ASP:O	2:B:58:THR:OG1	0.66	2.11	13	3
2:B:119:ASP:C	2:B:120:LEU:HD23	0.66	2.15	19	12
2:B:161:LEU:H	2:B:161:LEU:CD2	0.66	1.99	6	6
1:A:81:TYR:O	1:A:81:TYR:CG	0.66	2.48	9	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:82:TYR:CD2	2:B:90:PHE:CZ	0.66	2.83	16	4
2:B:155:ASN:HD22	2:B:155:ASN:N	0.66	1.89	6	1
2:B:53:LEU:HD13	2:B:53:LEU:N	0.66	2.05	2	2
2:B:111:MET:SD	2:B:141:CYS:SG	0.66	2.94	10	13
2:B:2:ARG:HE	2:B:49:GLN:NE2	0.66	1.88	9	1
2:B:40:TYR:CD1	2:B:55:ILE:HD13	0.66	2.25	19	1
2:B:100:ILE:N	2:B:100:ILE:HD12	0.66	2.06	7	3
1:A:16:THR:N	2:B:38:ASP:CG	0.66	2.54	9	2
2:B:19:LEU:O	2:B:23:PHE:CD2	0.66	2.48	7	1
1:A:18:GLN:OE1	2:B:36:ILE:HD13	0.66	1.90	16	1
2:B:53:LEU:N	2:B:53:LEU:HD23	0.65	2.06	12	4
2:B:82:TYR:CD1	2:B:93:LEU:HD12	0.65	2.26	16	3
1:A:12:ASN:ND2	2:B:41:ARG:CB	0.65	2.60	13	6
1:A:6:LEU:HD12	1:A:6:LEU:H	0.65	1.50	2	5
2:B:53:LEU:H	2:B:53:LEU:CD1	0.65	2.05	2	4
2:B:58:THR:HG22	2:B:59:ALA:N	0.65	2.05	16	2
1:A:27:ASP:O	1:A:30:ARG:N	0.65	2.29	11	20
1:A:18:GLN:NE2	2:B:36:ILE:HG23	0.65	2.07	13	16
1:A:47:PHE:CD2	1:A:81:TYR:CE2	0.65	2.84	8	2
2:B:14:VAL:HG23	2:B:15:GLY:N	0.65	2.06	12	15
1:A:14:VAL:HG12	1:A:14:VAL:O	0.65	1.90	8	3
2:B:93:LEU:H	2:B:93:LEU:CD2	0.65	2.04	8	1
1:A:5:SER:N	1:A:75:ASN:ND2	0.65	2.44	19	2
2:B:2:ARG:NH1	2:B:4:TYR:CZ	0.65	2.65	5	1
2:B:2:ARG:CD	2:B:4:TYR:CE2	0.65	2.79	17	1
2:B:33:ASP:O	2:B:34:PRO:O	0.65	2.15	20	20
1:A:37:PRO:CD	2:B:29:VAL:HG11	0.65	2.22	14	4
2:B:143:PHE:CD1	2:B:144:LEU:N	0.64	2.65	11	2
2:B:155:ASN:ND2	2:B:156:GLU:H	0.64	1.90	6	1
2:B:62:GLU:O	2:B:65:THR:HG23	0.64	1.91	16	10
1:A:47:PHE:CD1	1:A:81:TYR:CE2	0.64	2.85	14	1
2:B:4:TYR:CZ	2:B:162:VAL:HG23	0.64	2.27	17	4
2:B:143:PHE:CG	2:B:144:LEU:N	0.64	2.66	1	3
1:A:12:ASN:O	1:A:12:ASN:CG	0.64	2.40	6	9
2:B:61:THR:O	2:B:64:PHE:CD1	0.64	2.50	15	5
2:B:82:TYR:N	2:B:82:TYR:CD1	0.64	2.66	8	6
2:B:4:TYR:CE2	2:B:51:CYS:CB	0.64	2.81	15	1
2:B:71:TYR:O	2:B:75:GLY:N	0.64	2.30	6	7
1:A:15:LYS:NZ	2:B:25:GLN:NE2	0.64	2.46	2	3
2:B:112:ILE:HD13	2:B:160:ASP:OD2	0.64	1.93	17	2
1:A:19:PHE:CE2	1:A:31:MET:SD	0.64	2.91	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ARG:NE	1:A:36:ILE:N	0.64	2.46	13	1
2:B:164:GLN:NE2	2:B:167:ARG:NH1	0.64	2.46	10	1
2:B:82:TYR:CD2	2:B:82:TYR:N	0.64	2.65	19	2
2:B:82:TYR:CE2	2:B:93:LEU:HD22	0.64	2.28	8	1
2:B:70:LEU:HD12	2:B:70:LEU:C	0.64	2.18	11	1
1:A:4:LEU:HD23	1:A:74:ARG:O	0.63	1.92	1	10
2:B:21:VAL:O	2:B:26:GLY:N	0.63	2.31	6	7
1:A:35:ARG:NE	1:A:35:ARG:N	0.63	2.45	13	1
2:B:2:ARG:HE	2:B:49:GLN:HE22	0.63	1.36	9	1
1:A:61:TRP:CD1	1:A:61:TRP:H	0.63	2.11	11	9
2:B:112:ILE:HD13	2:B:160:ASP:CG	0.63	2.17	4	8
2:B:4:TYR:CD1	2:B:6:LEU:HD21	0.63	2.28	7	2
1:A:51:LEU:HD23	1:A:78:THR:O	0.63	1.93	6	13
2:B:90:PHE:CE1	2:B:134:LEU:HD22	0.63	2.29	1	4
2:B:73:LYS:O	2:B:104:LYS:NZ	0.63	2.32	5	7
2:B:9:LEU:HD23	2:B:97:ARG:NH2	0.63	2.09	9	1
2:B:58:THR:HG21	2:B:64:PHE:CG	0.63	2.29	16	1
1:A:47:PHE:CG	1:A:81:TYR:CZ	0.63	2.87	1	2
1:A:18:GLN:NE2	2:B:63:GLN:NE2	0.63	2.47	12	2
2:B:82:TYR:CE2	2:B:90:PHE:CD1	0.63	2.86	7	1
2:B:155:ASN:ND2	2:B:158:PHE:CZ	0.63	2.66	12	1
2:B:82:TYR:CE2	2:B:90:PHE:CE2	0.63	2.86	17	4
2:B:72:MET:SD	2:B:103:VAL:HG11	0.63	2.34	13	4
1:A:17:MET:SD	1:A:19:PHE:CZ	0.63	2.91	15	2
2:B:64:PHE:CD1	2:B:64:PHE:N	0.63	2.63	17	1
2:B:21:VAL:O	2:B:22:GLN:C	0.63	2.42	7	2
2:B:80:LEU:CD2	2:B:97:ARG:CZ	0.63	2.76	18	1
1:A:47:PHE:CE2	1:A:81:TYR:CD2	0.62	2.87	1	1
2:B:97:ARG:NH1	2:B:138:TRP:CE2	0.62	2.67	5	1
2:B:89:THR:O	2:B:91:ASN:N	0.62	2.32	8	1
2:B:97:ARG:NE	2:B:138:TRP:CE3	0.62	2.67	14	2
1:A:17:MET:HE3	1:A:35:ARG:CZ	0.62	2.23	16	1
2:B:166:ASN:O	2:B:167:ARG:C	0.62	2.43	5	10
1:A:47:PHE:CD1	1:A:81:TYR:CE1	0.62	2.88	6	1
1:A:74:ARG:N	1:A:74:ARG:CD	0.62	2.63	10	1
1:A:35:ARG:N	1:A:35:ARG:HE	0.62	1.92	13	1
2:B:23:PHE:CZ	2:B:155:ASN:ND2	0.62	2.68	19	1
2:B:50:GLN:NE2	2:B:50:GLN:N	0.62	2.47	3	1
2:B:72:MET:SD	2:B:73:LYS:N	0.62	2.72	15	4
2:B:135:ALA:O	2:B:140:ASN:N	0.62	2.32	1	20
2:B:97:ARG:NH1	2:B:138:TRP:CZ3	0.62	2.68	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:THR:HG23	2:B:38:ASP:OD1	0.62	1.94	14	1
2:B:21:VAL:O	2:B:25:GLN:N	0.62	2.30	20	8
1:A:30:ARG:NE	1:A:33:ARG:NH2	0.62	2.47	6	1
1:A:20:GLU:O	1:A:22:SER:N	0.62	2.32	18	20
2:B:100:ILE:N	2:B:100:ILE:CD1	0.62	2.63	14	3
2:B:40:TYR:CD2	2:B:41:ARG:N	0.62	2.68	19	1
2:B:2:ARG:NH1	2:B:76:GLN:HE21	0.61	1.93	6	1
2:B:4:TYR:CE1	2:B:52:MET:O	0.61	2.53	11	5
2:B:71:TYR:C	2:B:71:TYR:CD2	0.61	2.78	15	2
2:B:97:ARG:CZ	2:B:138:TRP:CE3	0.61	2.83	2	2
2:B:4:TYR:O	2:B:4:TYR:CD1	0.61	2.54	10	4
1:A:45:ASN:O	1:A:85:GLN:N	0.61	2.33	3	2
2:B:116:ASN:ND2	2:B:117:LYS:N	0.61	2.47	14	4
1:A:26:TYR:N	1:A:64:ALA:O	0.61	2.32	17	16
2:B:97:ARG:HD2	2:B:97:ARG:N	0.61	2.10	9	1
2:B:1:MET:HE3	2:B:43:GLN:OE1	0.61	1.95	19	1
2:B:4:TYR:CE2	2:B:6:LEU:HD11	0.61	2.30	3	1
2:B:21:VAL:O	2:B:27:ILE:N	0.61	2.25	15	1
1:A:11:GLY:O	1:A:13:VAL:N	0.61	2.34	8	6
2:B:97:ARG:NH1	2:B:138:TRP:NE1	0.61	2.49	5	1
1:A:81:TYR:CD2	1:A:81:TYR:O	0.61	2.54	15	3
2:B:97:ARG:NH1	2:B:141:CYS:SG	0.61	2.74	3	1
1:A:50:PHE:CD2	1:A:82:ARG:NH2	0.61	2.69	11	1
2:B:57:ASP:CG	2:B:58:THR:N	0.61	2.59	11	4
1:A:12:ASN:ND2	2:B:41:ARG:O	0.61	2.34	13	14
2:B:143:PHE:N	2:B:143:PHE:CD2	0.60	2.69	15	8
2:B:97:ARG:NE	2:B:97:ARG:CA	0.60	2.64	18	1
2:B:16:LYS:CD	2:B:16:LYS:H	0.60	2.08	11	7
2:B:2:ARG:NH1	2:B:49:GLN:NE2	0.60	2.49	3	1
2:B:116:ASN:ND2	2:B:117:LYS:H	0.60	1.95	3	4
2:B:55:ILE:HD12	2:B:55:ILE:N	0.60	2.10	19	3
2:B:155:ASN:H	2:B:155:ASN:ND2	0.60	1.92	6	1
2:B:82:TYR:CD2	2:B:93:LEU:HD12	0.60	2.31	9	1
1:A:30:ARG:HE	1:A:33:ARG:HH11	0.60	1.39	12	1
2:B:19:LEU:N	2:B:19:LEU:HD12	0.60	2.10	15	1
2:B:49:GLN:NE2	2:B:51:CYS:SG	0.60	2.75	9	1
1:A:50:PHE:CG	1:A:60:ILE:O	0.60	2.54	15	16
2:B:81:VAL:C	2:B:82:TYR:CD1	0.60	2.80	8	1
1:A:8:ILE:N	1:A:8:ILE:HD12	0.60	2.11	19	3
2:B:67:MET:O	2:B:71:TYR:N	0.60	2.29	14	3
2:B:97:ARG:NH2	2:B:138:TRP:CE3	0.60	2.70	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:128:LYS:O	2:B:132:GLN:N	0.60	2.33	3	19
2:B:5:LYS:NZ	2:B:76:GLN:NE2	0.60	2.49	5	2
2:B:163:ARG:NH1	2:B:166:ASN:ND2	0.60	2.49	5	1
2:B:1:MET:CB	2:B:50:GLN:O	0.60	2.49	10	3
2:B:78:PHE:CG	2:B:80:LEU:HD11	0.60	2.31	10	1
2:B:22:GLN:HE21	2:B:28:PHE:N	0.60	1.95	13	1
2:B:2:ARG:HH12	2:B:49:GLN:NE2	0.60	1.93	3	1
2:B:71:TYR:CD1	2:B:72:MET:N	0.60	2.70	20	1
2:B:53:LEU:H	2:B:53:LEU:HD12	0.59	1.57	1	1
2:B:44:VAL:HG21	2:B:158:PHE:CE2	0.59	2.32	11	1
2:B:2:ARG:HH12	2:B:49:GLN:HE22	0.59	1.41	3	1
1:A:20:GLU:N	1:A:23:THR:OG1	0.59	2.36	14	19
1:A:47:PHE:CE2	1:A:81:TYR:CE2	0.59	2.89	1	2
2:B:82:TYR:CZ	2:B:115:GLY:CA	0.59	2.86	13	8
2:B:68:ARG:HE	2:B:99:GLN:NE2	0.59	1.94	10	1
2:B:53:LEU:HD23	2:B:53:LEU:H	0.59	1.56	12	1
2:B:7:VAL:CG1	2:B:71:TYR:CE1	0.59	2.86	14	1
1:A:2:VAL:O	1:A:3:ALA:HB2	0.59	1.98	13	16
2:B:4:TYR:CE2	2:B:51:CYS:SG	0.59	2.96	15	1
2:B:37:GLU:OE2	2:B:56:LEU:HD11	0.59	1.96	20	1
2:B:57:ASP:OD2	2:B:58:THR:N	0.59	2.36	7	5
1:A:16:THR:O	1:A:17:MET:O	0.59	2.20	3	1
2:B:120:LEU:O	2:B:123:GLU:N	0.59	2.31	2	10
2:B:143:PHE:CD1	2:B:143:PHE:C	0.59	2.81	1	2
2:B:22:GLN:O	2:B:26:GLY:N	0.59	2.35	7	5
2:B:57:ASP:OD1	2:B:58:THR:N	0.59	2.35	11	3
2:B:97:ARG:CZ	2:B:111:MET:HE3	0.59	2.27	14	1
2:B:56:LEU:HD21	2:B:71:TYR:CG	0.59	2.33	18	1
2:B:4:TYR:CD2	2:B:52:MET:O	0.59	2.55	13	4
1:A:18:GLN:HE21	2:B:63:GLN:NE2	0.59	1.96	15	2
1:A:4:LEU:N	1:A:19:PHE:O	0.59	2.35	19	3
1:A:37:PRO:HA	1:A:40:LEU:HD13	0.59	1.75	3	3
2:B:50:GLN:N	2:B:50:GLN:HE21	0.59	1.96	3	1
2:B:82:TYR:OH	2:B:113:LEU:HD12	0.59	1.98	19	3
1:A:26:TYR:HB2	1:A:64:ALA:HB1	0.58	1.75	14	16
2:B:20:THR:O	2:B:24:VAL:HG12	0.58	1.97	5	4
2:B:37:GLU:CD	2:B:64:PHE:CE2	0.58	2.81	5	1
2:B:47:ASP:O	2:B:48:ALA:HB3	0.58	1.99	20	20
2:B:6:LEU:N	2:B:6:LEU:CD2	0.58	2.65	5	6
1:A:12:ASN:OD1	1:A:12:ASN:O	0.58	2.21	7	4
1:A:3:ALA:N	2:B:63:GLN:NE2	0.58	2.51	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:40:TYR:CE2	2:B:57:ASP:OD1	0.58	2.56	15	1
2:B:40:TYR:CZ	2:B:57:ASP:CG	0.58	2.81	15	1
1:A:5:SER:H	1:A:75:ASN:ND2	0.58	1.95	19	1
2:B:6:LEU:N	2:B:6:LEU:HD23	0.58	2.13	1	8
1:A:3:ALA:N	2:B:63:GLN:HE22	0.58	1.96	6	2
2:B:21:VAL:CG1	2:B:27:ILE:O	0.58	2.51	14	1
1:A:50:PHE:CD2	1:A:60:ILE:O	0.58	2.57	13	9
2:B:35:THR:O	2:B:59:ALA:HB3	0.58	1.99	1	2
2:B:41:ARG:HA	2:B:53:LEU:O	0.58	1.98	4	15
1:A:62:LEU:CD2	1:A:71:TYR:CE1	0.58	2.87	15	5
2:B:75:GLY:O	2:B:76:GLN:C	0.58	2.47	16	10
2:B:82:TYR:CE2	2:B:114:VAL:O	0.58	2.57	5	4
1:A:51:LEU:HD11	1:A:73:LEU:HD21	0.58	1.74	18	7
2:B:61:THR:O	2:B:64:PHE:CD2	0.58	2.56	4	2
2:B:113:LEU:CD1	2:B:138:TRP:CZ3	0.58	2.86	12	1
2:B:4:TYR:CZ	2:B:51:CYS:SG	0.58	2.96	15	1
1:A:74:ARG:O	1:A:75:ASN:ND2	0.58	2.36	18	8
2:B:123:GLU:O	2:B:124:ARG:O	0.58	2.22	10	20
1:A:46:ASP:O	1:A:47:PHE:CD2	0.58	2.57	3	3
1:A:12:ASN:ND2	2:B:41:ARG:HB3	0.58	2.14	13	6
1:A:81:TYR:O	1:A:81:TYR:CD1	0.58	2.57	13	6
2:B:21:VAL:O	2:B:24:VAL:N	0.58	2.37	20	2
2:B:37:GLU:N	2:B:37:GLU:OE1	0.58	2.37	8	2
2:B:2:ARG:HH22	2:B:76:GLN:NE2	0.58	1.97	15	1
2:B:116:ASN:HD21	2:B:148:ALA:N	0.58	1.97	1	5
1:A:10:ILE:HD11	1:A:35:ARG:HH12	0.58	1.58	4	1
2:B:58:THR:OG1	2:B:64:PHE:CD2	0.58	2.54	6	2
1:A:18:GLN:HE21	2:B:63:GLN:HE21	0.57	1.42	15	2
2:B:56:LEU:HD21	2:B:71:TYR:CD1	0.57	2.34	18	1
1:A:47:PHE:CD2	1:A:81:TYR:CZ	0.57	2.92	8	3
2:B:130:GLN:O	2:B:134:LEU:N	0.57	2.37	19	17
1:A:62:LEU:CD2	1:A:71:TYR:CE2	0.57	2.87	18	8
2:B:5:LYS:NZ	2:B:76:GLN:HE21	0.57	1.97	10	1
2:B:71:TYR:CD1	2:B:71:TYR:C	0.57	2.82	20	2
2:B:123:GLU:O	2:B:124:ARG:C	0.57	2.47	15	20
2:B:97:ARG:N	2:B:97:ARG:CD	0.57	2.66	9	1
1:A:36:ILE:HD11	2:B:21:VAL:CG2	0.57	2.28	19	1
2:B:22:GLN:N	2:B:22:GLN:OE1	0.57	2.35	20	1
2:B:37:GLU:CG	2:B:56:LEU:HD11	0.57	2.30	16	5
2:B:56:LEU:O	2:B:71:TYR:OH	0.57	2.22	4	1
1:A:74:ARG:O	1:A:75:ASN:CG	0.57	2.47	2	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:164:GLN:C	2:B:166:ASN:N	0.57	2.61	19	11
1:A:67:ALA:O	1:A:70:TYR:N	0.57	2.33	1	20
1:A:15:LYS:NZ	2:B:21:VAL:HG22	0.57	2.15	10	1
2:B:9:LEU:HD13	2:B:71:TYR:CE1	0.57	2.35	10	1
2:B:136:ARG:O	2:B:139:ASN:N	0.57	2.37	13	20
1:A:33:ARG:NH1	1:A:47:PHE:CG	0.57	2.73	10	1
1:A:68:LEU:O	1:A:70:TYR:N	0.57	2.38	5	20
2:B:147:SER:O	2:B:151:LYS:N	0.57	2.38	14	20
1:A:33:ARG:HH11	1:A:47:PHE:CB	0.57	2.13	10	1
1:A:10:ILE:O	1:A:12:ASN:N	0.57	2.38	19	2
2:B:68:ARG:CZ	2:B:99:GLN:NE2	0.57	2.68	20	2
2:B:82:TYR:CE1	2:B:114:VAL:O	0.57	2.57	2	7
2:B:141:CYS:O	2:B:142:ALA:HB2	0.57	2.00	5	6
2:B:116:ASN:OD1	2:B:117:LYS:N	0.57	2.37	17	2
2:B:2:ARG:HE	2:B:3:GLU:H	0.57	1.42	6	1
2:B:17:SER:O	2:B:21:VAL:HG13	0.57	2.00	8	1
2:B:61:THR:O	2:B:64:PHE:CG	0.57	2.57	18	1
2:B:140:ASN:C	2:B:142:ALA:H	0.57	2.05	2	14
2:B:2:ARG:NH1	2:B:76:GLN:NE2	0.57	2.53	16	2
2:B:68:ARG:O	2:B:72:MET:SD	0.57	2.63	6	1
2:B:19:LEU:O	2:B:23:PHE:CG	0.57	2.58	7	1
2:B:61:THR:OG1	2:B:64:PHE:CE2	0.57	2.56	17	1
2:B:167:ARG:N	2:B:167:ARG:CD	0.57	2.67	18	1
1:A:50:PHE:CD1	1:A:60:ILE:O	0.56	2.58	20	10
2:B:126:VAL:HG13	2:B:126:VAL:O	0.56	1.99	19	12
1:A:6:LEU:O	1:A:16:THR:HG23	0.56	2.00	5	3
1:A:19:PHE:CE1	1:A:28:ALA:HB1	0.56	2.35	9	1
2:B:80:LEU:HD11	2:B:111:MET:SD	0.56	2.40	14	1
2:B:116:ASN:CG	2:B:117:LYS:H	0.56	2.08	5	18
2:B:53:LEU:HD12	2:B:53:LEU:C	0.56	2.25	3	2
2:B:71:TYR:N	2:B:71:TYR:CD2	0.56	2.68	7	1
1:A:63:GLU:N	1:A:63:GLU:CD	0.56	2.62	20	2
2:B:2:ARG:NH2	2:B:165:ILE:CG2	0.56	2.68	9	1
1:A:81:TYR:O	1:A:81:TYR:CD2	0.56	2.58	10	2
1:A:4:LEU:HD23	1:A:74:ARG:C	0.56	2.25	17	16
1:A:5:SER:CB	1:A:75:ASN:HD22	0.56	2.13	2	2
2:B:64:PHE:CD1	2:B:64:PHE:C	0.56	2.82	2	5
2:B:82:TYR:CE2	2:B:114:VAL:C	0.56	2.83	13	4
1:A:12:ASN:C	1:A:13:VAL:HG12	0.56	2.25	6	1
2:B:21:VAL:HG12	2:B:27:ILE:O	0.56	1.99	9	4
1:A:85:GLN:CG	1:A:86:ARG:H	0.56	2.13	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:143:PHE:CD2	2:B:143:PHE:C	0.56	2.83	20	1
2:B:40:TYR:CD1	2:B:40:TYR:N	0.56	2.73	11	2
2:B:155:ASN:ND2	2:B:156:GLU:N	0.56	2.53	6	1
1:A:30:ARG:HE	1:A:33:ARG:NH1	0.56	1.98	12	1
2:B:143:PHE:O	2:B:144:LEU:HD22	0.56	2.01	16	3
2:B:40:TYR:CE2	2:B:55:ILE:HG21	0.56	2.35	16	1
1:A:17:MET:SD	1:A:19:PHE:CE2	0.56	2.98	11	3
2:B:143:PHE:CE1	2:B:144:LEU:C	0.56	2.83	1	2
2:B:74:ASN:ND2	2:B:76:GLN:H	0.56	1.97	19	2
1:A:35:ARG:C	2:B:31:LYS:HZ3	0.56	2.07	13	1
1:A:35:ARG:NH2	1:A:39:ALA:HB2	0.56	2.16	20	1
1:A:68:LEU:C	1:A:70:TYR:N	0.56	2.63	2	20
1:A:84:LYS:O	1:A:85:GLN:C	0.56	2.48	1	3
2:B:47:ASP:O	2:B:48:ALA:CB	0.56	2.53	9	20
1:A:35:ARG:CD	1:A:36:ILE:H	0.56	2.14	13	1
1:A:18:GLN:NE2	2:B:63:GLN:OE1	0.56	2.39	13	4
2:B:82:TYR:CE1	2:B:114:VAL:C	0.56	2.84	17	7
1:A:53:ASP:OD1	1:A:54:ASP:N	0.56	2.38	11	6
1:A:12:ASN:OD1	2:B:24:VAL:HG13	0.56	2.00	15	3
1:A:47:PHE:CD1	1:A:47:PHE:C	0.56	2.83	20	4
2:B:128:LYS:HZ1	2:B:145:GLU:CD	0.56	2.09	12	1
1:A:74:ARG:NH2	1:A:75:ASN:O	0.56	2.39	13	1
2:B:64:PHE:O	2:B:67:MET:N	0.56	2.39	17	2
2:B:17:SER:O	2:B:20:THR:N	0.56	2.38	16	8
2:B:62:GLU:O	2:B:65:THR:OG1	0.56	2.24	8	7
2:B:113:LEU:CD2	2:B:131:GLY:O	0.56	2.53	4	14
2:B:116:ASN:CG	2:B:117:LYS:N	0.56	2.64	5	19
2:B:147:SER:C	2:B:149:LYS:H	0.56	2.09	3	20
1:A:75:ASN:ND2	2:B:63:GLN:HE22	0.56	1.99	2	1
2:B:64:PHE:CD2	2:B:64:PHE:C	0.56	2.84	4	1
1:A:36:ILE:HD12	2:B:25:GLN:HE22	0.56	1.61	10	1
2:B:14:VAL:CG2	2:B:16:LYS:NZ	0.56	2.68	13	1
1:A:4:LEU:O	2:B:63:GLN:NE2	0.56	2.39	16	1
2:B:104:LYS:O	2:B:105:ASP:CB	0.56	2.54	2	19
2:B:37:GLU:CD	2:B:37:GLU:H	0.56	2.09	9	2
1:A:80:GLU:CD	1:A:82:ARG:HH11	0.56	2.09	6	1
2:B:78:PHE:CD2	2:B:80:LEU:HD11	0.56	2.35	10	1
1:A:16:THR:O	1:A:17:MET:CB	0.55	2.53	2	1
1:A:12:ASN:O	2:B:41:ARG:NE	0.55	2.39	14	3
2:B:143:PHE:CE2	2:B:144:LEU:C	0.55	2.83	20	1
1:A:7:LYS:O	1:A:9:SER:N	0.55	2.39	3	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ASP:OD2	1:A:54:ASP:N	0.55	2.39	16	4
2:B:17:SER:O	2:B:21:VAL:CG2	0.55	2.55	5	4
2:B:7:VAL:HG11	2:B:71:TYR:CD1	0.55	2.36	11	1
2:B:3:GLU:O	2:B:76:GLN:NE2	0.55	2.39	15	2
2:B:100:ILE:O	2:B:103:VAL:N	0.55	2.39	9	10
1:A:24:MET:O	1:A:27:ASP:N	0.55	2.40	6	17
2:B:83:SER:OG	2:B:86:ALA:N	0.55	2.40	7	5
1:A:25:VAL:O	1:A:29:CYS:SG	0.55	2.65	17	9
2:B:41:ARG:CB	2:B:53:LEU:O	0.55	2.54	20	8
2:B:141:CYS:O	2:B:142:ALA:CB	0.55	2.54	7	6
2:B:53:LEU:H	2:B:53:LEU:CD2	0.55	2.14	12	1
2:B:35:THR:HB	2:B:59:ALA:HB3	0.55	1.78	14	2
2:B:97:ARG:NH2	2:B:111:MET:HE3	0.55	2.17	14	2
1:A:16:THR:N	2:B:38:ASP:OD1	0.55	2.40	15	9
2:B:153:ASN:O	2:B:157:ILE:HD11	0.55	2.01	12	5
2:B:22:GLN:OE1	2:B:22:GLN:N	0.55	2.40	4	3
1:A:10:ILE:O	1:A:11:GLY:C	0.55	2.49	6	4
2:B:16:LYS:NZ	2:B:40:TYR:OH	0.55	2.39	9	1
1:A:13:VAL:HG11	1:A:15:LYS:HZ3	0.55	1.61	18	1
1:A:5:SER:H	1:A:75:ASN:HD22	0.55	1.41	19	1
2:B:147:SER:C	2:B:149:LYS:N	0.55	2.64	10	20
2:B:56:LEU:HD22	2:B:71:TYR:CD1	0.55	2.37	13	4
2:B:89:THR:O	2:B:92:ASP:N	0.55	2.38	5	15
2:B:16:LYS:O	2:B:19:LEU:N	0.55	2.40	8	2
2:B:38:ASP:N	2:B:57:ASP:OD1	0.55	2.38	7	2
2:B:35:THR:O	2:B:58:THR:HG22	0.55	2.00	13	1
1:A:36:ILE:HG23	1:A:36:ILE:O	0.55	2.01	2	1
2:B:57:ASP:N	2:B:57:ASP:OD2	0.55	2.40	12	2
2:B:93:LEU:O	2:B:97:ARG:NH2	0.55	2.40	18	1
1:A:20:GLU:O	1:A:23:THR:OG1	0.55	2.25	13	20
2:B:127:GLY:C	2:B:129:GLU:N	0.55	2.64	16	17
2:B:127:GLY:O	2:B:131:GLY:N	0.55	2.27	19	10
2:B:70:LEU:HD13	2:B:71:TYR:N	0.55	2.16	5	1
2:B:40:TYR:CZ	2:B:55:ILE:HG21	0.55	2.36	12	3
2:B:154:VAL:O	2:B:157:ILE:CD1	0.55	2.54	20	11
2:B:111:MET:CG	2:B:141:CYS:SG	0.55	2.95	16	7
2:B:124:ARG:C	2:B:124:ARG:NE	0.55	2.65	13	4
2:B:94:GLN:O	2:B:97:ARG:NH2	0.55	2.39	4	1
2:B:160:ASP:CG	2:B:161:LEU:N	0.55	2.65	4	2
1:A:26:TYR:O	1:A:26:TYR:CD2	0.55	2.60	5	3
2:B:37:GLU:CD	2:B:57:ASP:O	0.55	2.49	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:82:TYR:CE1	2:B:93:LEU:HD13	0.55	2.37	8	1
2:B:2:ARG:NH2	2:B:165:ILE:HG21	0.55	2.16	16	2
2:B:49:GLN:O	2:B:51:CYS:SG	0.54	2.65	15	16
2:B:97:ARG:O	2:B:100:ILE:N	0.54	2.40	18	19
2:B:70:LEU:HD13	2:B:70:LEU:O	0.54	2.02	14	2
2:B:37:GLU:CB	2:B:64:PHE:CZ	0.54	2.89	5	1
2:B:20:THR:HG21	2:B:40:TYR:CD1	0.54	2.38	8	2
2:B:49:GLN:CD	2:B:51:CYS:SG	0.54	2.91	9	1
2:B:21:VAL:C	2:B:23:PHE:N	0.54	2.64	10	4
2:B:68:ARG:NH1	2:B:99:GLN:CD	0.54	2.66	20	2
2:B:138:TRP:O	2:B:139:ASN:CB	0.54	2.56	11	20
2:B:2:ARG:NH2	2:B:162:VAL:CG2	0.54	2.70	3	1
1:A:32:ILE:O	1:A:34:GLU:N	0.54	2.40	20	2
2:B:82:TYR:CE1	2:B:90:PHE:CD2	0.54	2.95	15	1
1:A:55:ASP:C	1:A:57:LYS:H	0.54	2.10	3	20
2:B:18:ALA:O	2:B:22:GLN:NE2	0.54	2.41	17	5
2:B:7:VAL:CG1	2:B:71:TYR:O	0.54	2.55	5	1
2:B:53:LEU:N	2:B:53:LEU:CD2	0.54	2.71	6	4
2:B:23:PHE:CE2	2:B:154:VAL:HG22	0.54	2.37	7	1
2:B:75:GLY:O	2:B:78:PHE:CE2	0.54	2.61	16	1
2:B:124:ARG:NH2	2:B:130:GLN:HE21	0.54	2.01	16	1
1:A:46:ASP:OD2	1:A:47:PHE:CD2	0.54	2.60	18	1
2:B:4:TYR:OH	2:B:162:VAL:N	0.54	2.40	5	2
2:B:22:GLN:NE2	2:B:148:ALA:C	0.54	2.65	7	1
2:B:74:ASN:ND2	2:B:74:ASN:C	0.54	2.65	19	1
2:B:140:ASN:O	2:B:140:ASN:ND2	0.54	2.40	3	2
2:B:4:TYR:CD1	2:B:52:MET:O	0.54	2.60	12	4
1:A:85:GLN:CG	1:A:86:ARG:N	0.54	2.70	14	2
2:B:19:LEU:HD21	2:B:116:ASN:HB2	0.54	1.77	19	1
2:B:97:ARG:NH2	2:B:138:TRP:CE2	0.54	2.75	20	1
1:A:14:VAL:O	1:A:16:THR:N	0.54	2.41	19	6
2:B:46:VAL:O	2:B:49:GLN:NE2	0.54	2.40	3	2
2:B:36:ILE:O	2:B:38:ASP:OD2	0.54	2.25	15	8
2:B:155:ASN:O	2:B:158:PHE:CE2	0.54	2.60	7	2
1:A:15:LYS:NZ	2:B:25:GLN:OE1	0.54	2.41	8	2
2:B:161:LEU:O	2:B:165:ILE:N	0.54	2.36	20	4
2:B:4:TYR:CG	2:B:4:TYR:O	0.54	2.60	13	1
2:B:64:PHE:CD1	2:B:65:THR:N	0.54	2.76	20	3
1:A:26:TYR:O	1:A:26:TYR:CD1	0.54	2.61	13	5
1:A:39:ALA:O	1:A:41:ALA:N	0.54	2.39	13	14
1:A:48:GLY:N	1:A:82:ARG:O	0.54	2.40	10	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:38:ASP:OD1	2:B:38:ASP:N	0.54	2.40	20	2
2:B:100:ILE:HG22	2:B:104:LYS:HG3	0.54	1.79	1	8
2:B:164:GLN:O	2:B:166:ASN:N	0.54	2.41	13	6
2:B:5:LYS:NZ	2:B:76:GLN:CD	0.54	2.66	6	1
2:B:111:MET:CE	2:B:141:CYS:SG	0.54	2.96	7	2
1:A:35:ARG:HE	1:A:36:ILE:N	0.54	1.98	13	1
2:B:82:TYR:CE2	2:B:90:PHE:CD2	0.54	2.96	17	1
2:B:111:MET:C	2:B:161:LEU:HD21	0.54	2.27	19	1
1:A:55:ASP:C	1:A:57:LYS:N	0.54	2.66	6	19
2:B:39:SER:CB	2:B:55:ILE:O	0.54	2.56	2	10
2:B:146:SER:OG	2:B:147:SER:N	0.54	2.39	13	5
2:B:37:GLU:OE2	2:B:64:PHE:CZ	0.54	2.60	3	1
2:B:80:LEU:CD1	2:B:111:MET:HE2	0.54	2.33	5	1
2:B:68:ARG:NH2	2:B:99:GLN:OE1	0.54	2.41	9	2
1:A:16:THR:N	2:B:38:ASP:OD2	0.54	2.41	3	2
1:A:33:ARG:O	1:A:40:LEU:HD22	0.54	2.02	19	10
1:A:47:PHE:CD2	1:A:47:PHE:C	0.54	2.84	1	1
1:A:68:LEU:C	1:A:70:TYR:H	0.54	2.11	19	20
2:B:74:ASN:O	2:B:75:GLY:C	0.54	2.51	16	20
2:B:17:SER:O	2:B:21:VAL:N	0.54	2.40	19	6
2:B:22:GLN:NE2	2:B:28:PHE:CD2	0.54	2.76	8	1
2:B:50:GLN:N	2:B:50:GLN:OE1	0.54	2.41	11	4
1:A:15:LYS:HZ1	1:A:36:ILE:HD13	0.54	1.61	13	1
2:B:75:GLY:O	2:B:77:GLY:N	0.54	2.41	16	1
2:B:156:GLU:N	2:B:156:GLU:CD	0.54	2.66	10	3
2:B:70:LEU:C	2:B:70:LEU:CD1	0.54	2.78	5	5
2:B:19:LEU:HD21	2:B:116:ASN:CG	0.54	2.27	5	2
2:B:30:GLU:OE2	2:B:31:LYS:N	0.54	2.41	5	2
1:A:77:ASP:OD2	1:A:78:THR:N	0.54	2.41	20	6
2:B:158:PHE:CD1	2:B:158:PHE:C	0.54	2.86	10	4
1:A:32:ILE:O	1:A:35:ARG:NH2	0.54	2.41	13	1
2:B:38:ASP:O	2:B:57:ASP:OD1	0.54	2.25	15	2
2:B:2:ARG:HE	2:B:3:GLU:C	0.54	2.11	16	2
2:B:72:MET:CG	2:B:99:GLN:HE22	0.54	2.16	17	1
2:B:121:GLU:C	2:B:123:GLU:N	0.53	2.63	14	17
2:B:153:ASN:ND2	2:B:156:GLU:OE1	0.53	2.41	16	3
2:B:161:LEU:O	2:B:164:GLN:N	0.53	2.41	6	9
1:A:33:ARG:NH2	1:A:39:ALA:O	0.53	2.41	20	2
1:A:39:ALA:O	1:A:47:PHE:CZ	0.53	2.61	18	1
2:B:53:LEU:HD12	2:B:53:LEU:N	0.53	2.17	1	1
2:B:120:LEU:C	2:B:122:ASP:N	0.53	2.65	3	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ASN:O	1:A:84:LYS:CB	0.53	2.57	3	2
2:B:37:GLU:CD	2:B:56:LEU:HD11	0.53	2.28	16	5
2:B:21:VAL:HG22	2:B:25:GLN:NE2	0.53	2.18	14	2
1:A:50:PHE:CD1	1:A:82:ARG:NH2	0.53	2.77	17	1
2:B:116:ASN:ND2	2:B:147:SER:N	0.53	2.56	1	4
2:B:32:TYR:O	2:B:32:TYR:CD1	0.53	2.62	14	4
2:B:164:GLN:O	2:B:164:GLN:NE2	0.53	2.41	4	1
2:B:164:GLN:O	2:B:167:ARG:N	0.53	2.41	5	7
2:B:155:ASN:HD22	2:B:156:GLU:H	0.53	1.47	6	1
1:A:15:LYS:C	2:B:38:ASP:OD2	0.53	2.52	14	1
1:A:4:LEU:O	1:A:18:GLN:HG3	0.53	2.04	1	14
2:B:155:ASN:O	2:B:158:PHE:CD1	0.53	2.62	1	1
2:B:156:GLU:N	2:B:156:GLU:OE1	0.53	2.41	13	3
2:B:28:PHE:O	2:B:28:PHE:CD2	0.53	2.61	2	1
2:B:163:ARG:O	2:B:167:ARG:NH2	0.53	2.41	20	3
2:B:28:PHE:CD1	2:B:28:PHE:O	0.53	2.61	5	3
2:B:46:VAL:HG11	2:B:162:VAL:HG11	0.53	1.79	5	1
2:B:23:PHE:CD2	2:B:154:VAL:HG13	0.53	2.39	7	1
2:B:157:ILE:O	2:B:160:ASP:N	0.53	2.40	8	3
1:A:74:ARG:C	1:A:75:ASN:ND2	0.53	2.66	15	3
2:B:97:ARG:NH1	2:B:101:LEU:CD1	0.53	2.71	13	1
2:B:166:ASN:N	2:B:166:ASN:ND2	0.53	2.57	14	1
2:B:68:ARG:NH1	2:B:99:GLN:NE2	0.53	2.57	20	1
1:A:47:PHE:CZ	1:A:81:TYR:CE2	0.53	2.97	1	1
2:B:117:LYS:C	2:B:119:ASP:N	0.53	2.66	11	13
1:A:16:THR:HB	2:B:36:ILE:HD12	0.53	1.79	2	1
1:A:15:LYS:O	1:A:17:MET:N	0.53	2.41	3	1
2:B:37:GLU:OE2	2:B:64:PHE:CE2	0.53	2.61	3	1
2:B:67:MET:O	2:B:70:LEU:N	0.53	2.42	10	2
1:A:19:PHE:CE2	1:A:28:ALA:HB1	0.53	2.39	18	2
2:B:22:GLN:CD	2:B:22:GLN:H	0.53	2.12	10	1
2:B:9:LEU:CD2	2:B:97:ARG:NH1	0.53	2.72	18	1
1:A:38:GLU:OE1	2:B:25:GLN:NE2	0.53	2.42	20	1
1:A:8:ILE:N	1:A:8:ILE:CD1	0.53	2.71	1	4
2:B:126:VAL:HG23	2:B:130:GLN:HB2	0.53	1.80	4	10
2:B:147:SER:O	2:B:149:LYS:N	0.53	2.42	19	16
1:A:18:GLN:HE21	2:B:63:GLN:CD	0.53	2.12	4	4
2:B:128:LYS:NZ	2:B:145:GLU:CD	0.53	2.66	12	1
2:B:61:THR:O	2:B:63:GLN:N	0.53	2.41	13	1
2:B:2:ARG:HH21	2:B:2:ARG:HG3	0.53	1.63	16	1
1:A:26:TYR:CE2	1:A:27:ASP:OD2	0.53	2.62	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:116:ASN:HD21	2:B:148:ALA:H	0.53	1.47	4	5
2:B:162:VAL:O	2:B:166:ASN:ND2	0.53	2.42	14	6
2:B:4:TYR:O	2:B:4:TYR:CG	0.53	2.62	11	4
2:B:156:GLU:O	2:B:160:ASP:N	0.53	2.42	8	3
1:A:40:LEU:O	1:A:42:GLY:N	0.53	2.40	18	3
2:B:82:TYR:CD2	2:B:90:PHE:CE2	0.53	2.97	6	3
1:A:66:LYS:NZ	1:A:70:TYR:CD1	0.53	2.67	13	2
1:A:39:ALA:O	1:A:47:PHE:CE2	0.53	2.62	16	2
2:B:97:ARG:HH12	2:B:113:LEU:CD1	0.53	2.16	17	1
2:B:36:ILE:CG1	2:B:37:GLU:N	0.53	2.71	19	1
1:A:15:LYS:NZ	2:B:20:THR:OG1	0.53	2.42	1	1
2:B:158:PHE:C	2:B:158:PHE:CD2	0.53	2.86	2	4
1:A:12:ASN:OD1	2:B:24:VAL:CG2	0.53	2.56	5	5
1:A:29:CYS:SG	1:A:49:LEU:HD12	0.53	2.43	2	6
1:A:77:ASP:OD1	1:A:78:THR:N	0.53	2.41	17	6
1:A:6:LEU:HD23	1:A:77:ASP:N	0.53	2.18	3	1
2:B:16:LYS:HZ3	2:B:16:LYS:HB2	0.53	1.64	7	1
2:B:58:THR:OG1	2:B:64:PHE:CE2	0.53	2.61	9	1
2:B:58:THR:OG1	2:B:64:PHE:CZ	0.53	2.60	9	1
2:B:44:VAL:HG21	2:B:158:PHE:CZ	0.53	2.39	11	1
1:A:33:ARG:NH1	1:A:43:PRO:C	0.53	2.67	13	1
2:B:78:PHE:CG	2:B:111:MET:SD	0.53	3.02	14	1
1:A:26:TYR:CE2	1:A:27:ASP:OD1	0.53	2.62	17	1
1:A:4:LEU:O	1:A:18:GLN:CG	0.53	2.57	1	18
1:A:38:GLU:OE2	2:B:25:GLN:NE2	0.53	2.42	1	1
2:B:28:PHE:O	2:B:28:PHE:CG	0.53	2.62	5	5
2:B:54:GLU:N	2:B:54:GLU:CD	0.53	2.67	1	1
1:A:26:TYR:CE1	1:A:27:ASP:OD2	0.53	2.62	18	3
2:B:16:LYS:NZ	2:B:57:ASP:OD2	0.53	2.42	9	1
2:B:38:ASP:N	2:B:57:ASP:OD2	0.53	2.39	11	1
1:A:47:PHE:C	1:A:47:PHE:CD2	0.53	2.85	15	1
2:B:4:TYR:OH	2:B:51:CYS:SG	0.53	2.66	15	1
2:B:80:LEU:O	2:B:82:TYR:CZ	0.53	2.62	16	1
2:B:3:GLU:OE2	2:B:5:LYS:NZ	0.53	2.42	20	1
1:A:5:SER:OG	2:B:36:ILE:HG21	0.53	2.04	10	7
2:B:116:ASN:HD22	2:B:146:SER:CB	0.53	2.17	12	7
1:A:60:ILE:CD1	1:A:71:TYR:CZ	0.53	2.92	3	12
1:A:36:ILE:CG2	1:A:36:ILE:O	0.53	2.57	3	1
2:B:97:ARG:NH1	2:B:138:TRP:CD1	0.53	2.76	5	2
2:B:7:VAL:HG21	2:B:78:PHE:CE1	0.53	2.39	19	3
2:B:144:LEU:HD13	2:B:153:ASN:HD21	0.53	1.64	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:30:GLU:OE1	2:B:31:LYS:N	0.52	2.41	8	3
