Full wwPDB NMR Structure Validation Report (i)

May 7, 2024 – 12:30 pm BST

PDB ID	:	2WC2
Title	:	Nmr structure of catabolite activator protein in the unliganded state
Authors	:	Popovych, N.; Tzeng, S.R.; Kalodimos, C.G.
Deposited on	:	2009-03-06

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

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

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

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

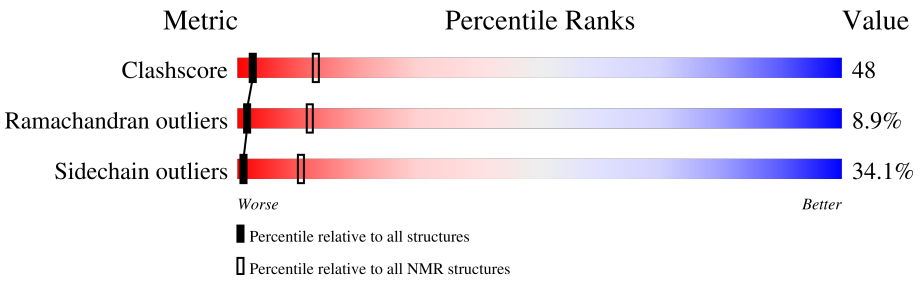
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	209	25% 51% 20% • •
1	B	209	26% 49% 20% • •

2 Ensemble composition and analysis (i)

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:8-A:209, B:8-B:209 (404)	1.10	3

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6704 atoms, of which 3404 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CATABOLITE GENE ACTIVATOR.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	209	3352	1044	1702	290	307	9	0
1	B	209	3352	1044	1702	290	307	9	0

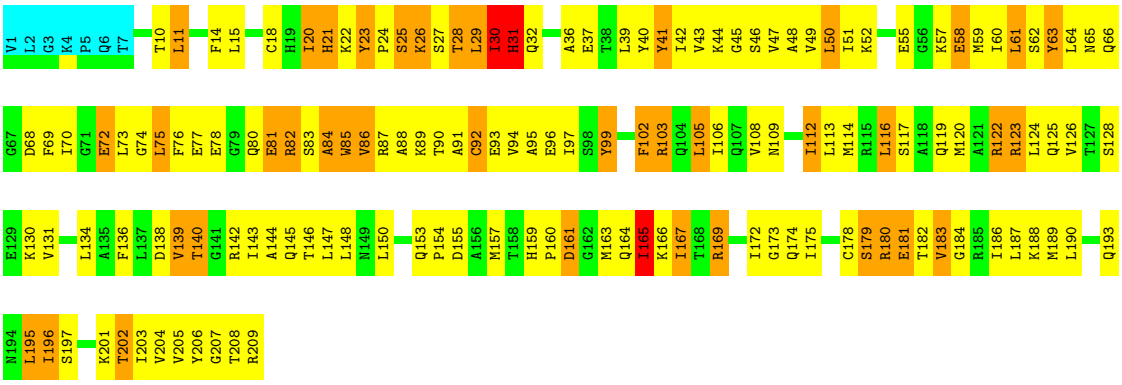
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

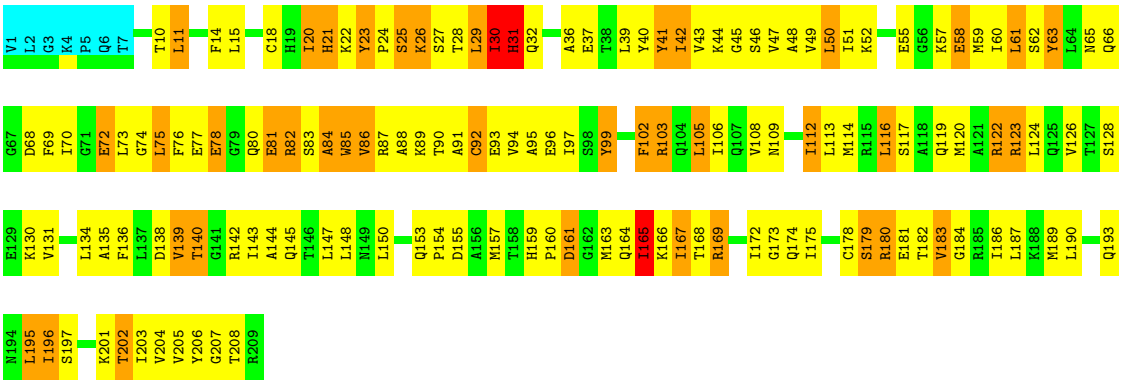
• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 25% 51% 20%



• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B: 26% 49% 20%



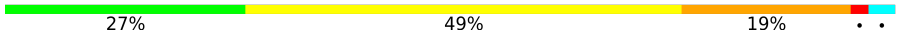
4.2 Scores per residue for each member of the ensemble

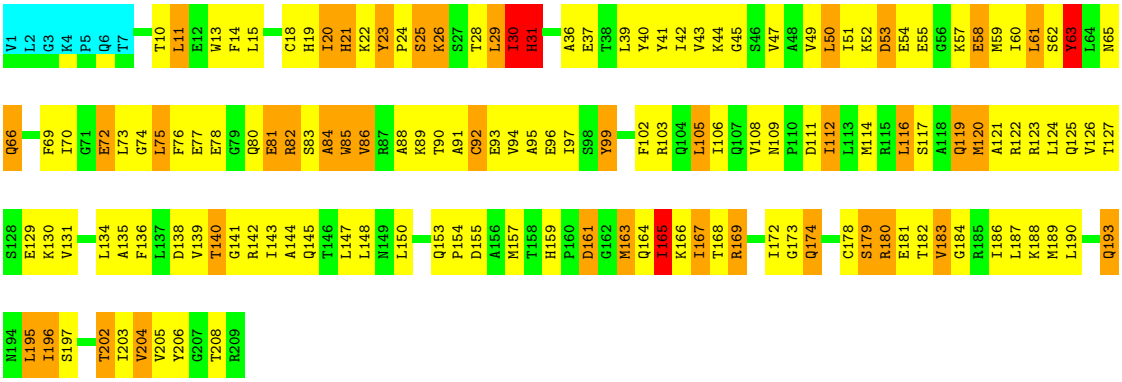
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: CATABOLITE GENE ACTIVATOR

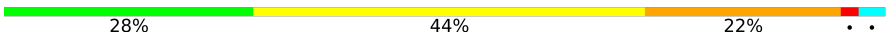
Chain A:

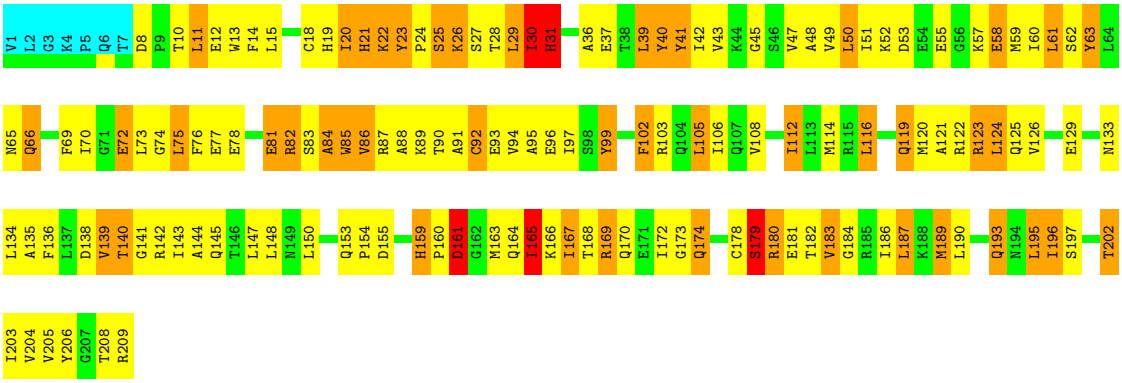




- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B:

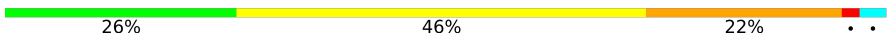


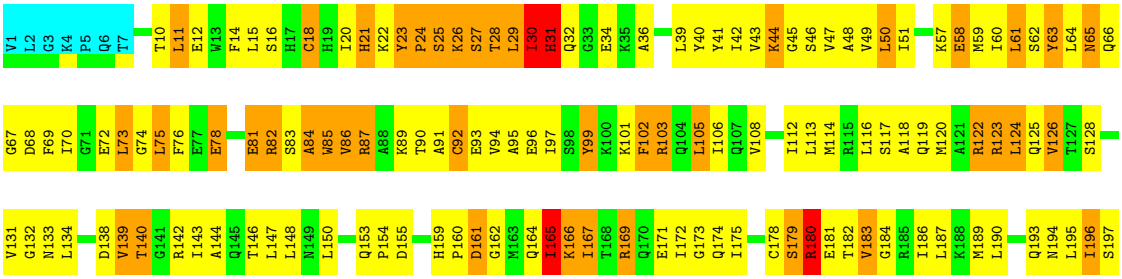


4.2.2 Score per residue for model 2

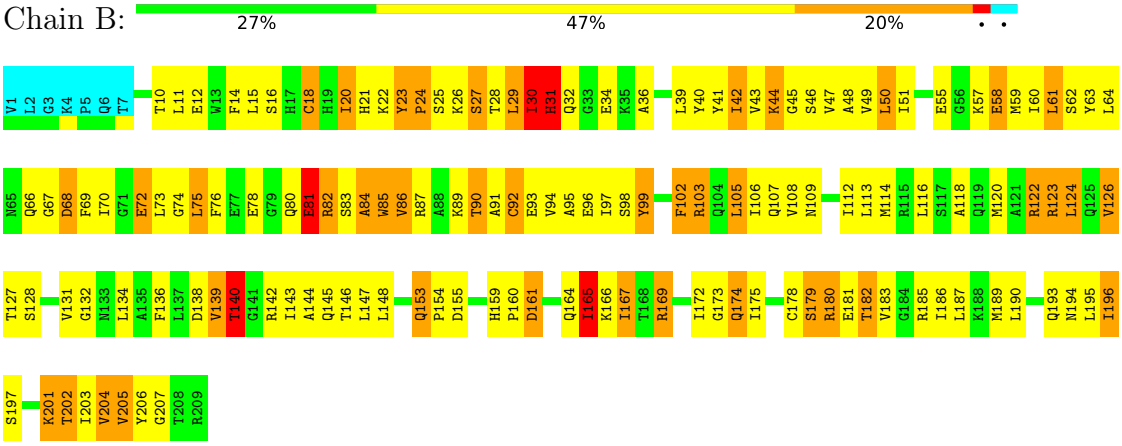
- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A:



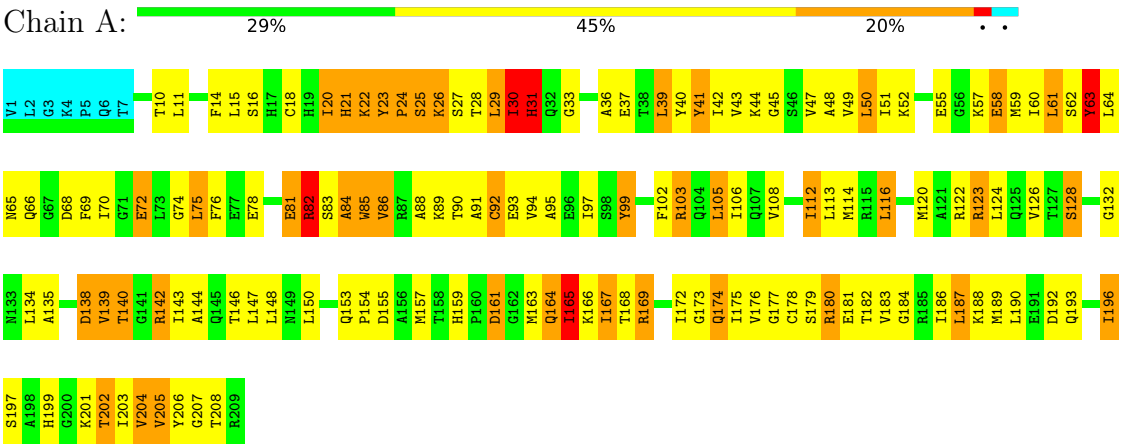


• Molecule 1: CATABOLITE GENE ACTIVATOR

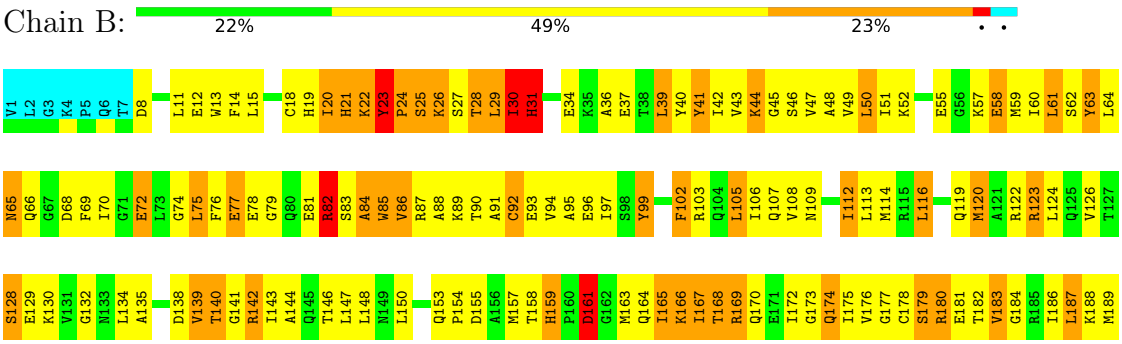


4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: CATABOLITE GENE ACTIVATOR



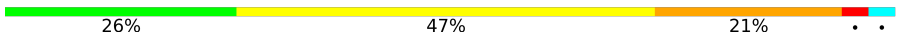
• Molecule 1: CATABOLITE GENE ACTIVATOR

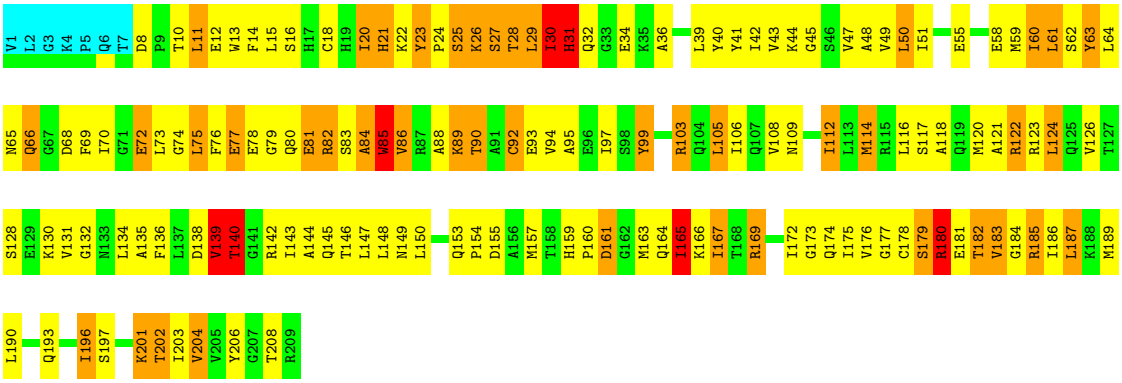


4.2.4 Score per residue for model 4

• Molecule 1: CATABOLITE GENE ACTIVATOR

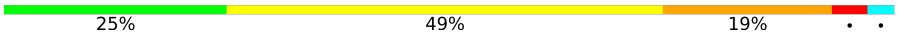
Chain A:

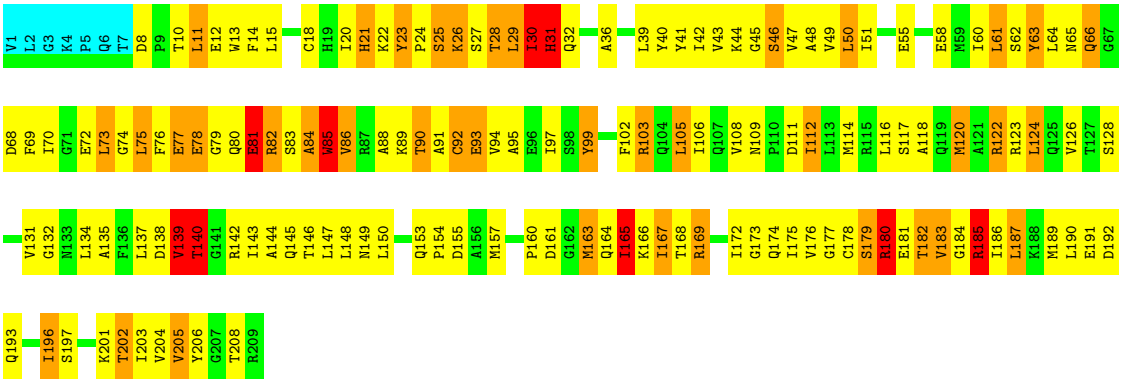




• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B:

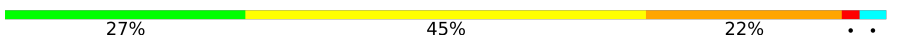


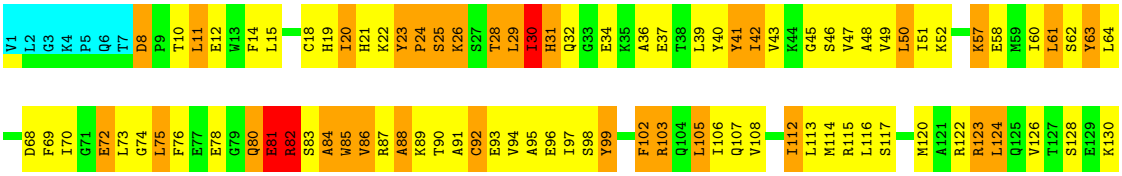


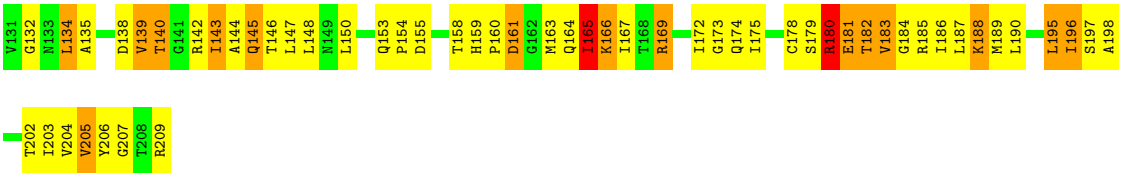
4.2.5 Score per residue for model 5

• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A:

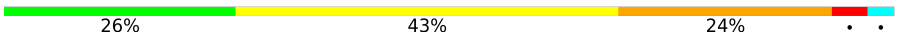


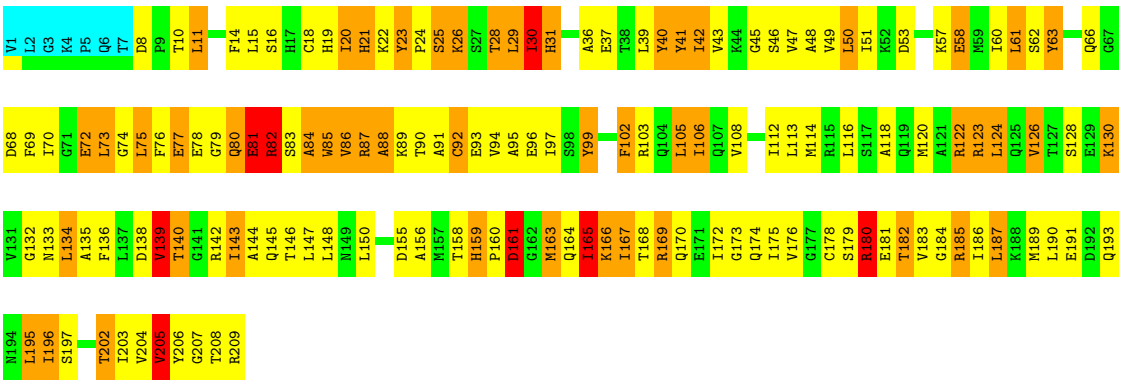




• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B:

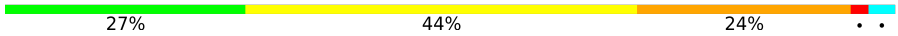


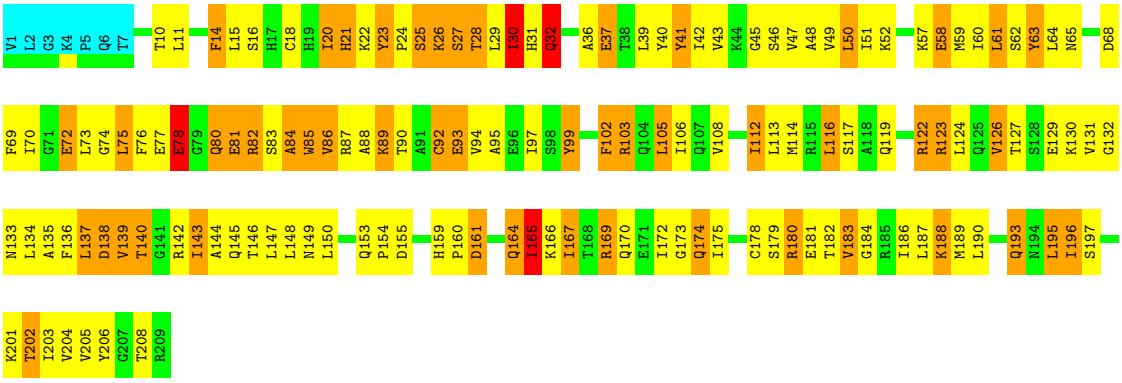


4.2.6 Score per residue for model 6

• Molecule 1: CATABOLITE GENE ACTIVATOR

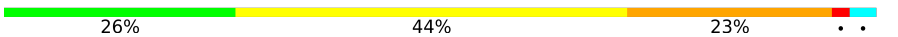
Chain A:

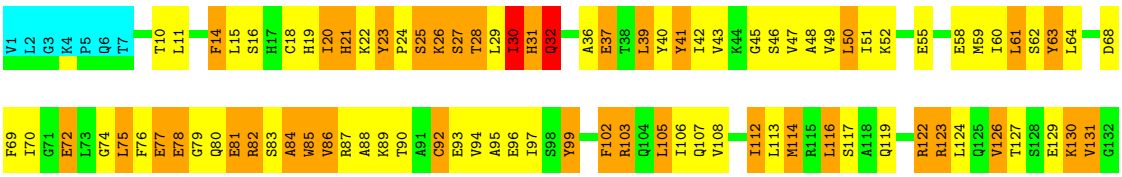


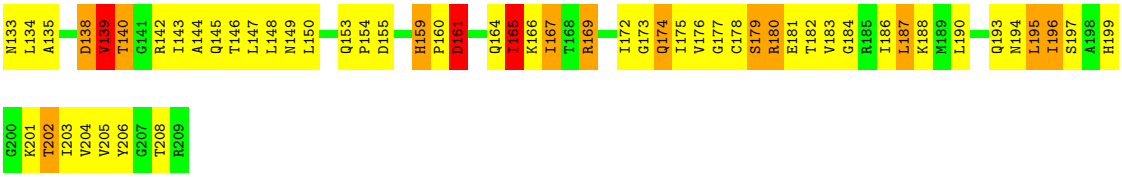


• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B:



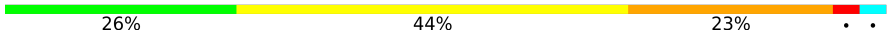