2:B:7:VAL:HG22	2:B:71:TYR:CE2	0.52	2.39	4	1
2:B:84:ILE:HD13	2:B:84:ILE:N	0.52	2.19	14	2
2:B:67:MET:O	2:B:71:TYR:CD2	0.52	2.62	18	1
2:B:108:ASP:OD2	2:B:167:ARG:NH1	0.52	2.42	19	1
1:A:5:SER:C	1:A:76:GLY:H	0.52	2.13	5	10
1:A:30:ARG:C	1:A:32:ILE:N	0.52	2.66	9	4
2:B:97:ARG:HH11	2:B:101:LEU:CD2	0.52	2.17	2	1
2:B:111:MET:SD	2:B:111:MET:C	0.52	2.92	5	2
2:B:22:GLN:NE2	2:B:148:ALA:O	0.52	2.42	7	2
2:B:17:SER:C	2:B:21:VAL:HG23	0.52	2.28	9	4
1:A:32:ILE:HG21	1:A:81:TYR:CD1	0.52	2.40	14	1
1:A:18:GLN:O	1:A:19:PHE:CD1	0.52	2.63	17	1
1:A:53:ASP:CG	1:A:54:ASP:H	0.52	2.12	4	16
2:B:116:ASN:HD22	2:B:146:SER:C	0.52	2.12	1	5
2:B:154:VAL:O	2:B:157:ILE:CG1	0.52	2.58	2	12
1:A:16:THR:HG1	2:B:38:ASP:CG	0.52	2.12	12	1
2:B:87:GLN:HE21	2:B:125:VAL:CG1	0.52	2.17	16	1
2:B:96:LEU:C	2:B:97:ARG:NH1	0.52	2.67	18	1
2:B:74:ASN:ND2	2:B:75:GLY:N	0.52	2.57	19	1
1:A:25:VAL:N	1:A:64:ALA:O	0.52	2.42	8	16
1:A:74:ARG:C	1:A:75:ASN:CG	0.52	2.77	17	15
2:B:4:TYR:CD2	2:B:6:LEU:HD21	0.52	2.40	3	1
2:B:7:VAL:HG23	2:B:77:GLY:O	0.52	2.03	6	1
1:A:74:ARG:NH1	1:A:77:ASP:CG	0.52	2.68	14	1
2:B:8:VAL:C	2:B:71:TYR:HH	0.52	2.11	14	1
2:B:40:TYR:CE1	2:B:57:ASP:OD2	0.52	2.62	15	1
1:A:3:ALA:N	2:B:63:GLN:OE1	0.52	2.42	20	1
2:B:11:SER:O	2:B:16:LYS:NZ	0.52	2.41	2	2
2:B:64:PHE:CD2	2:B:64:PHE:O	0.52	2.62	6	1
2:B:155:ASN:N	2:B:155:ASN:ND2	0.52	2.56	6	1
1:A:30:ARG:NE	1:A:34:GLU:OE2	0.52	2.42	9	1
2:B:45:GLU:OE1	2:B:50:GLN:NE2	0.52	2.43	12	2
2:B:2:ARG:NH2	2:B:2:ARG:CG	0.52	2.71	16	1
2:B:2:ARG:NH1	2:B:76:GLN:OE1	0.52	2.43	20	1
1:A:20:GLU:C	1:A:22:SER:N	0.52	2.66	17	20
2:B:162:VAL:HG13	2:B:163:ARG:N	0.52	2.20	20	14
1:A:12:ASN:O	1:A:12:ASN:OD1	0.52	2.28	5	5
1:A:18:GLN:NE2	2:B:63:GLN:CD	0.52	2.67	6	4
2:B:121:GLU:O	2:B:124:ARG:N	0.52	2.42	4	7
1:A:80:GLU:OE2	1:A:82:ARG:NH1	0.52	2.42	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:4:TYR:OH	2:B:162:VAL:HG23	0.52	2.04	8	1
1:A:63:GLU:N	1:A:63:GLU:OE2	0.52	2.42	9	2
2:B:28:PHE:CD1	2:B:28:PHE:N	0.52	2.78	14	1
2:B:2:ARG:NE	2:B:4:TYR:CE2	0.52	2.78	17	1
2:B:35:THR:O	2:B:36:ILE:O	0.52	2.28	5	19
2:B:32:TYR:CD2	2:B:32:TYR:O	0.52	2.62	5	5
2:B:5:LYS:CE	2:B:76:GLN:NE2	0.52	2.73	6	1
2:B:131:GLY:O	2:B:135:ALA:N	0.52	2.40	15	7
2:B:112:ILE:HB	2:B:161:LEU:HD22	0.52	1.80	16	1
1:A:46:ASP:OD2	1:A:47:PHE:CE2	0.52	2.62	18	1
2:B:35:THR:O	2:B:36:ILE:C	0.52	2.52	12	20
2:B:87:GLN:CG	2:B:88:SER:N	0.52	2.73	2	14
2:B:108:ASP:OD1	2:B:167:ARG:NH1	0.52	2.43	12	1
1:A:17:MET:O	1:A:19:PHE:CD1	0.52	2.62	14	1
1:A:74:ARG:NH1	1:A:77:ASP:OD2	0.52	2.42	14	1
2:B:7:VAL:CG1	2:B:71:TYR:CZ	0.52	2.93	14	1
2:B:144:LEU:HD12	2:B:153:ASN:HB3	0.52	1.82	16	1
2:B:2:ARG:HE	2:B:3:GLU:N	0.52	2.02	6	1
2:B:116:ASN:OD1	2:B:147:SER:N	0.52	2.43	16	4
2:B:28:PHE:CZ	2:B:149:LYS:NZ	0.52	2.78	7	1
2:B:16:LYS:C	2:B:18:ALA:N	0.52	2.65	8	2
2:B:82:TYR:OH	2:B:113:LEU:CD1	0.52	2.58	9	3
1:A:17:MET:O	1:A:19:PHE:CE1	0.52	2.63	14	1
1:A:17:MET:HE3	1:A:35:ARG:NE	0.52	2.19	14	1
2:B:42:LYS:O	2:B:53:LEU:CB	0.52	2.57	14	1
2:B:155:ASN:ND2	2:B:156:GLU:CD	0.52	2.67	20	1
2:B:15:GLY:O	2:B:19:LEU:CD1	0.52	2.58	19	9
2:B:127:GLY:O	2:B:129:GLU:N	0.52	2.43	8	10
2:B:4:TYR:CG	2:B:6:LEU:HD21	0.52	2.39	7	2
2:B:8:VAL:N	2:B:56:LEU:O	0.52	2.39	3	7
2:B:143:PHE:CD1	2:B:143:PHE:N	0.52	2.78	18	5
2:B:37:GLU:CG	2:B:64:PHE:CE2	0.52	2.93	5	1
2:B:78:PHE:CD1	2:B:78:PHE:N	0.52	2.78	5	1
1:A:26:TYR:O	1:A:29:CYS:SG	0.52	2.68	11	4
1:A:81:TYR:OH	1:A:83:LYS:NZ	0.52	2.41	20	1
2:B:128:LYS:O	2:B:132:GLN:CG	0.51	2.59	7	20
2:B:136:ARG:CA	2:B:140:ASN:H	0.51	2.18	20	20
1:A:13:VAL:CG1	1:A:15:LYS:NZ	0.51	2.73	15	3
2:B:57:ASP:C	2:B:58:THR:HG22	0.51	2.29	9	5
2:B:82:TYR:CD2	2:B:90:PHE:CD1	0.51	2.98	7	1
2:B:58:THR:OG1	2:B:64:PHE:CE1	0.51	2.60	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:40:TYR:CD2	2:B:57:ASP:OD1	0.51	2.63	15	1
2:B:144:LEU:CD1	2:B:153:ASN:HD21	0.51	2.18	17	1
2:B:128:LYS:CB	2:B:143:PHE:CE2	0.51	2.93	20	1
1:A:36:ILE:O	1:A:36:ILE:CG2	0.51	2.58	2	2
2:B:90:PHE:CE2	2:B:134:LEU:HD22	0.51	2.40	10	5
2:B:124:ARG:C	2:B:124:ARG:HE	0.51	2.12	13	4
2:B:162:VAL:O	2:B:165:ILE:N	0.51	2.42	3	1
2:B:16:LYS:NZ	2:B:34:PRO:O	0.51	2.36	18	3
2:B:164:GLN:C	2:B:166:ASN:H	0.51	2.13	10	5
1:A:37:PRO:O	1:A:40:LEU:N	0.51	2.43	3	1
2:B:28:PHE:CG	2:B:28:PHE:O	0.51	2.64	3	1
2:B:39:SER:C	2:B:40:TYR:CD1	0.51	2.87	4	2
1:A:80:GLU:CD	1:A:82:ARG:HE	0.51	2.13	6	1
2:B:117:LYS:O	2:B:119:ASP:N	0.51	2.43	11	5
1:A:80:GLU:OE1	1:A:82:ARG:NH2	0.51	2.44	16	2
1:A:36:ILE:O	1:A:39:ALA:N	0.51	2.33	20	2
2:B:111:MET:H	2:B:164:GLN:NE2	0.51	2.04	14	1
1:A:26:TYR:OH	1:A:30:ARG:NH1	0.51	2.43	15	1
2:B:78:PHE:N	2:B:78:PHE:CD2	0.51	2.78	15	1
1:A:49:LEU:HD23	1:A:80:GLU:O	0.51	2.05	17	1
2:B:37:GLU:OE1	2:B:71:TYR:CE1	0.51	2.62	18	1
1:A:38:GLU:CD	2:B:25:GLN:HE21	0.51	2.12	20	1
2:B:90:PHE:CG	2:B:126:VAL:HG11	0.51	2.40	20	1
2:B:23:PHE:CD1	2:B:155:ASN:OD1	0.51	2.64	2	1
2:B:41:ARG:CA	2:B:53:LEU:O	0.51	2.59	11	8
2:B:89:THR:OG1	2:B:90:PHE:N	0.51	2.43	15	8
2:B:40:TYR:OH	2:B:158:PHE:CZ	0.51	2.62	16	1
2:B:91:ASN:O	2:B:94:GLN:NE2	0.51	2.43	19	1
1:A:38:GLU:CD	2:B:25:GLN:NE2	0.51	2.69	20	1
1:A:32:ILE:O	1:A:35:ARG:N	0.51	2.38	11	6
1:A:64:ALA:C	1:A:66:LYS:N	0.51	2.68	19	15
2:B:39:SER:OG	2:B:55:ILE:O	0.51	2.22	19	8
2:B:116:ASN:ND2	2:B:146:SER:C	0.51	2.69	1	4
1:A:36:ILE:O	1:A:40:LEU:CD1	0.51	2.58	2	2
1:A:30:ARG:O	1:A:33:ARG:NH2	0.51	2.43	3	1
1:A:13:VAL:N	2:B:41:ARG:HE	0.51	2.04	6	1
1:A:30:ARG:CZ	1:A:33:ARG:HH22	0.51	2.19	6	1
2:B:20:THR:O	2:B:21:VAL:C	0.51	2.51	7	2
2:B:49:GLN:CD	2:B:49:GLN:O	0.51	2.54	9	1
1:A:16:THR:H	2:B:38:ASP:CG	0.51	2.14	1	1
1:A:4:LEU:C	1:A:75:ASN:ND2	0.51	2.69	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LYS:NZ	2:B:40:TYR:CE1	0.51	2.79	5	2
2:B:23:PHE:CE2	2:B:154:VAL:HG13	0.51	2.40	7	1
2:B:28:PHE:CD2	2:B:28:PHE:N	0.51	2.79	8	1
1:A:15:LYS:N	2:B:38:ASP:OD1	0.51	2.43	9	1
2:B:37:GLU:OE1	2:B:59:ALA:HB3	0.51	2.04	12	1
2:B:22:GLN:O	2:B:22:GLN:NE2	0.51	2.44	14	2
2:B:45:GLU:OE2	2:B:50:GLN:NE2	0.51	2.42	7	1
1:A:84:LYS:O	1:A:85:GLN:O	0.51	2.29	12	2
2:B:56:LEU:HD23	2:B:71:TYR:CG	0.51	2.40	12	1
2:B:20:THR:O	2:B:40:TYR:CD1	0.51	2.64	13	1
1:A:39:ALA:C	1:A:41:ALA:H	0.51	2.14	10	12
2:B:30:GLU:CD	2:B:30:GLU:H	0.51	2.14	17	6
1:A:74:ARG:NE	1:A:75:ASN:O	0.51	2.41	2	1
2:B:97:ARG:NH2	2:B:138:TRP:CZ3	0.51	2.79	2	1
1:A:15:LYS:C	1:A:17:MET:N	0.51	2.66	3	1
1:A:17:MET:SD	1:A:18:GLN:O	0.51	2.68	6	1
2:B:74:ASN:C	2:B:74:ASN:ND2	0.51	2.69	7	1
1:A:37:PRO:C	1:A:39:ALA:N	0.51	2.65	13	4
2:B:97:ARG:NE	2:B:97:ARG:HA	0.51	2.21	18	1
2:B:97:ARG:NH2	2:B:138:TRP:NE1	0.51	2.59	20	1
2:B:19:LEU:C	2:B:21:VAL:H	0.51	2.13	15	7
2:B:157:ILE:C	2:B:159:TYR:N	0.51	2.66	7	12
1:A:20:GLU:N	1:A:20:GLU:OE2	0.51	2.43	4	1
2:B:97:ARG:NE	2:B:138:TRP:CD2	0.51	2.79	5	1
1:A:15:LYS:HZ1	2:B:21:VAL:HG12	0.51	1.65	8	1
2:B:57:ASP:CG	2:B:58:THR:H	0.51	2.13	18	2
1:A:85:GLN:O	1:A:86:ARG:CB	0.51	2.58	13	1
2:B:2:ARG:HH11	2:B:76:GLN:CD	0.51	2.13	16	1
2:B:58:THR:HG21	2:B:64:PHE:CZ	0.51	2.41	19	1
1:A:69:ASP:C	1:A:72:MET:H	0.51	2.13	17	13
2:B:157:ILE:O	2:B:161:LEU:CD2	0.51	2.59	13	6
1:A:16:THR:OG1	2:B:38:ASP:CB	0.51	2.59	9	4
2:B:16:LYS:CG	2:B:17:SER:N	0.51	2.74	9	2
2:B:58:THR:OG1	2:B:64:PHE:CG	0.51	2.63	9	1
2:B:5:LYS:C	2:B:6:LEU:HD23	0.50	2.30	1	9
2:B:76:GLN:O	2:B:165:ILE:CG1	0.50	2.58	10	4
2:B:82:TYR:CD1	2:B:114:VAL:O	0.50	2.65	18	2
2:B:16:LYS:O	2:B:20:THR:N	0.50	2.38	5	1
2:B:21:VAL:HG23	2:B:27:ILE:O	0.50	2.06	6	2
1:A:35:ARG:O	2:B:31:LYS:NZ	0.50	2.42	13	1
2:B:144:LEU:HD12	2:B:153:ASN:CG	0.50	2.31	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ARG:CB	2:B:31:LYS:HZ3	0.50	2.19	19	1
2:B:155:ASN:ND2	2:B:156:GLU:OE1	0.50	2.41	20	1
2:B:132:GLN:O	2:B:132:GLN:NE2	0.50	2.44	13	1
2:B:166:ASN:N	2:B:166:ASN:HD22	0.50	2.04	14	1
1:A:13:VAL:CG1	1:A:15:LYS:HZ3	0.50	2.19	18	2
2:B:118:CYS:SG	2:B:145:GLU:OE2	0.50	2.69	17	2
2:B:37:GLU:CD	2:B:71:TYR:CE1	0.50	2.89	18	1
2:B:23:PHE:CE1	2:B:155:ASN:OD1	0.50	2.64	2	2
2:B:162:VAL:CG1	2:B:163:ARG:N	0.50	2.74	20	13
2:B:68:ARG:NE	2:B:99:GLN:NE2	0.50	2.59	10	1
2:B:90:PHE:CD2	2:B:134:LEU:HD22	0.50	2.42	11	1
2:B:22:GLN:CD	2:B:23:PHE:N	0.50	2.68	19	1
1:A:3:ALA:HB3	1:A:18:GLN:HG2	0.50	1.82	16	11
1:A:53:ASP:CG	1:A:54:ASP:N	0.50	2.69	2	16
2:B:165:ILE:C	2:B:167:ARG:H	0.50	2.13	11	8
2:B:17:SER:O	2:B:18:ALA:C	0.50	2.54	18	13
1:A:40:LEU:C	1:A:42:GLY:H	0.50	2.15	14	10
2:B:37:GLU:CD	2:B:64:PHE:CD1	0.50	2.89	8	1
2:B:37:GLU:OE1	2:B:56:LEU:HD23	0.50	2.07	13	1
1:A:18:GLN:CD	2:B:63:GLN:NE2	0.50	2.69	16	1
2:B:38:ASP:O	2:B:57:ASP:CG	0.50	2.55	16	5
1:A:16:THR:OG1	2:B:38:ASP:CA	0.50	2.60	4	2
2:B:64:PHE:CG	2:B:64:PHE:O	0.50	2.64	9	1
2:B:72:MET:CB	2:B:103:VAL:HG21	0.50	2.36	11	1
1:A:16:THR:OG1	2:B:38:ASP:CG	0.50	2.54	14	6
1:A:4:LEU:O	1:A:18:GLN:HA	0.50	2.05	19	2
2:B:157:ILE:O	2:B:161:LEU:HD23	0.50	2.06	8	4
2:B:40:TYR:N	2:B:40:TYR:CD2	0.50	2.79	7	1
2:B:80:LEU:HD13	2:B:111:MET:SD	0.50	2.46	8	1
1:A:73:LEU:CD2	1:A:77:ASP:OD1	0.50	2.60	11	2
2:B:38:ASP:OD2	2:B:38:ASP:N	0.50	2.45	19	2
1:A:4:LEU:O	1:A:19:PHE:N	0.50	2.39	19	1
1:A:12:ASN:OD1	2:B:41:ARG:O	0.50	2.30	7	6
2:B:92:ASP:C	2:B:94:GLN:N	0.50	2.68	19	17
1:A:30:ARG:O	1:A:32:ILE:N	0.50	2.45	2	4
2:B:68:ARG:O	2:B:72:MET:CG	0.50	2.59	12	5
2:B:37:GLU:OE1	2:B:64:PHE:CG	0.50	2.65	8	1
2:B:16:LYS:HZ3	2:B:57:ASP:CG	0.50	2.15	9	1
2:B:158:PHE:CD1	2:B:158:PHE:N	0.50	2.79	9	1
1:A:18:GLN:OE1	2:B:36:ILE:HG21	0.50	2.07	16	1
2:B:9:LEU:CD2	2:B:97:ARG:HH12	0.50	2.20	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LYS:HZ3	2:B:25:GLN:NE2	0.50	2.03	2	1
2:B:76:GLN:O	2:B:165:ILE:CD1	0.50	2.60	20	8
2:B:28:PHE:O	2:B:28:PHE:CD1	0.50	2.65	3	1
2:B:62:GLU:HA	2:B:65:THR:HG23	0.50	1.83	5	1
2:B:57:ASP:C	2:B:58:THR:OG1	0.50	2.55	17	3
2:B:111:MET:C	2:B:141:CYS:SG	0.50	2.95	10	1
2:B:2:ARG:NH2	2:B:76:GLN:NE2	0.50	2.60	15	1
2:B:82:TYR:OH	2:B:113:LEU:HD23	0.50	2.06	20	1
2:B:140:ASN:C	2:B:142:ALA:N	0.49	2.68	2	11
2:B:92:ASP:O	2:B:94:GLN:N	0.49	2.45	19	7
2:B:6:LEU:N	2:B:6:LEU:HD22	0.49	2.21	5	1
1:A:24:MET:SD	1:A:27:ASP:OD2	0.49	2.70	6	1
2:B:125:VAL:O	2:B:130:GLN:NE2	0.49	2.45	16	2
1:A:18:GLN:OE1	2:B:36:ILE:CD1	0.49	2.58	16	1
2:B:2:ARG:HH21	2:B:2:ARG:CG	0.49	2.20	16	1
2:B:7:VAL:HG12	2:B:9:LEU:CD1	0.49	2.36	18	1
2:B:21:VAL:O	2:B:23:PHE:N	0.49	2.45	20	1
2:B:133:ASN:ND2	2:B:136:ARG:NH2	0.49	2.60	3	2
1:A:16:THR:OG1	2:B:37:GLU:C	0.49	2.56	12	1
2:B:90:PHE:CD2	2:B:126:VAL:CG2	0.49	2.94	12	2
2:B:2:ARG:NE	2:B:3:GLU:C	0.49	2.70	16	1
1:A:31:MET:O	1:A:35:ARG:NH2	0.49	2.42	17	1
2:B:72:MET:CB	2:B:99:GLN:NE2	0.49	2.75	17	1
2:B:74:ASN:HD22	2:B:76:GLN:H	0.49	1.49	7	1
2:B:35:THR:CB	2:B:59:ALA:HB3	0.49	2.36	14	3
1:A:6:LEU:C	1:A:16:THR:HG23	0.49	2.32	17	1
2:B:156:GLU:OE2	2:B:156:GLU:N	0.49	2.39	20	1
2:B:65:THR:O	2:B:69:ASP:N	0.49	2.45	1	2
2:B:107:ASP:C	2:B:109:VAL:H	0.49	2.16	10	15
2:B:118:CYS:SG	2:B:145:GLU:CD	0.49	2.95	11	8
2:B:5:LYS:HZ1	2:B:76:GLN:NE2	0.49	2.04	5	1
2:B:118:CYS:SG	2:B:146:SER:O	0.49	2.69	5	3
1:A:53:ASP:OD1	1:A:58:LYS:NZ	0.49	2.40	13	1
2:B:19:LEU:HD11	2:B:116:ASN:ND2	0.49	2.22	15	1
1:A:26:TYR:CD1	1:A:26:TYR:C	0.49	2.90	1	5
2:B:19:LEU:HD11	2:B:116:ASN:CG	0.49	2.33	8	1
2:B:68:ARG:HH12	2:B:96:LEU:HD22	0.49	1.68	9	1
1:A:37:PRO:O	1:A:39:ALA:N	0.49	2.45	13	3
1:A:74:ARG:O	1:A:75:ASN:CB	0.49	2.60	3	17
1:A:14:VAL:C	2:B:38:ASP:OD1	0.49	2.55	9	1
2:B:21:VAL:CG1	2:B:22:GLN:N	0.49	2.75	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:GLU:O	1:A:21:PRO:C	0.49	2.56	8	20
1:A:27:ASP:C	1:A:29:CYS:N	0.49	2.68	3	12
1:A:35:ARG:O	1:A:36:ILE:O	0.49	2.31	1	8
2:B:140:ASN:O	2:B:140:ASN:CG	0.49	2.56	10	11
2:B:8:VAL:HA	2:B:79:ALA:HB3	0.49	1.84	2	2
2:B:89:THR:C	2:B:91:ASN:N	0.49	2.70	8	1
2:B:108:ASP:O	2:B:167:ARG:NH2	0.49	2.41	19	1
2:B:97:ARG:CZ	2:B:138:TRP:CD2	0.49	2.95	5	1
2:B:90:PHE:CD2	2:B:93:LEU:HD11	0.49	2.43	8	1
2:B:69:ASP:O	2:B:72:MET:SD	0.49	2.70	15	1
2:B:2:ARG:NE	2:B:3:GLU:O	0.49	2.46	16	1
2:B:16:LYS:CG	2:B:17:SER:H	0.49	2.20	20	1
2:B:9:LEU:HD13	2:B:10:GLY:H	0.49	1.67	1	1
2:B:146:SER:CB	2:B:152:ILE:O	0.49	2.60	13	10
1:A:15:LYS:C	2:B:38:ASP:OD1	0.49	2.56	9	2
2:B:20:THR:HG21	2:B:40:TYR:CZ	0.49	2.42	7	1
2:B:78:PHE:CD2	2:B:80:LEU:CD1	0.49	2.96	10	1
1:A:33:ARG:NH1	1:A:44:PRO:N	0.49	2.60	13	1
2:B:61:THR:C	2:B:63:GLN:H	0.49	2.16	13	1
2:B:40:TYR:CE1	2:B:57:ASP:CG	0.49	2.91	15	1
2:B:95:ASP:C	2:B:97:ARG:N	0.49	2.69	11	7
1:A:3:ALA:O	1:A:4:LEU:O	0.49	2.31	20	11
2:B:38:ASP:O	2:B:57:ASP:N	0.49	2.41	9	5
2:B:153:ASN:N	2:B:153:ASN:HD22	0.49	2.05	12	3
1:A:50:PHE:O	1:A:52:SER:N	0.49	2.43	18	3
1:A:46:ASP:O	1:A:47:PHE:CG	0.49	2.66	14	1
1:A:29:CYS:SG	1:A:49:LEU:CD1	0.48	3.01	3	3
1:A:74:ARG:O	1:A:75:ASN:OD1	0.48	2.30	6	4
2:B:78:PHE:CE1	2:B:100:ILE:CD1	0.48	2.95	3	2
1:A:16:THR:HG1	2:B:37:GLU:C	0.48	2.15	18	2
1:A:18:GLN:N	2:B:36:ILE:CD1	0.48	2.76	9	4
2:B:3:GLU:CD	2:B:52:MET:SD	0.48	2.96	6	1
2:B:40:TYR:CE1	2:B:55:ILE:CG2	0.48	2.93	6	1
2:B:132:GLN:HE21	2:B:132:GLN:C	0.48	2.15	13	1
1:A:18:GLN:OE1	2:B:36:ILE:CG2	0.48	2.60	16	1
1:A:5:SER:N	1:A:75:ASN:OD1	0.48	2.46	1	3
1:A:21:PRO:O	1:A:69:ASP:N	0.48	2.43	9	7
1:A:35:ARG:O	1:A:40:LEU:HD11	0.48	2.08	2	1
2:B:118:CYS:O	2:B:121:GLU:CG	0.48	2.61	19	6
1:A:27:ASP:OD2	1:A:31:MET:SD	0.48	2.72	7	2
1:A:33:ARG:NH1	1:A:47:PHE:CD2	0.48	2.81	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:72:MET:SD	2:B:103:VAL:CG1	0.48	3.01	13	1
2:B:4:TYR:CZ	2:B:162:VAL:CG2	0.48	2.96	17	2
1:A:64:ALA:C	1:A:66:LYS:H	0.48	2.17	19	16
2:B:152:ILE:O	2:B:153:ASN:C	0.48	2.57	12	17
2:B:59:ALA:O	2:B:60:GLY:C	0.48	2.56	19	15
2:B:111:MET:CG	2:B:112:ILE:N	0.48	2.75	2	5
2:B:137:GLN:C	2:B:139:ASN:H	0.48	2.14	13	15
2:B:2:ARG:O	2:B:52:MET:N	0.48	2.43	4	3
2:B:81:VAL:HG23	2:B:81:VAL:O	0.48	2.07	5	3
2:B:158:PHE:CD2	2:B:158:PHE:C	0.48	2.91	12	1
1:A:33:ARG:C	1:A:35:ARG:NH1	0.48	2.72	13	1
2:B:111:MET:C	2:B:161:LEU:CD2	0.48	2.86	15	1
1:A:17:MET:HE3	1:A:35:ARG:NH2	0.48	2.23	19	1
2:B:37:GLU:CB	2:B:64:PHE:CD2	0.48	2.97	1	1
2:B:62:GLU:O	2:B:65:THR:CG2	0.48	2.61	19	6
2:B:74:ASN:CG	2:B:75:GLY:N	0.48	2.71	3	2
2:B:38:ASP:O	2:B:57:ASP:CB	0.48	2.62	17	3
2:B:90:PHE:CD1	2:B:126:VAL:CG2	0.48	2.92	9	2
2:B:153:ASN:O	2:B:153:ASN:ND2	0.48	2.46	17	1
1:A:67:ALA:O	1:A:70:TYR:CB	0.48	2.62	12	20
2:B:64:PHE:O	2:B:65:THR:C	0.48	2.56	17	11
1:A:18:GLN:NE2	2:B:36:ILE:CG2	0.48	2.76	9	8
2:B:53:LEU:C	2:B:53:LEU:CD2	0.48	2.87	5	4
2:B:64:PHE:O	2:B:68:ARG:CB	0.48	2.62	16	4
1:A:15:LYS:C	1:A:17:MET:H	0.48	2.15	3	1
2:B:56:LEU:C	2:B:57:ASP:OD1	0.48	2.56	4	1
2:B:77:GLY:C	2:B:78:PHE:CD2	0.48	2.91	4	1
2:B:32:TYR:O	2:B:32:TYR:CG	0.48	2.66	12	2
1:A:80:GLU:CD	1:A:82:ARG:NH1	0.48	2.71	6	1
1:A:15:LYS:HZ3	2:B:21:VAL:HG22	0.48	1.67	10	1
1:A:4:LEU:C	1:A:75:ASN:OD1	0.48	2.56	14	3
2:B:109:VAL:O	2:B:110:PRO:C	0.48	2.57	14	20
2:B:118:CYS:C	2:B:120:LEU:H	0.48	2.17	20	11
2:B:2:ARG:HG2	2:B:3:GLU:N	0.48	2.22	8	2
2:B:78:PHE:CE1	2:B:100:ILE:HD11	0.48	2.43	3	1
2:B:22:GLN:NE2	2:B:22:GLN:C	0.48	2.71	5	1
2:B:163:ARG:NH1	2:B:166:ASN:HD22	0.48	2.05	5	1
2:B:68:ARG:CZ	2:B:99:GLN:HE22	0.48	2.20	16	1
2:B:107:ASP:OD1	2:B:107:ASP:N	0.48	2.47	17	1
2:B:37:GLU:CD	2:B:56:LEU:HD21	0.48	2.34	1	1
1:A:24:MET:O	1:A:28:ALA:N	0.48	2.42	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:155:ASN:O	2:B:158:PHE:CD2	0.48	2.66	15	3
1:A:14:VAL:O	1:A:14:VAL:CG1	0.48	2.61	8	2
2:B:68:ARG:NH1	2:B:99:GLN:OE1	0.48	2.41	10	3
2:B:42:LYS:O	2:B:53:LEU:N	0.48	2.45	14	1
1:A:80:GLU:C	1:A:82:ARG:H	0.48	2.16	18	2
2:B:5:LYS:HZ3	2:B:76:GLN:NE2	0.48	2.07	6	1
1:A:12:ASN:ND2	2:B:41:ARG:C	0.48	2.71	18	2
2:B:40:TYR:CE2	2:B:55:ILE:CG2	0.48	2.96	16	1
1:A:36:ILE:CG1	2:B:25:GLN:OE1	0.48	2.61	19	1
1:A:40:LEU:HD23	1:A:40:LEU:H	0.48	1.68	20	12
1:A:67:ALA:O	1:A:68:LEU:C	0.48	2.57	19	20
1:A:14:VAL:HG21	2:B:39:SER:OG	0.48	2.09	3	2
2:B:100:ILE:O	2:B:102:ARG:N	0.48	2.47	9	1
2:B:68:ARG:HH11	2:B:99:GLN:CD	0.48	2.16	10	1
2:B:138:TRP:C	2:B:139:ASN:CG	0.48	2.82	10	1
2:B:4:TYR:O	2:B:4:TYR:CD2	0.48	2.67	11	1
2:B:132:GLN:NE2	2:B:132:GLN:C	0.48	2.72	13	1
2:B:37:GLU:OE2	2:B:67:MET:CB	0.48	2.62	18	1
1:A:16:THR:OG1	2:B:38:ASP:OD1	0.48	2.32	14	3
2:B:14:VAL:CG2	2:B:15:GLY:N	0.48	2.74	16	8
2:B:152:ILE:O	2:B:154:VAL:N	0.48	2.47	2	8
2:B:63:GLN:C	2:B:65:THR:H	0.48	2.17	19	5
2:B:162:VAL:C	2:B:164:GLN:N	0.48	2.70	3	2
2:B:103:VAL:CG1	2:B:104:LYS:N	0.48	2.76	20	5
2:B:121:GLU:O	2:B:124:ARG:CB	0.48	2.62	20	5
2:B:143:PHE:CD2	2:B:143:PHE:N	0.48	2.81	7	4
2:B:82:TYR:CE1	2:B:93:LEU:HD22	0.48	2.43	8	1
2:B:21:VAL:HG13	2:B:25:GLN:HE21	0.48	1.69	11	1
2:B:117:LYS:O	2:B:120:LEU:N	0.48	2.46	17	2
2:B:158:PHE:O	2:B:162:VAL:CG1	0.47	2.62	2	4
2:B:70:LEU:HD22	2:B:70:LEU:C	0.47	2.34	5	1
2:B:37:GLU:CG	2:B:64:PHE:CD1	0.47	2.97	8	1
1:A:32:ILE:HG22	1:A:33:ARG:N	0.47	2.24	9	1
2:B:7:VAL:O	2:B:7:VAL:HG12	0.47	2.08	10	1
1:A:32:ILE:O	1:A:32:ILE:HG22	0.47	2.09	13	1
2:B:61:THR:O	2:B:64:PHE:N	0.47	2.41	16	1
2:B:14:VAL:HG23	2:B:15:GLY:H	0.47	1.68	12	3
2:B:32:TYR:O	2:B:33:ASP:C	0.47	2.57	3	12
2:B:36:ILE:O	2:B:38:ASP:OD1	0.47	2.32	10	5
2:B:6:LEU:O	2:B:56:LEU:N	0.47	2.44	18	4
2:B:158:PHE:O	2:B:162:VAL:HG12	0.47	2.09	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:68:ARG:O	2:B:68:ARG:CD	0.47	2.62	3	1
2:B:140:ASN:CG	2:B:140:ASN:O	0.47	2.57	14	5
1:A:7:LYS:NZ	1:A:76:GLY:CA	0.47	2.77	6	1
2:B:20:THR:CG2	2:B:40:TYR:CE2	0.47	2.93	7	1
2:B:82:TYR:CD2	2:B:114:VAL:O	0.47	2.67	13	2
1:A:15:LYS:CE	2:B:33:ASP:CG	0.47	2.88	13	1
2:B:5:LYS:NZ	2:B:76:GLN:OE1	0.47	2.41	14	1
2:B:9:LEU:O	2:B:81:VAL:CG2	0.47	2.62	14	1
2:B:37:GLU:N	2:B:58:THR:HG23	0.47	2.23	14	2
2:B:19:LEU:N	2:B:19:LEU:CD1	0.47	2.76	15	1
1:A:14:VAL:O	1:A:15:LYS:O	0.47	2.32	17	1
2:B:31:LYS:O	2:B:31:LYS:CG	0.47	2.62	15	10
2:B:108:ASP:CG	2:B:108:ASP:O	0.47	2.57	14	11
2:B:93:LEU:HA	2:B:96:LEU:HD12	0.47	1.86	15	6
1:A:26:TYR:CD2	1:A:26:TYR:C	0.47	2.92	14	4
1:A:43:PRO:O	1:A:46:ASP:OD2	0.47	2.32	18	4
2:B:21:VAL:CG2	2:B:27:ILE:O	0.47	2.62	12	2
2:B:16:LYS:HE3	2:B:59:ALA:HB2	0.47	1.85	7	1
2:B:9:LEU:HD23	2:B:97:ARG:HH22	0.47	1.67	9	1
1:A:2:VAL:CA	2:B:63:GLN:NE2	0.47	2.76	12	1
1:A:30:ARG:CZ	1:A:34:GLU:OE1	0.47	2.62	16	2
2:B:78:PHE:CE2	2:B:100:ILE:CD1	0.47	2.98	12	2
2:B:97:ARG:CZ	2:B:97:ARG:N	0.47	2.78	18	1
2:B:89:THR:O	2:B:90:PHE:C	0.47	2.57	5	17
2:B:101:LEU:CD1	2:B:101:LEU:N	0.47	2.77	3	15
1:A:15:LYS:NZ	2:B:40:TYR:OH	0.47	2.38	14	3
1:A:27:ASP:O	1:A:31:MET:N	0.47	2.46	3	1
1:A:46:ASP:OD2	1:A:47:PHE:CE1	0.47	2.67	3	1
1:A:47:PHE:CD2	1:A:81:TYR:OH	0.47	2.61	3	1
2:B:153:ASN:O	2:B:157:ILE:CD1	0.47	2.63	18	4
2:B:4:TYR:HB2	2:B:6:LEU:HD21	0.47	1.86	6	1
2:B:58:THR:OG1	2:B:64:PHE:CD1	0.47	2.63	9	2
2:B:68:ARG:HD3	2:B:69:ASP:N	0.47	2.24	11	1
2:B:22:GLN:HG3	2:B:148:ALA:HB1	0.47	1.86	13	1
2:B:84:ILE:N	2:B:84:ILE:CD1	0.47	2.77	14	1
2:B:46:VAL:O	2:B:47:ASP:CB	0.47	2.62	9	20
2:B:112:ILE:CD1	2:B:142:ALA:O	0.47	2.63	1	3
2:B:18:ALA:O	2:B:22:GLN:CD	0.47	2.58	10	3
2:B:113:LEU:HD22	2:B:135:ALA:HB2	0.47	1.84	6	5
2:B:111:MET:HE3	2:B:141:CYS:SG	0.47	2.49	7	2
2:B:2:ARG:NH1	2:B:166:ASN:OD1	0.47	2.48	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:56:LEU:CD2	2:B:71:TYR:CD1	0.47	2.97	18	1
1:A:10:ILE:HG23	1:A:81:TYR:CD2	0.47	2.44	20	1
1:A:30:ARG:NE	1:A:34:GLU:OE1	0.47	2.48	2	1
2:B:90:PHE:CE2	2:B:134:LEU:CD2	0.47	2.98	2	3
2:B:30:GLU:OE1	2:B:30:GLU:N	0.47	2.48	8	1
1:A:31:MET:O	1:A:32:ILE:C	0.47	2.56	18	1
2:B:55:ILE:N	2:B:55:ILE:CD1	0.47	2.78	19	1
2:B:100:ILE:C	2:B:102:ARG:N	0.47	2.70	9	6
2:B:128:LYS:O	2:B:132:GLN:CB	0.47	2.62	15	19
1:A:15:LYS:CE	2:B:33:ASP:OD2	0.47	2.63	3	1
1:A:16:THR:O	1:A:17:MET:C	0.47	2.58	3	1
1:A:46:ASP:OD2	1:A:46:ASP:C	0.47	2.58	3	3
1:A:47:PHE:CD2	1:A:81:TYR:CE1	0.47	3.02	3	1
2:B:145:GLU:O	2:B:145:GLU:CG	0.47	2.63	4	1
2:B:19:LEU:O	2:B:20:THR:O	0.47	2.33	7	1
2:B:46:VAL:HG21	2:B:162:VAL:HG21	0.47	1.86	7	1
2:B:2:ARG:CG	2:B:3:GLU:N	0.47	2.76	8	1
1:A:13:VAL:HG11	2:B:25:GLN:CD	0.47	2.35	12	2
1:A:16:THR:CG2	2:B:38:ASP:OD1	0.47	2.61	14	1
1:A:74:ARG:CZ	1:A:77:ASP:CG	0.47	2.87	14	1
2:B:4:TYR:CE1	2:B:162:VAL:CG2	0.47	2.97	14	1
1:A:10:ILE:HD12	1:A:35:ARG:NH1	0.47	2.25	20	1
2:B:127:GLY:C	2:B:129:GLU:H	0.47	2.18	12	14
1:A:37:PRO:CA	1:A:40:LEU:HD13	0.47	2.40	11	3
1:A:26:TYR:C	1:A:26:TYR:CD2	0.47	2.91	6	2
2:B:75:GLY:HA3	2:B:104:LYS:HZ1	0.47	1.68	9	1
2:B:93:LEU:O	2:B:97:ARG:CD	0.47	2.62	9	1
1:A:30:ARG:CZ	1:A:34:GLU:CD	0.47	2.87	16	1
1:A:32:ILE:C	1:A:34:GLU:N	0.47	2.72	20	4
2:B:31:LYS:CG	2:B:31:LYS:O	0.47	2.63	12	2
1:A:8:ILE:HD11	1:A:19:PHE:CE2	0.47	2.45	6	1
2:B:56:LEU:CD2	2:B:71:TYR:CG	0.47	2.97	19	3
2:B:96:LEU:HD23	2:B:99:GLN:NE2	0.47	2.25	11	2
1:A:26:TYR:CD2	1:A:27:ASP:OD2	0.47	2.67	16	1
2:B:58:THR:CG2	2:B:59:ALA:N	0.47	2.77	16	1
2:B:28:PHE:CD1	2:B:28:PHE:C	0.47	2.92	19	1
1:A:51:LEU:HD22	1:A:77:ASP:OD2	0.47	2.10	20	1
2:B:104:LYS:HG3	2:B:109:VAL:HG21	0.47	1.87	5	1
2:B:159:TYR:O	2:B:159:TYR:CD2	0.47	2.68	6	1
1:A:16:THR:HG23	2:B:38:ASP:OD2	0.47	2.09	9	1
1:A:74:ARG:CD	1:A:75:ASN:H	0.47	2.23	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:PRO:O	1:A:46:ASP:OD1	0.47	2.33	17	1
1:A:52:SER:O	1:A:53:ASP:O	0.46	2.34	18	20
2:B:90:PHE:CE1	2:B:134:LEU:CD2	0.46	2.98	3	3
1:A:58:LYS:O	1:A:59:GLY:O	0.46	2.33	13	9
2:B:161:LEU:N	2:B:161:LEU:CD2	0.46	2.76	3	6
2:B:156:GLU:O	2:B:159:TYR:N	0.46	2.47	5	1
2:B:61:THR:CB	2:B:64:PHE:CE2	0.46	2.98	17	1
2:B:157:ILE:O	2:B:160:ASP:OD1	0.46	2.33	17	2
2:B:2:ARG:NH1	2:B:162:VAL:CG2	0.46	2.78	7	1
2:B:61:THR:C	2:B:63:GLN:N	0.46	2.73	13	1
2:B:13:GLY:O	2:B:14:VAL:O	0.46	2.34	11	19
2:B:162:VAL:O	2:B:166:ASN:CG	0.46	2.58	10	7
1:A:3:ALA:C	1:A:4:LEU:O	0.46	2.58	11	15
1:A:51:LEU:HD22	1:A:77:ASP:OD1	0.46	2.10	9	1
1:A:16:THR:O	2:B:38:ASP:OD2	0.46	2.34	10	1
1:A:45:ASN:C	1:A:45:ASN:HD22	0.46	2.17	17	1
2:B:23:PHE:CE1	2:B:40:TYR:OH	0.46	2.62	19	1
1:A:2:VAL:O	1:A:3:ALA:CB	0.46	2.62	13	12
2:B:22:GLN:OE1	2:B:27:ILE:O	0.46	2.34	10	6
2:B:28:PHE:CD2	2:B:28:PHE:C	0.46	2.94	1	1
2:B:128:LYS:CB	2:B:143:PHE:CE1	0.46	2.97	1	2
2:B:100:ILE:O	2:B:101:LEU:C	0.46	2.59	2	11
2:B:53:LEU:C	2:B:53:LEU:CD1	0.46	2.88	20	2
1:A:69:ASP:O	1:A:72:MET:N	0.46	2.44	17	2
2:B:19:LEU:C	2:B:20:THR:O	0.46	2.56	7	2
2:B:56:LEU:HD11	2:B:71:TYR:CE1	0.46	2.45	18	1
1:A:33:ARG:HH11	1:A:43:PRO:C	0.46	2.19	20	1
1:A:40:LEU:HD12	1:A:40:LEU:N	0.46	2.26	2	3
2:B:140:ASN:O	2:B:141:CYS:C	0.46	2.59	14	6
1:A:32:ILE:O	1:A:33:ARG:C	0.46	2.58	20	4
1:A:74:ARG:CZ	1:A:75:ASN:O	0.46	2.64	8	1
2:B:15:GLY:O	2:B:18:ALA:HB3	0.46	2.11	8	1
2:B:22:GLN:HE21	2:B:28:PHE:CB	0.46	2.24	13	1
1:A:74:ARG:CZ	1:A:77:ASP:OD2	0.46	2.64	14	1
2:B:167:ARG:H	2:B:167:ARG:HD2	0.46	1.71	18	1
1:A:12:ASN:ND2	2:B:41:ARG:HB2	0.46	2.24	19	4
2:B:32:TYR:O	2:B:33:ASP:O	0.46	2.34	12	5
2:B:42:LYS:O	2:B:53:LEU:HA	0.46	2.10	7	5
2:B:82:TYR:CD2	2:B:90:PHE:CE1	0.46	3.04	19	3
2:B:22:GLN:O	2:B:23:PHE:C	0.46	2.57	7	3
1:A:8:ILE:HG21	1:A:32:ILE:CD1	0.46	2.40	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:16:LYS:NZ	2:B:57:ASP:CG	0.46	2.73	9	1
1:A:15:LYS:HZ1	2:B:33:ASP:CG	0.46	2.17	3	1
2:B:111:MET:SD	2:B:112:ILE:C	0.46	2.99	3	1
2:B:97:ARG:CG	2:B:98:GLU:N	0.46	2.79	4	4
1:A:7:LYS:HZ2	1:A:76:GLY:CA	0.46	2.24	6	1
1:A:12:ASN:OD1	2:B:41:ARG:N	0.46	2.47	7	1
2:B:16:LYS:CB	2:B:16:LYS:NZ	0.46	2.79	7	1
1:A:3:ALA:O	2:B:63:GLN:OE1	0.46	2.34	12	1
2:B:84:ILE:CD1	2:B:84:ILE:H	0.46	2.24	14	1
2:B:68:ARG:CD	2:B:68:ARG:C	0.46	2.88	13	2
2:B:18:ALA:O	2:B:22:GLN:OE1	0.46	2.34	7	2
1:A:12:ASN:O	1:A:13:VAL:CB	0.46	2.64	6	1
2:B:2:ARG:NE	2:B:49:GLN:NE2	0.46	2.62	9	1
2:B:49:GLN:O	2:B:49:GLN:CG	0.46	2.64	9	1
1:A:60:ILE:CD1	1:A:71:TYR:CE1	0.46	2.99	18	2
2:B:5:LYS:HA	2:B:54:GLU:O	0.46	2.10	13	1
2:B:37:GLU:C	2:B:37:GLU:CD	0.46	2.84	15	2
1:A:72:MET:O	1:A:73:LEU:O	0.46	2.34	8	9
1:A:36:ILE:O	1:A:36:ILE:HG23	0.46	2.10	3	1
2:B:65:THR:C	2:B:67:MET:N	0.46	2.72	14	4
2:B:163:ARG:HE	2:B:163:ARG:CA	0.46	2.22	9	1
2:B:8:VAL:O	2:B:57:ASP:OD1	0.46	2.34	10	2
2:B:64:PHE:O	2:B:64:PHE:CG	0.46	2.68	14	2
2:B:111:MET:SD	2:B:138:TRP:CE3	0.46	3.09	4	1
1:A:30:ARG:CZ	1:A:34:GLU:OE2	0.46	2.63	5	1
2:B:81:VAL:O	2:B:81:VAL:CG2	0.46	2.64	18	4
2:B:167:ARG:CG	2:B:167:ARG:NH2	0.46	2.78	5	1
2:B:57:ASP:OD2	2:B:57:ASP:N	0.46	2.47	19	2
2:B:37:GLU:HG3	2:B:57:ASP:O	0.46	2.11	8	1
2:B:37:GLU:CB	2:B:64:PHE:CD1	0.46	2.99	11	1
2:B:97:ARG:NH2	2:B:138:TRP:O	0.46	2.48	11	1
1:A:14:VAL:C	2:B:38:ASP:OD2	0.46	2.59	14	1
2:B:79:ALA:O	2:B:81:VAL:HG23	0.46	2.11	15	1
2:B:2:ARG:HH11	2:B:76:GLN:NE2	0.46	2.09	16	1
2:B:61:THR:O	2:B:62:GLU:C	0.46	2.59	16	1
2:B:46:VAL:O	2:B:49:GLN:CG	0.45	2.64	5	16
2:B:65:THR:O	2:B:66:ALA:C	0.45	2.59	1	4
1:A:16:THR:OG1	2:B:37:GLU:O	0.45	2.34	12	6
2:B:121:GLU:O	2:B:122:ASP:C	0.45	2.59	7	13
1:A:10:ILE:O	1:A:11:GLY:O	0.45	2.34	14	4
2:B:64:PHE:CD1	2:B:67:MET:CB	0.45	2.99	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:90:PHE:CD1	2:B:134:LEU:HD23	0.45	2.45	15	2
2:B:67:MET:O	2:B:71:TYR:CB	0.45	2.63	14	1
2:B:100:ILE:O	2:B:103:VAL:HG12	0.45	2.11	3	1
2:B:16:LYS:O	2:B:17:SER:C	0.45	2.59	5	1
2:B:4:TYR:CE1	2:B:51:CYS:HB3	0.45	2.46	17	2
2:B:22:GLN:CD	2:B:22:GLN:O	0.45	2.59	9	1
1:A:64:ALA:O	1:A:66:LYS:N	0.45	2.50	19	2
2:B:8:VAL:O	2:B:57:ASP:OD2	0.45	2.33	17	2
2:B:141:CYS:O	2:B:142:ALA:C	0.45	2.59	10	7
2:B:4:TYR:OH	2:B:162:VAL:CG2	0.45	2.64	17	1
1:A:77:ASP:CG	1:A:78:THR:H	0.45	2.19	18	5
2:B:146:SER:OG	2:B:152:ILE:O	0.45	2.35	15	5
2:B:17:SER:OG	2:B:40:TYR:OH	0.45	2.33	3	2
2:B:87:GLN:O	2:B:88:SER:C	0.45	2.59	8	11
1:A:12:ASN:C	1:A:13:VAL:CG2	0.45	2.90	7	2
2:B:17:SER:HA	2:B:20:THR:OG1	0.45	2.12	7	1
2:B:117:LYS:O	2:B:118:CYS:C	0.45	2.60	11	4
2:B:22:GLN:CD	2:B:22:GLN:N	0.45	2.73	10	1
2:B:6:LEU:HD23	2:B:6:LEU:N	0.45	2.26	12	1
1:A:30:ARG:O	1:A:31:MET:C	0.45	2.60	18	9
2:B:108:ASP:O	2:B:108:ASP:CG	0.45	2.59	6	8
2:B:16:LYS:CE	2:B:59:ALA:HB2	0.45	2.42	7	1
2:B:84:ILE:HG21	2:B:145:GLU:OE1	0.45	2.12	8	1
1:A:32:ILE:O	1:A:32:ILE:CG2	0.45	2.63	13	1
1:A:53:ASP:H	1:A:59:GLY:CA	0.45	2.24	15	10
2:B:54:GLU:N	2:B:54:GLU:OE2	0.45	2.49	1	1
2:B:68:ARG:O	2:B:71:TYR:CE2	0.45	2.67	3	1
1:A:10:ILE:CD1	1:A:35:ARG:HH12	0.45	2.24	4	1
2:B:2:ARG:NH1	2:B:4:TYR:CE2	0.45	2.85	5	1
2:B:7:VAL:C	2:B:71:TYR:OH	0.45	2.60	5	1
1:A:85:GLN:O	1:A:86:ARG:C	0.45	2.60	12	4
1:A:14:VAL:N	2:B:39:SER:O	0.45	2.44	11	1
2:B:31:LYS:O	2:B:31:LYS:HG3	0.45	2.12	12	3
2:B:128:LYS:NZ	2:B:144:LEU:O	0.45	2.40	19	1
1:A:47:PHE:CG	1:A:81:TYR:OH	0.45	2.59	3	1
2:B:37:GLU:CD	2:B:37:GLU:N	0.45	2.74	9	2
2:B:71:TYR:CD2	2:B:71:TYR:C	0.45	2.95	5	1
1:A:80:GLU:CG	1:A:82:ARG:HE	0.45	2.24	6	1
2:B:78:PHE:CE1	2:B:111:MET:HG3	0.45	2.47	15	1
2:B:68:ARG:CD	2:B:68:ARG:O	0.45	2.65	1	1
2:B:67:MET:C	2:B:69:ASP:N	0.45	2.74	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:92:ASP:O	2:B:93:LEU:C	0.45	2.60	8	5
1:A:51:LEU:O	1:A:52:SER:C	0.45	2.59	13	5
2:B:157:ILE:O	2:B:159:TYR:N	0.45	2.49	16	2
2:B:71:TYR:OH	2:B:96:LEU:O	0.45	2.35	15	1
2:B:153:ASN:OD1	2:B:156:GLU:OE1	0.45	2.34	8	2
1:A:35:ARG:CD	1:A:36:ILE:N	0.45	2.80	13	1
1:A:36:ILE:H	2:B:31:LYS:HZ3	0.45	1.54	19	1
2:B:82:TYR:CD1	2:B:90:PHE:CZ	0.45	3.05	20	1
1:A:5:SER:OG	2:B:36:ILE:CG2	0.45	2.65	9	4
2:B:2:ARG:HH11	2:B:162:VAL:HG23	0.45	1.72	5	1
2:B:22:GLN:C	2:B:22:GLN:CD	0.45	2.85	5	3
1:A:16:THR:OG1	2:B:38:ASP:OD2	0.45	2.35	9	2
2:B:32:TYR:C	2:B:33:ASP:O	0.45	2.59	12	1
2:B:155:ASN:CG	2:B:158:PHE:CE1	0.45	2.95	12	1
1:A:83:LYS:HG2	1:A:85:GLN:N	0.45	2.27	17	1
2:B:56:LEU:C	2:B:57:ASP:OD2	0.44	2.60	13	2
1:A:14:VAL:CG1	2:B:38:ASP:OD2	0.44	2.65	2	1
1:A:75:ASN:ND2	2:B:63:GLN:NE2	0.44	2.65	2	1
2:B:128:LYS:NZ	2:B:128:LYS:CB	0.44	2.79	14	2
2:B:19:LEU:C	2:B:21:VAL:N	0.44	2.76	15	1
2:B:53:LEU:CD2	2:B:53:LEU:H	0.44	2.26	16	1
2:B:145:GLU:OE2	2:B:145:GLU:C	0.44	2.61	17	1
2:B:118:CYS:C	2:B:120:LEU:N	0.44	2.74	19	10
2:B:11:SER:O	2:B:14:VAL:CG2	0.44	2.66	4	3
2:B:58:THR:CB	2:B:64:PHE:CE1	0.44	3.00	9	2
2:B:3:GLU:O	2:B:76:GLN:OE1	0.44	2.34	15	2
2:B:96:LEU:HD23	2:B:99:GLN:OE1	0.44	2.11	18	1
1:A:10:ILE:CD1	1:A:35:ARG:NH1	0.44	2.80	20	1
1:A:40:LEU:H	1:A:40:LEU:CD2	0.44	2.25	4	8
2:B:78:PHE:CB	2:B:111:MET:SD	0.44	3.06	1	2
2:B:38:ASP:O	2:B:57:ASP:OD2	0.44	2.36	3	2
1:A:74:ARG:C	1:A:75:ASN:OD1	0.44	2.61	6	2
2:B:6:LEU:HD11	2:B:158:PHE:CE1	0.44	2.47	8	1
1:A:37:PRO:C	1:A:39:ALA:H	0.44	2.19	13	2
2:B:153:ASN:ND2	2:B:153:ASN:N	0.44	2.65	16	1
2:B:117:LYS:NZ	2:B:117:LYS:CB	0.44	2.80	19	1
2:B:22:GLN:OE1	2:B:27:ILE:C	0.44	2.60	1	1
1:A:37:PRO:O	1:A:38:GLU:C	0.44	2.61	13	6
2:B:162:VAL:O	2:B:163:ARG:C	0.44	2.61	3	1
2:B:16:LYS:CD	2:B:16:LYS:N	0.44	2.78	11	3
2:B:37:GLU:OE2	2:B:58:THR:CB	0.44	2.66	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:141:CYS:C	2:B:142:ALA:O	0.44	2.61	12	2
2:B:153:ASN:ND2	2:B:156:GLU:CD	0.44	2.76	9	1
1:A:35:ARG:NH1	1:A:40:LEU:CD2	0.44	2.81	13	1
1:A:24:MET:O	1:A:25:VAL:C	0.44	2.61	20	10
2:B:37:GLU:HB3	2:B:64:PHE:CD2	0.44	2.48	1	1
2:B:111:MET:HG2	2:B:141:CYS:SG	0.44	2.52	2	4
1:A:80:GLU:O	1:A:82:ARG:N	0.44	2.50	3	1
2:B:124:ARG:C	2:B:124:ARG:CD	0.44	2.91	13	3
2:B:160:ASP:OD2	2:B:161:LEU:N	0.44	2.50	4	1
1:A:30:ARG:CZ	1:A:33:ARG:NH2	0.44	2.81	6	1
1:A:3:ALA:O	1:A:75:ASN:OD1	0.44	2.36	12	2
2:B:155:ASN:OD1	2:B:156:GLU:OE2	0.44	2.35	20	1
2:B:134:LEU:CD1	2:B:138:TRP:NE1	0.44	2.78	12	6
1:A:3:ALA:O	1:A:75:ASN:ND2	0.44	2.41	2	1
2:B:2:ARG:NE	2:B:3:GLU:N	0.44	2.62	6	3
2:B:2:ARG:CG	2:B:4:TYR:CE1	0.44	3.00	4	1
2:B:37:GLU:C	2:B:37:GLU:OE1	0.44	2.60	14	3
1:A:75:ASN:N	1:A:75:ASN:ND2	0.44	2.64	17	1
1:A:51:LEU:HD12	1:A:62:LEU:HD21	0.44	1.88	13	2
2:B:145:GLU:O	2:B:153:ASN:OD1	0.44	2.36	15	2
2:B:139:ASN:O	2:B:140:ASN:OD1	0.44	2.35	3	1
2:B:45:GLU:OE2	2:B:50:GLN:OE1	0.44	2.35	4	2
2:B:62:GLU:O	2:B:65:THR:N	0.44	2.40	6	2
2:B:49:GLN:C	2:B:49:GLN:OE1	0.44	2.60	9	1
2:B:71:TYR:OH	2:B:100:ILE:CG1	0.44	2.66	15	1
2:B:61:THR:OG1	2:B:64:PHE:CZ	0.44	2.62	17	1
2:B:101:LEU:N	2:B:101:LEU:CD1	0.44	2.81	17	2
1:A:6:LEU:O	1:A:16:THR:O	0.44	2.36	2	2
2:B:37:GLU:CD	2:B:37:GLU:O	0.44	2.61	3	5
1:A:80:GLU:CD	1:A:82:ARG:NE	0.44	2.76	6	1
1:A:16:THR:OG1	2:B:38:ASP:HB2	0.44	2.13	9	1
1:A:69:ASP:C	1:A:69:ASP:OD1	0.44	2.61	9	1
1:A:26:TYR:C	1:A:29:CYS:SG	0.44	3.00	15	3
1:A:13:VAL:HG11	2:B:25:GLN:NE2	0.44	2.27	15	1
2:B:127:GLY:O	2:B:130:GLN:N	0.44	2.51	15	1
2:B:6:LEU:O	2:B:56:LEU:O	0.44	2.35	18	1
1:A:36:ILE:H	2:B:31:LYS:NZ	0.44	2.11	19	1
2:B:53:LEU:CD1	2:B:53:LEU:N	0.44	2.79	1	1
2:B:121:GLU:C	2:B:121:GLU:CD	0.44	2.86	18	12
2:B:155:ASN:O	2:B:158:PHE:CE1	0.44	2.71	1	1
1:A:14:VAL:HG12	2:B:38:ASP:OD2	0.44	2.12	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:TYR:CD2	1:A:26:TYR:O	0.44	2.71	3	1
2:B:64:PHE:CZ	2:B:67:MET:CB	0.44	3.01	3	1
2:B:166:ASN:ND2	2:B:166:ASN:N	0.44	2.64	17	2
2:B:97:ARG:HH11	2:B:138:TRP:NE1	0.44	2.11	5	1
1:A:13:VAL:HG21	2:B:25:GLN:NE2	0.44	2.27	8	1
1:A:33:ARG:O	1:A:40:LEU:HD11	0.44	2.12	11	1
1:A:69:ASP:OD2	1:A:69:ASP:C	0.44	2.61	12	1
1:A:37:PRO:CG	2:B:29:VAL:HG11	0.44	2.42	14	1
2:B:21:VAL:CG2	2:B:22:GLN:N	0.44	2.81	16	1
1:A:27:ASP:O	1:A:28:ALA:C	0.43	2.61	4	6
2:B:74:ASN:H	2:B:74:ASN:HD22	0.43	1.56	3	1
1:A:12:ASN:OD1	1:A:12:ASN:C	0.43	2.61	14	5
2:B:40:TYR:CD2	2:B:40:TYR:C	0.43	2.96	17	2
1:A:19:PHE:N	1:A:19:PHE:CD2	0.43	2.86	11	1
2:B:84:ILE:O	2:B:125:VAL:N	0.43	2.35	11	3
1:A:20:GLU:C	1:A:22:SER:H	0.43	2.20	17	2
2:B:4:TYR:HB3	2:B:6:LEU:HD21	0.43	1.90	17	1
1:A:35:ARG:HE	2:B:34:PRO:CD	0.43	2.26	1	1
2:B:62:GLU:CD	2:B:62:GLU:C	0.43	2.87	4	7
2:B:118:CYS:SG	2:B:145:GLU:OE1	0.43	2.73	1	2
2:B:10:GLY:O	2:B:11:SER:O	0.43	2.36	4	2
2:B:84:ILE:HA	2:B:126:VAL:HG13	0.43	1.90	4	3
2:B:16:LYS:O	2:B:20:THR:HG23	0.43	2.13	7	1
2:B:74:ASN:HD22	2:B:76:GLN:N	0.43	2.11	7	1
1:A:35:ARG:HB3	2:B:31:LYS:HZ3	0.43	1.73	19	1
2:B:124:ARG:O	2:B:124:ARG:CG	0.43	2.65	19	1
2:B:18:ALA:O	2:B:21:VAL:CG2	0.43	2.66	8	2
1:A:46:ASP:OD2	1:A:47:PHE:CD1	0.43	2.71	3	1
2:B:121:GLU:C	2:B:121:GLU:OE2	0.43	2.61	4	3
2:B:8:VAL:C	2:B:71:TYR:OH	0.43	2.61	14	2
2:B:91:ASN:O	2:B:94:GLN:OE1	0.43	2.37	5	2
2:B:97:ARG:C	2:B:99:GLN:N	0.43	2.76	6	2
2:B:121:GLU:C	2:B:121:GLU:OE1	0.43	2.61	8	2
1:A:15:LYS:HZ1	2:B:25:GLN:NE2	0.43	2.11	11	1
2:B:153:ASN:HD22	2:B:153:ASN:H	0.43	1.55	12	1
2:B:140:ASN:O	2:B:140:ASN:OD1	0.43	2.37	13	2
1:A:17:MET:HE3	1:A:35:ARG:HE	0.43	1.73	14	1
1:A:17:MET:HE1	1:A:31:MET:C	0.43	2.38	14	1
1:A:36:ILE:H	2:B:31:LYS:HE3	0.43	1.73	18	1
2:B:46:VAL:O	2:B:49:GLN:CD	0.43	2.62	1	14
1:A:15:LYS:O	1:A:16:THR:O	0.43	2.36	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:162:VAL:O	2:B:166:ASN:OD1	0.43	2.37	10	5
2:B:1:MET:HE3	2:B:1:MET:N	0.43	2.28	3	1
2:B:53:LEU:CD1	2:B:53:LEU:C	0.43	2.91	7	2
2:B:49:GLN:O	2:B:49:GLN:OE1	0.43	2.37	9	1
2:B:78:PHE:O	2:B:161:LEU:HD11	0.43	2.13	10	1
2:B:68:ARG:O	2:B:71:TYR:CG	0.43	2.71	11	1
2:B:7:VAL:HG12	2:B:71:TYR:CZ	0.43	2.48	14	1
2:B:46:VAL:O	2:B:49:GLN:OE1	0.43	2.37	18	3
2:B:156:GLU:CD	2:B:156:GLU:O	0.43	2.62	15	1
2:B:62:GLU:O	2:B:63:GLN:C	0.43	2.60	3	4
2:B:150:SER:O	2:B:151:LYS:C	0.43	2.61	10	11
1:A:33:ARG:NH2	1:A:42:GLY:O	0.43	2.42	5	1
1:A:33:ARG:O	1:A:40:LEU:CD2	0.43	2.67	8	1
2:B:92:ASP:OD2	2:B:96:LEU:HD11	0.43	2.14	8	1
2:B:64:PHE:CE2	2:B:68:ARG:NE	0.43	2.87	9	1
1:A:26:TYR:CD1	1:A:27:ASP:OD2	0.43	2.72	15	1
2:B:20:THR:HG1	2:B:21:VAL:HG13	0.43	1.74	16	1
2:B:72:MET:SD	2:B:72:MET:C	0.43	3.01	16	1
2:B:99:GLN:CD	2:B:99:GLN:C	0.43	2.86	17	1
2:B:16:LYS:NZ	2:B:59:ALA:CB	0.43	2.81	20	1
2:B:62:GLU:O	2:B:62:GLU:CD	0.43	2.62	7	2
2:B:37:GLU:CD	2:B:37:GLU:C	0.43	2.86	3	4
2:B:64:PHE:CD2	2:B:67:MET:HB2	0.43	2.49	5	1
2:B:96:LEU:O	2:B:100:ILE:HD13	0.43	2.13	7	1
2:B:145:GLU:C	2:B:145:GLU:OE2	0.43	2.62	13	1
2:B:20:THR:O	2:B:40:TYR:CE2	0.43	2.72	14	1
2:B:132:GLN:O	2:B:136:ARG:CB	0.43	2.67	14	1
1:A:35:ARG:NH2	1:A:39:ALA:CB	0.43	2.81	20	1
2:B:78:PHE:CE2	2:B:100:ILE:HG21	0.43	2.49	20	1
2:B:106:THR:OG1	2:B:107:ASP:N	0.43	2.51	6	5
2:B:97:ARG:CZ	2:B:138:TRP:CZ3	0.43	3.00	2	1
2:B:125:VAL:O	2:B:130:GLN:OE1	0.43	2.36	4	3
2:B:38:ASP:C	2:B:57:ASP:OD1	0.43	2.62	9	1
2:B:37:GLU:O	2:B:37:GLU:OE2	0.43	2.37	10	1
2:B:37:GLU:C	2:B:37:GLU:OE2	0.43	2.62	10	1
1:A:15:LYS:HZ3	1:A:36:ILE:HD13	0.43	1.69	13	1
2:B:107:ASP:OD1	2:B:138:TRP:O	0.43	2.37	13	1
2:B:62:GLU:OE2	2:B:63:GLN:OE1	0.43	2.37	17	1
1:A:10:ILE:C	1:A:12:ASN:N	0.43	2.76	19	1
2:B:45:GLU:OE1	2:B:50:GLN:OE1	0.43	2.37	16	2
2:B:74:ASN:C	2:B:74:ASN:HD22	0.43	2.21	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:VAL:HG21	2:B:25:GLN:CD	0.43	2.39	20	2
2:B:78:PHE:CE1	2:B:100:ILE:HG13	0.43	2.48	10	1
2:B:138:TRP:O	2:B:139:ASN:OD1	0.43	2.36	10	1
2:B:31:LYS:O	2:B:31:LYS:NZ	0.43	2.37	11	2
1:A:13:VAL:HG11	2:B:25:GLN:OE1	0.43	2.14	12	1
2:B:60:GLY:O	2:B:61:THR:HG23	0.43	2.13	12	1
2:B:56:LEU:HD21	2:B:71:TYR:CD2	0.43	2.48	18	1
2:B:37:GLU:C	2:B:38:ASP:OD1	0.43	2.61	20	1
1:A:43:PRO:C	1:A:45:ASN:N	0.43	2.74	18	2
1:A:85:GLN:O	1:A:86:ARG:OXT	0.43	2.37	12	1
2:B:78:PHE:CE2	2:B:100:ILE:HD11	0.43	2.49	12	1
2:B:35:THR:CG2	2:B:59:ALA:HB3	0.43	2.44	14	1
2:B:40:TYR:CE2	2:B:55:ILE:HD13	0.43	2.49	17	1
2:B:153:ASN:OD1	2:B:156:GLU:CD	0.43	2.62	19	2
2:B:53:LEU:C	2:B:53:LEU:HD22	0.43	2.39	2	1
2:B:16:LYS:HZ3	2:B:16:LYS:CB	0.43	2.25	7	1
1:A:34:GLU:O	1:A:35:ARG:O	0.43	2.37	8	1
2:B:74:ASN:O	2:B:76:GLN:OE1	0.43	2.36	10	1
1:A:85:GLN:O	1:A:86:ARG:O	0.43	2.37	11	1
2:B:119:ASP:OD1	2:B:119:ASP:O	0.43	2.37	12	1
1:A:15:LYS:NZ	1:A:36:ILE:CD1	0.43	2.80	13	1
2:B:76:GLN:C	2:B:76:GLN:OE1	0.43	2.61	13	1
2:B:5:LYS:N	2:B:76:GLN:OE1	0.43	2.42	16	1
1:A:46:ASP:O	1:A:46:ASP:CG	0.43	2.62	17	1
2:B:58:THR:OG1	2:B:68:ARG:NE	0.42	2.52	1	1
1:A:36:ILE:O	1:A:37:PRO:C	0.42	2.62	8	3
2:B:136:ARG:HA	2:B:140:ASN:H	0.42	1.72	20	11
2:B:62:GLU:OE2	2:B:62:GLU:O	0.42	2.36	5	1
2:B:132:GLN:C	2:B:132:GLN:OE1	0.42	2.61	5	4
2:B:138:TRP:CD1	2:B:138:TRP:N	0.42	2.87	5	1
2:B:156:GLU:CD	2:B:156:GLU:H	0.42	2.22	13	2
1:A:69:ASP:OD1	1:A:69:ASP:C	0.42	2.62	13	3
2:B:146:SER:OG	2:B:153:ASN:O	0.42	2.37	12	2
2:B:22:GLN:NE2	2:B:28:PHE:N	0.42	2.66	13	1
2:B:37:GLU:OE2	2:B:58:THR:O	0.42	2.36	13	1
1:A:13:VAL:O	1:A:13:VAL:CG1	0.42	2.66	16	1
2:B:124:ARG:O	2:B:124:ARG:CD	0.42	2.66	19	1
2:B:62:GLU:C	2:B:62:GLU:CD	0.42	2.87	17	4
1:A:6:LEU:CD2	1:A:77:ASP:CB	0.42	2.97	3	1
2:B:46:VAL:HG11	2:B:162:VAL:CG1	0.42	2.45	5	1
1:A:69:ASP:C	1:A:69:ASP:OD2	0.42	2.62	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:116:ASN:OD1	2:B:146:SER:C	0.42	2.62	6	4
2:B:22:GLN:CD	2:B:148:ALA:HB1	0.42	2.39	7	1
2:B:57:ASP:OD2	2:B:57:ASP:C	0.42	2.61	9	3
2:B:97:ARG:HH11	2:B:101:LEU:CD1	0.42	2.26	13	1
2:B:137:GLN:OE1	2:B:137:GLN:O	0.42	2.37	13	1
2:B:63:GLN:C	2:B:65:THR:N	0.42	2.76	14	2
2:B:20:THR:HG23	2:B:20:THR:O	0.42	2.13	15	1
2:B:145:GLU:OE2	2:B:145:GLU:O	0.42	2.36	17	1
2:B:152:ILE:C	2:B:154:VAL:N	0.42	2.75	11	4
1:A:15:LYS:NZ	2:B:33:ASP:CG	0.42	2.77	3	1
2:B:101:LEU:N	2:B:101:LEU:HD12	0.42	2.30	10	8
2:B:56:LEU:C	2:B:71:TYR:OH	0.42	2.61	4	1
2:B:58:THR:CG2	2:B:68:ARG:HE	0.42	2.26	5	1
2:B:67:MET:O	2:B:69:ASP:N	0.42	2.51	10	1
2:B:77:GLY:CA	2:B:161:LEU:HD12	0.42	2.44	13	1
1:A:17:MET:HE3	1:A:19:PHE:CZ	0.42	2.49	20	1
1:A:58:LYS:C	1:A:59:GLY:O	0.42	2.62	8	8
1:A:45:ASN:O	1:A:84:LYS:C	0.42	2.63	3	1
2:B:161:LEU:CD2	2:B:161:LEU:N	0.42	2.76	4	1
2:B:92:ASP:C	2:B:94:GLN:H	0.42	2.22	19	3
2:B:161:LEU:O	2:B:162:VAL:C	0.42	2.62	6	1
2:B:64:PHE:CD1	2:B:67:MET:HB2	0.42	2.49	11	2
2:B:153:ASN:CG	2:B:156:GLU:OE2	0.42	2.62	9	1
2:B:122:ASP:OD1	2:B:122:ASP:C	0.42	2.62	12	1
2:B:111:MET:CE	2:B:141:CYS:HG	0.42	2.27	13	1
2:B:96:LEU:HB2	2:B:97:ARG:NH2	0.42	2.29	18	1
2:B:82:TYR:OH	2:B:113:LEU:CD2	0.42	2.68	20	1
2:B:33:ASP:C	2:B:33:ASP:OD2	0.42	2.62	2	1
2:B:35:THR:C	2:B:36:ILE:O	0.42	2.62	5	5
2:B:17:SER:C	2:B:19:LEU:N	0.42	2.74	3	1
2:B:22:GLN:NE2	2:B:26:GLY:C	0.42	2.77	3	1
2:B:164:GLN:O	2:B:165:ILE:C	0.42	2.61	19	3
2:B:37:GLU:HB2	2:B:64:PHE:CE1	0.42	2.50	8	1
2:B:153:ASN:CG	2:B:156:GLU:OE1	0.42	2.62	16	2
2:B:56:LEU:C	2:B:57:ASP:CG	0.42	2.87	13	1
2:B:33:ASP:OD1	2:B:33:ASP:C	0.42	2.62	17	1
2:B:82:TYR:CD1	2:B:82:TYR:N	0.42	2.83	20	2
2:B:1:MET:HG3	2:B:2:ARG:H	0.42	1.74	18	1
2:B:36:ILE:HG13	2:B:37:GLU:N	0.42	2.28	19	1
1:A:27:ASP:C	1:A:30:ARG:H	0.42	2.21	20	1
2:B:37:GLU:OE2	2:B:57:ASP:O	0.42	2.37	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:129:GLU:O	2:B:133:ASN:N	0.42	2.52	2	1
1:A:6:LEU:O	1:A:8:ILE:N	0.42	2.53	3	1
2:B:167:ARG:CG	2:B:167:ARG:HH21	0.42	2.26	5	1
1:A:35:ARG:O	1:A:39:ALA:HB3	0.42	2.14	9	1
2:B:80:LEU:HD12	2:B:80:LEU:N	0.42	2.30	9	1
2:B:21:VAL:C	2:B:23:PHE:H	0.42	2.20	10	1
2:B:80:LEU:CD1	2:B:111:MET:SD	0.42	3.08	11	2
1:A:47:PHE:CD1	1:A:81:TYR:CZ	0.42	3.08	14	1
2:B:97:ARG:NH2	2:B:138:TRP:CD1	0.42	2.88	20	1
2:B:107:ASP:OD2	2:B:107:ASP:N	0.42	2.51	2	1
2:B:164:GLN:C	2:B:164:GLN:CD	0.42	2.87	4	1
2:B:15:GLY:O	2:B:19:LEU:HD12	0.42	2.14	6	2
2:B:80:LEU:CD1	2:B:80:LEU:N	0.42	2.81	12	1
2:B:22:GLN:CD	2:B:148:ALA:O	0.42	2.62	13	1
2:B:37:GLU:OE1	2:B:37:GLU:O	0.42	2.37	16	1
2:B:18:ALA:HB1	2:B:28:PHE:CD1	0.42	2.49	18	1
1:A:72:MET:C	1:A:73:LEU:O	0.42	2.63	1	6
2:B:121:GLU:CD	2:B:122:ASP:N	0.42	2.78	2	4
1:A:23:THR:CG2	1:A:27:ASP:OD1	0.42	2.68	9	1
2:B:167:ARG:NH2	2:B:167:ARG:CG	0.42	2.83	11	1
2:B:78:PHE:CE1	2:B:111:MET:CG	0.42	3.02	15	1
2:B:19:LEU:O	2:B:23:PHE:CB	0.42	2.67	16	1
2:B:112:ILE:HD12	2:B:142:ALA:C	0.42	2.38	17	1
1:A:12:ASN:HD21	2:B:41:ARG:CB	0.42	2.27	19	1
2:B:91:ASN:CG	2:B:94:GLN:OE1	0.42	2.62	20	1
1:A:72:MET:O	1:A:73:LEU:C	0.42	2.63	1	1
1:A:46:ASP:OD2	1:A:47:PHE:CZ	0.42	2.73	3	1
2:B:82:TYR:CZ	2:B:90:PHE:CZ	0.42	3.07	15	2
2:B:136:ARG:HA	2:B:140:ASN:N	0.42	2.29	20	4
2:B:139:ASN:O	2:B:140:ASN:C	0.42	2.62	7	3
2:B:62:GLU:OE2	2:B:62:GLU:N	0.42	2.40	8	1
1:A:30:ARG:C	1:A:32:ILE:H	0.42	2.21	9	1
2:B:112:ILE:HD12	2:B:142:ALA:HB3	0.42	1.91	12	2
2:B:155:ASN:CG	2:B:156:GLU:N	0.42	2.77	18	1
2:B:108:ASP:O	2:B:108:ASP:OD1	0.42	2.37	19	1
2:B:112:ILE:HB	2:B:161:LEU:HD21	0.42	1.91	19	1
2:B:19:LEU:HD21	2:B:116:ASN:CB	0.42	2.45	5	1
2:B:97:ARG:O	2:B:98:GLU:C	0.42	2.62	10	3
2:B:82:TYR:CG	2:B:90:PHE:CD2	0.42	3.08	13	1
2:B:21:VAL:C	2:B:27:ILE:O	0.42	2.63	15	1
1:A:17:MET:CE	1:A:35:ARG:CZ	0.42	2.96	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:VAL:C	1:A:15:LYS:O	0.42	2.62	17	1
2:B:4:TYR:CE1	2:B:51:CYS:CB	0.42	3.03	17	1
2:B:22:GLN:CD	2:B:22:GLN:C	0.42	2.87	19	1
2:B:33:ASP:OD1	2:B:40:TYR:OH	0.41	2.38	2	1
2:B:101:LEU:CD1	2:B:101:LEU:H	0.41	2.28	2	3
1:A:3:ALA:O	2:B:63:GLN:NE2	0.41	2.52	3	1
2:B:14:VAL:HG11	2:B:82:TYR:HA	0.41	1.92	4	1
1:A:31:MET:O	1:A:35:ARG:CD	0.41	2.68	5	2
2:B:58:THR:HB	2:B:64:PHE:CZ	0.41	2.50	6	1
2:B:78:PHE:CZ	2:B:100:ILE:CG1	0.41	3.03	7	1
1:A:40:LEU:HD12	1:A:40:LEU:H	0.41	1.74	8	1
2:B:113:LEU:HD23	2:B:131:GLY:O	0.41	2.15	11	1
2:B:80:LEU:CD2	2:B:97:ARG:NH2	0.41	2.82	18	1
1:A:5:SER:HB3	1:A:75:ASN:HD22	0.41	1.74	19	1
1:A:11:GLY:O	1:A:12:ASN:CB	0.41	2.68	19	1
1:A:17:MET:SD	1:A:17:MET:C	0.41	3.02	1	1
2:B:156:GLU:O	2:B:157:ILE:C	0.41	2.61	5	3
1:A:39:ALA:C	1:A:41:ALA:N	0.41	2.78	5	8
1:A:83:LYS:HB2	1:A:83:LYS:HZ2	0.41	1.76	5	1
2:B:134:LEU:CD1	2:B:138:TRP:HE1	0.41	2.26	5	1
2:B:81:VAL:C	2:B:82:TYR:CG	0.41	2.98	8	1
2:B:89:THR:C	2:B:91:ASN:H	0.41	2.24	8	1
1:A:40:LEU:C	1:A:42:GLY:N	0.41	2.78	14	3
2:B:78:PHE:CD1	2:B:97:ARG:NH1	0.41	2.88	9	1
2:B:121:GLU:CD	2:B:121:GLU:C	0.41	2.88	10	1
2:B:108:ASP:CG	2:B:167:ARG:NH1	0.41	2.79	19	1
2:B:72:MET:HE1	2:B:99:GLN:CB	0.41	2.45	1	1
1:A:8:ILE:HD11	1:A:79:MET:SD	0.41	2.55	2	1
2:B:67:MET:O	2:B:68:ARG:C	0.41	2.61	10	2
1:A:76:GLY:O	1:A:77:ASP:O	0.41	2.38	5	2
2:B:101:LEU:HD12	2:B:101:LEU:N	0.41	2.31	6	2
2:B:127:GLY:O	2:B:128:LYS:C	0.41	2.62	15	2
2:B:38:ASP:CA	2:B:57:ASP:OD1	0.41	2.68	9	1
1:A:17:MET:HE1	1:A:32:ILE:N	0.41	2.29	14	1
2:B:106:THR:O	2:B:109:VAL:HG23	0.41	2.15	16	2
2:B:157:ILE:O	2:B:158:PHE:C	0.41	2.62	16	1
2:B:53:LEU:O	2:B:55:ILE:CD1	0.41	2.69	19	1
1:A:15:LYS:HZ3	2:B:25:GLN:CD	0.41	2.24	2	1
1:A:17:MET:HE2	1:A:19:PHE:CE2	0.41	2.51	3	1
1:A:16:THR:O	2:B:38:ASP:OD1	0.41	2.38	11	2
2:B:62:GLU:H	2:B:62:GLU:CD	0.41	2.21	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:82:TYR:CE2	2:B:93:LEU:HD12	0.41	2.49	9	1
2:B:116:ASN:O	2:B:117:LYS:CB	0.41	2.69	17	3
2:B:64:PHE:CE2	2:B:68:ARG:CB	0.41	3.03	13	1
2:B:121:GLU:O	2:B:124:ARG:HB2	0.41	2.15	14	1
1:A:3:ALA:HB3	1:A:18:GLN:HB3	0.41	1.92	19	1
2:B:126:VAL:O	2:B:126:VAL:CG1	0.41	2.68	20	1
1:A:54:ASP:OD1	1:A:54:ASP:O	0.41	2.39	1	1
1:A:6:LEU:HD22	1:A:79:MET:SD	0.41	2.55	2	1
2:B:3:GLU:OE2	2:B:52:MET:SD	0.41	2.78	4	1
1:A:15:LYS:NZ	2:B:40:TYR:CD1	0.41	2.86	5	1
1:A:40:LEU:H	1:A:40:LEU:HD23	0.41	1.75	17	2
2:B:19:LEU:HD22	2:B:81:VAL:HG11	0.41	1.91	7	1
2:B:56:LEU:HD22	2:B:71:TYR:CE1	0.41	2.50	9	1
1:A:33:ARG:O	1:A:40:LEU:HD21	0.41	2.16	11	1
2:B:22:GLN:OE1	2:B:148:ALA:O	0.41	2.38	12	1
2:B:153:ASN:N	2:B:153:ASN:ND2	0.41	2.66	12	1
1:A:39:ALA:O	1:A:81:TYR:CZ	0.41	2.74	14	1
2:B:94:GLN:O	2:B:97:ARG:CG	0.41	2.69	15	1
2:B:7:VAL:N	2:B:77:GLY:O	0.41	2.41	18	1
2:B:82:TYR:HB3	2:B:93:LEU:HD11	0.41	1.92	5	1
1:A:12:ASN:C	1:A:13:VAL:CG1	0.41	2.93	6	1
2:B:60:GLY:O	2:B:61:THR:C	0.41	2.61	6	1
1:A:33:ARG:NH2	1:A:39:ALA:C	0.41	2.78	10	1
2:B:13:GLY:C	2:B:14:VAL:O	0.41	2.64	15	1
2:B:36:ILE:CG2	2:B:64:PHE:CE1	0.41	3.04	17	1
2:B:4:TYR:HB2	2:B:52:MET:O	0.41	2.16	20	1
2:B:137:GLN:C	2:B:139:ASN:N	0.41	2.78	13	2
2:B:16:LYS:HZ2	2:B:58:THR:H	0.41	1.58	7	1
2:B:139:ASN:C	2:B:140:ASN:HD22	0.41	2.24	9	1
2:B:100:ILE:O	2:B:103:VAL:HG22	0.41	2.16	15	1
2:B:16:LYS:HB3	2:B:16:LYS:HZ2	0.41	1.74	16	1
2:B:18:ALA:O	2:B:21:VAL:HG22	0.41	2.15	12	2
2:B:37:GLU:OE1	2:B:64:PHE:CB	0.41	2.69	8	1
2:B:64:PHE:O	2:B:64:PHE:CD1	0.41	2.74	9	1
2:B:28:PHE:CD2	2:B:28:PHE:O	0.41	2.74	10	1
1:A:30:ARG:O	1:A:33:ARG:CG	0.41	2.69	12	1
2:B:60:GLY:O	2:B:61:THR:CG2	0.41	2.69	12	1
1:A:10:ILE:HG23	1:A:81:TYR:CG	0.41	2.51	13	1
2:B:164:GLN:O	2:B:167:ARG:CD	0.41	2.69	13	1
2:B:22:GLN:C	2:B:22:GLN:NE2	0.41	2.79	16	1
2:B:116:ASN:OD1	2:B:147:SER:CA	0.41	2.69	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:53:LEU:O	2:B:53:LEU:HG	0.41	2.16	19	1
2:B:160:ASP:OD2	2:B:160:ASP:C	0.41	2.64	4	1
2:B:8:VAL:O	2:B:58:THR:HG22	0.41	2.16	8	1
2:B:68:ARG:NH1	2:B:96:LEU:HD22	0.41	2.30	9	1
1:A:24:MET:HA	1:A:66:LYS:O	0.41	2.15	11	1
2:B:95:ASP:O	2:B:98:GLU:N	0.41	2.54	11	1
2:B:147:SER:OG	2:B:150:SER:N	0.41	2.42	11	1
2:B:78:PHE:CD2	2:B:100:ILE:CD1	0.41	3.04	12	1
2:B:58:THR:CG2	2:B:64:PHE:CD2	0.41	3.02	14	1
2:B:61:THR:CB	2:B:64:PHE:CZ	0.41	3.04	17	1
2:B:56:LEU:HD21	2:B:71:TYR:CE1	0.41	2.51	18	1
2:B:53:LEU:O	2:B:53:LEU:CG	0.41	2.69	19	1
2:B:100:ILE:HG22	2:B:104:LYS:CG	0.41	2.46	19	1
1:A:35:ARG:HH22	1:A:39:ALA:HB2	0.41	1.75	20	1
2:B:16:LYS:NZ	2:B:59:ALA:HB1	0.41	2.31	20	1
1:A:6:LEU:HD12	1:A:6:LEU:N	0.41	2.26	2	1
1:A:45:ASN:OD1	1:A:45:ASN:O	0.41	2.39	5	1
1:A:16:THR:CB	2:B:37:GLU:O	0.41	2.69	8	1
2:B:117:LYS:C	2:B:119:ASP:H	0.41	2.24	10	2
2:B:165:ILE:C	2:B:167:ARG:N	0.41	2.79	16	2
2:B:21:VAL:CG2	2:B:40:TYR:OH	0.41	2.69	13	1
2:B:84:ILE:HG23	2:B:116:ASN:O	0.41	2.16	14	1
2:B:7:VAL:HG12	2:B:9:LEU:HD13	0.41	1.93	15	1
2:B:6:LEU:HB2	2:B:55:ILE:HG23	0.41	1.93	17	1
1:A:18:GLN:N	2:B:36:ILE:HD13	0.41	2.31	20	1
1:A:18:GLN:CD	2:B:36:ILE:HG23	0.40	2.41	1	1
1:A:26:TYR:N	1:A:64:ALA:C	0.40	2.80	3	1
2:B:134:LEU:O	2:B:138:TRP:CD1	0.40	2.74	5	1
2:B:4:TYR:OH	2:B:44:VAL:HG13	0.40	2.16	6	1
2:B:121:GLU:OE2	2:B:122:ASP:N	0.40	2.55	12	1
2:B:62:GLU:OE2	2:B:62:GLU:C	0.40	2.64	17	1
2:B:56:LEU:HD21	2:B:71:TYR:CE2	0.40	2.50	7	1
2:B:143:PHE:CZ	2:B:144:LEU:O	0.40	2.74	11	1
1:A:39:ALA:O	1:A:81:TYR:CE2	0.40	2.74	14	1
1:A:80:GLU:C	1:A:82:ARG:N	0.40	2.80	18	1
2:B:103:VAL:HG13	2:B:104:LYS:N	0.40	2.31	20	1
1:A:8:ILE:N	1:A:15:LYS:O	0.40	2.54	7	1
1:A:60:ILE:CD1	1:A:71:TYR:CE2	0.40	3.05	16	1
2:B:90:PHE:CD2	2:B:126:VAL:HG11	0.40	2.52	20	1
2:B:133:ASN:HD21	2:B:136:ARG:NH2	0.40	2.15	3	1
2:B:57:ASP:OD1	2:B:57:ASP:N	0.40	2.54	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:64:PHE:CD2	2:B:65:THR:N	0.40	2.89	4	1
2:B:119:ASP:O	2:B:119:ASP:OD2	0.40	2.40	9	1
2:B:30:GLU:CD	2:B:30:GLU:N	0.40	2.79	10	1
1:A:6:LEU:CD1	1:A:19:PHE:CD2	0.40	3.05	11	1
1:A:35:ARG:NH2	1:A:40:LEU:HD23	0.40	2.31	13	1
2:B:2:ARG:HH22	2:B:76:GLN:HE21	0.40	1.55	15	1
2:B:155:ASN:O	2:B:156:GLU:C	0.40	2.63	18	1
2:B:8:VAL:O	2:B:8:VAL:HG12	0.40	2.14	19	1
2:B:156:GLU:CD	2:B:156:GLU:N	0.40	2.79	20	1
2:B:37:GLU:CG	2:B:64:PHE:CZ	0.40	3.05	3	1
2:B:74:ASN:ND2	2:B:76:GLN:N	0.40	2.69	7	1
1:A:74:ARG:HG2	1:A:75:ASN:N	0.40	2.31	10	1
2:B:72:MET:CG	2:B:99:GLN:NE2	0.40	2.85	17	1
2:B:163:ARG:NH2	2:B:167:ARG:CZ	0.40	2.84	17	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	84/93 (90%)	51±3 (61±3%)	17±3 (20±4%)	16±2 (19±3%)	0	2
2	B	165/168 (98%)	129±3 (78±2%)	24±3 (14±2%)	12±1 (7±1%)	1	15
All	All	4980/5220 (95%)	3602 (72%)	804 (16%)	574 (12%)	1	7

All 60 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	21	PRO	20
1	A	53	ASP	20
1	A	56	PRO	20
1	A	69	ASP	20
1	A	75	ASN	20
1	A	77	ASP	20
2	B	14	VAL	20

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Mol	Chain	Res	Type	Models (Total)
2	B	34	PRO	20
2	B	48	ALA	20
2	B	124	ARG	20
2	B	139	ASN	20
2	B	142	ALA	20
1	A	2	VAL	19
2	B	36	ILE	19
2	B	53	LEU	19
2	B	60	GLY	18
2	B	105	ASP	18
1	A	3	ALA	17
1	A	8	ILE	15
1	A	36	ILE	15
1	A	4	LEU	15
1	A	5	SER	15
2	B	141	CYS	14
1	A	11	GLY	13
1	A	40	LEU	13
2	B	15	GLY	13
1	A	73	LEU	12
1	A	85	GLN	10
1	A	15	LYS	8
1	A	52	SER	8
1	A	59	GLY	7
2	B	153	ASN	7
1	A	66	LYS	7
1	A	64	ALA	5
1	A	14	VAL	4
1	A	31	MET	3
1	A	35	ARG	3
1	A	37	PRO	3
2	B	20	THR	3
2	B	21	VAL	3
1	A	16	THR	2
1	A	17	MET	2
2	B	11	SER	2
1	A	7	LYS	2
2	B	148	ALA	2
1	A	63	GLU	2
2	B	118	CYS	2
1	A	12	ASN	2
1	A	13	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	60	ILE	1
2	B	90	PHE	1
2	B	128	LYS	1
2	B	165	ILE	1
1	A	62	LEU	1
2	B	33	ASP	1
2	B	62	GLU	1
1	A	41	ALA	1
2	B	76	GLN	1
2	B	93	LEU	1
1	A	33	ARG	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	73/79 (92%)	58±2 (80±3%)	15±2 (20±3%)	3	33
2	B	148/149 (99%)	114±4 (77±3%)	34±4 (23±3%)	2	28
All	All	4420/4560 (97%)	3447 (78%)	973 (22%)	2	30

All 140 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	26	TYR	20
1	A	61	TRP	20
1	A	84	LYS	20
2	B	27	ILE	20
2	B	36	ILE	20
2	B	83	SER	20
2	B	151	LYS	19
1	A	10	ILE	18
1	A	23	THR	18
2	B	42	LYS	18
1	A	40	LEU	17
1	A	60	ILE	17
1	A	55	ASP	16

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Mol	Chain	Res	Type	Models (Total)
1	A	18	GLN	15
2	B	51	CYS	15
2	B	84	ILE	15
2	B	150	SER	15
2	B	154	VAL	15
2	B	157	ILE	15
2	B	167	ARG	15
1	A	6	LEU	14
2	B	53	LEU	14
2	B	72	MET	14
2	B	12	VAL	13
2	B	16	LYS	13
2	B	68	ARG	13
2	B	20	THR	13
2	B	132	GLN	13
1	A	83	LYS	13
1	A	13	VAL	12
1	A	74	ARG	12
2	B	6	LEU	12
2	B	106	THR	12
1	A	75	ASN	12
2	B	58	THR	11
2	B	64	PHE	11
2	B	104	LYS	11
2	B	161	LEU	11
2	B	76	GLN	11
2	B	5	LYS	11
2	B	33	ASP	10
2	B	137	GLN	10
1	A	57	LYS	9
2	B	35	THR	9
2	B	165	ILE	9
2	B	7	VAL	9
2	B	38	ASP	9
2	B	8	VAL	8
2	B	57	ASP	8
2	B	41	ARG	8
1	A	16	THR	7
2	B	9	LEU	7
2	B	30	GLU	7
2	B	65	THR	7
2	B	81	VAL	7

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Mol	Chain	Res	Type	Models (Total)
2	B	107	ASP	7
2	B	124	ARG	7
2	B	71	TYR	7
2	B	4	TYR	6
2	B	22	GLN	6
1	A	80	GLU	6
2	B	50	GLN	6
2	B	63	GLN	6
2	B	1	MET	6
2	B	80	LEU	6
2	B	82	TYR	6
2	B	147	SER	6
2	B	32	TYR	5
2	B	62	GLU	5
2	B	69	ASP	5
2	B	160	ASP	5
2	B	2	ARG	5
2	B	90	PHE	5
1	A	17	MET	4
2	B	133	ASN	4
2	B	14	VAL	4
2	B	70	LEU	4
2	B	74	ASN	4
1	A	51	LEU	4
2	B	145	GLU	4
2	B	37	GLU	4
2	B	40	TYR	4
2	B	139	ASN	4
2	B	61	THR	4
2	B	31	LYS	4
2	B	156	GLU	3
1	A	15	LYS	3
2	B	103	VAL	3
1	A	34	GLU	3
2	B	97	ARG	3
1	A	24	MET	3
1	A	46	ASP	3
1	A	81	TYR	3
1	A	12	ASN	3
1	A	72	MET	3
2	B	17	SER	3
1	A	66	LYS	3

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Mol	Chain	Res	Type	Models (Total)
2	B	29	VAL	3
2	B	39	SER	3
2	B	21	VAL	3
2	B	164	GLN	2
2	B	78	PHE	2
2	B	140	ASN	2
2	B	128	LYS	2
2	B	85	THR	2
2	B	123	GLU	2
2	B	52	MET	2
2	B	155	ASN	2
1	A	35	ARG	2
2	B	117	LYS	2
1	A	32	ILE	2
2	B	113	LEU	2
2	B	163	ARG	2
2	B	24	VAL	2
1	A	58	LYS	2
1	A	85	GLN	2
2	B	112	ILE	2
1	A	14	VAL	1
2	B	141	CYS	1
1	A	29	CYS	1
1	A	38	GLU	1
2	B	88	SER	1
2	B	126	VAL	1
2	B	130	GLN	1
2	B	159	TYR	1
2	B	87	GLN	1
1	A	4	LEU	1
2	B	93	LEU	1
2	B	158	PHE	1
2	B	110	PRO	1
2	B	100	ILE	1
2	B	34	PRO	1
2	B	146	SER	1
1	A	45	ASN	1
2	B	99	GLN	1
2	B	153	ASN	1
1	A	36	ILE	1
1	A	77	ASP	1
2	B	120	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	56	PRO	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 oligosaccharides 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

The completeness of assignment taking into account all chemical shift lists is 73% for the well-defined parts and 73% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1695
Number of shifts mapped to atoms	1695
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	164	-0.10 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	153	0.55 ± 0.14	Should be checked
$^{13}\text{C}'$	156	0.32 ± 0.07	None needed (< 0.5 ppm)
^{15}N	159	0.36 ± 0.37	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 48%, i.e. 1688 atoms were assigned a chemical shift out of a possible 3504. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	808/1262 (64%)	331/513 (65%)	318/504 (63%)	159/245 (65%)
Sidechain	880/2028 (43%)	573/1310 (44%)	307/628 (49%)	0/90 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/214 (0%)	0/102 (0%)	0/110 (0%)	0/2 (0%)
Overall	1688/3504 (48%)	904/1925 (47%)	625/1242 (50%)	159/337 (47%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 48%, i.e. 1695 atoms were assigned a chemical shift out of a possible 3519. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	811/1267 (64%)	332/515 (64%)	320/506 (63%)	159/246 (65%)
Sidechain	884/2038 (43%)	575/1317 (44%)	309/631 (49%)	0/90 (0%)
Aromatic	0/214 (0%)	0/102 (0%)	0/110 (0%)	0/2 (0%)
Overall	1695/3519 (48%)	907/1934 (47%)	629/1247 (50%)	159/338 (47%)

7.1.4 Statistically unusual chemical shifts [i](#)

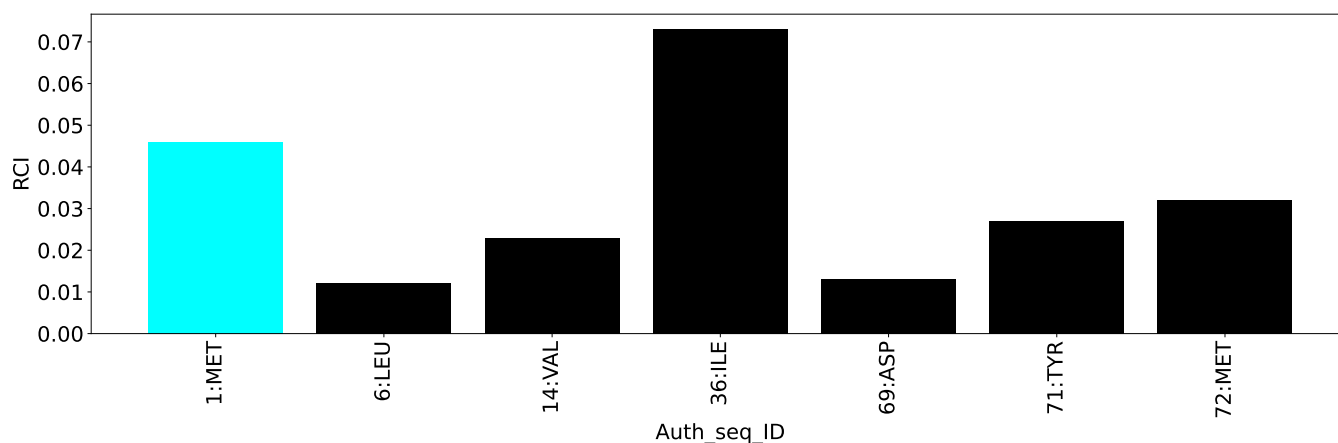
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	134	LEU	HG	-0.28	-0.13 – 3.16	-5.5

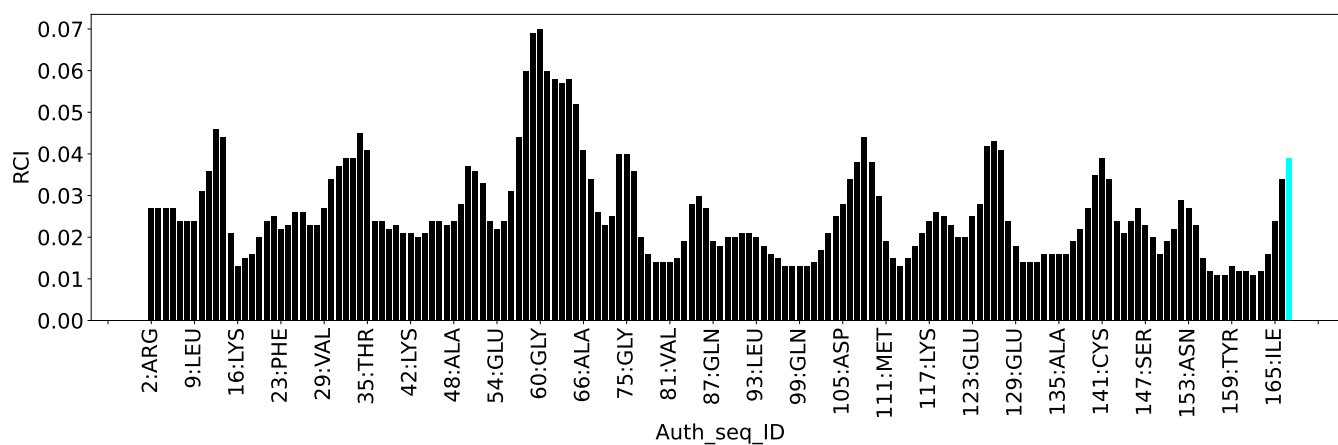
7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *taln-F0-bound-nc-noesy.str_assigned_chem_shift_list_1*

7.2.1 Bookkeeping ⓘ

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	884
Number of shifts mapped to atoms	884
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.2.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	84	0.19 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	79	0.42 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	73	-0.15 ± 0.57	None needed (< 0.5 ppm)

7.2.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 25%, i.e. 876 atoms were assigned a chemical shift out of a possible 3504. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	319/1262 (25%)	163/513 (32%)	83/504 (16%)	73/245 (30%)
Sidechain	555/2028 (27%)	367/1310 (28%)	183/628 (29%)	5/90 (6%)
Aromatic	2/214 (1%)	1/102 (1%)	0/110 (0%)	1/2 (50%)
Overall	876/3504 (25%)	531/1925 (28%)	266/1242 (21%)	79/337 (23%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 25%, i.e. 884 atoms were assigned a chemical shift out of a possible 3519. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	321/1267 (25%)	164/515 (32%)	84/506 (17%)	73/246 (30%)
Sidechain	561/2038 (28%)	371/1317 (28%)	185/631 (29%)	5/90 (6%)
Aromatic	2/214 (1%)	1/102 (1%)	0/110 (0%)	1/2 (50%)
Overall	884/3519 (25%)	536/1934 (28%)	269/1247 (22%)	79/338 (23%)

7.2.4 Statistically unusual chemical shifts ⓘ

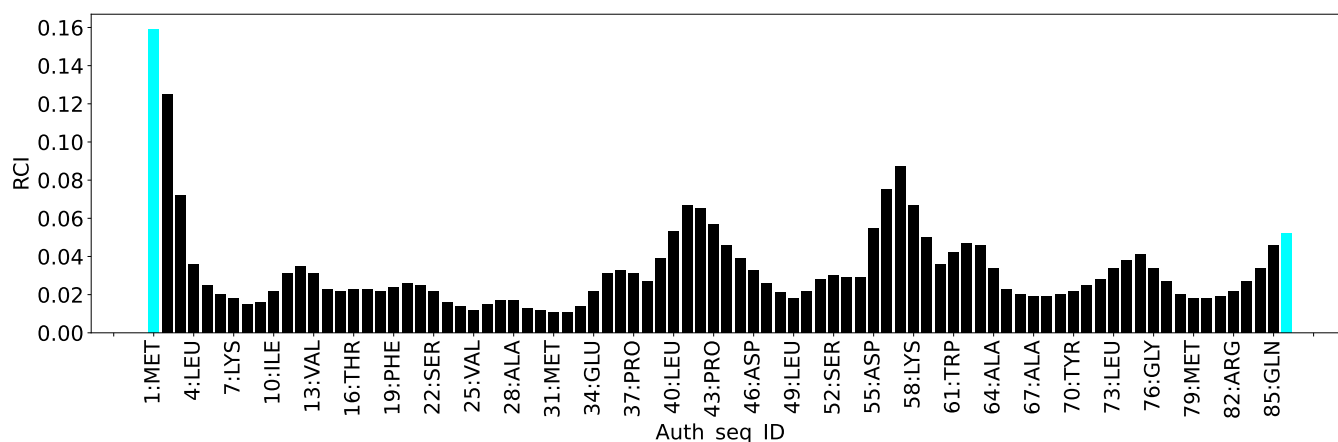
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	65	GLY	N	130.83	91.59 – 127.52	5.9
2	A	66	LYS	HD3	0.44	0.54 – 2.65	-5.5

7.2.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.3 Chemical shift list 3

File name: working_cs.cif

Chemical shift list name: *rap1b-bound-nc-noesy.str_assigned_chem_shift_list_1*

7.3.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1601
Number of shifts mapped to atoms	1601
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.3.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	166	0.05 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	156	0.50 ± 0.14	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	159	0.30 ± 0.40	None needed (< 0.5 ppm)

7.3.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 46%, i.e. 1595 atoms were assigned a chemical shift out of a possible 3504. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	658/1262 (52%)	334/513 (65%)	165/504 (33%)	159/245 (65%)
Sidechain	935/2028 (46%)	609/1310 (46%)	325/628 (52%)	1/90 (1%)
Aromatic	2/214 (1%)	1/102 (1%)	0/110 (0%)	1/2 (50%)
Overall	1595/3504 (46%)	944/1925 (49%)	490/1242 (39%)	161/337 (48%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 45%, i.e. 1601 atoms were assigned a chemical shift out of a possible 3519. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	660/1267 (52%)	335/515 (65%)	166/506 (33%)	159/246 (65%)
Sidechain	939/2038 (46%)	611/1317 (46%)	327/631 (52%)	1/90 (1%)
Aromatic	2/214 (1%)	1/102 (1%)	0/110 (0%)	1/2 (50%)
Overall	1601/3519 (45%)	947/1934 (49%)	493/1247 (40%)	161/338 (48%)

7.3.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

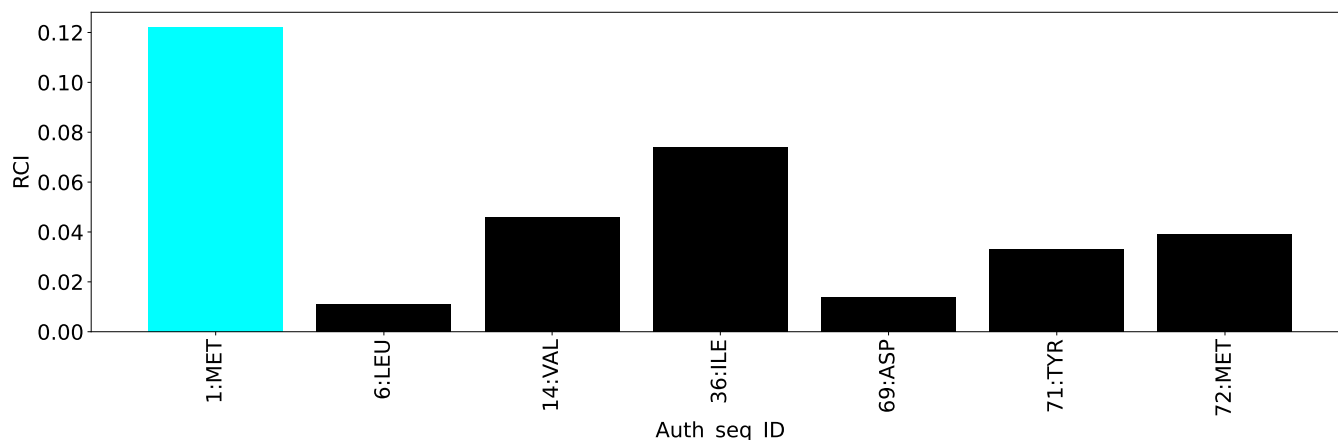
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
3	B	134	LEU	HG	-0.47	-0.13 – 3.16	-6.0

7.3.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication

of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

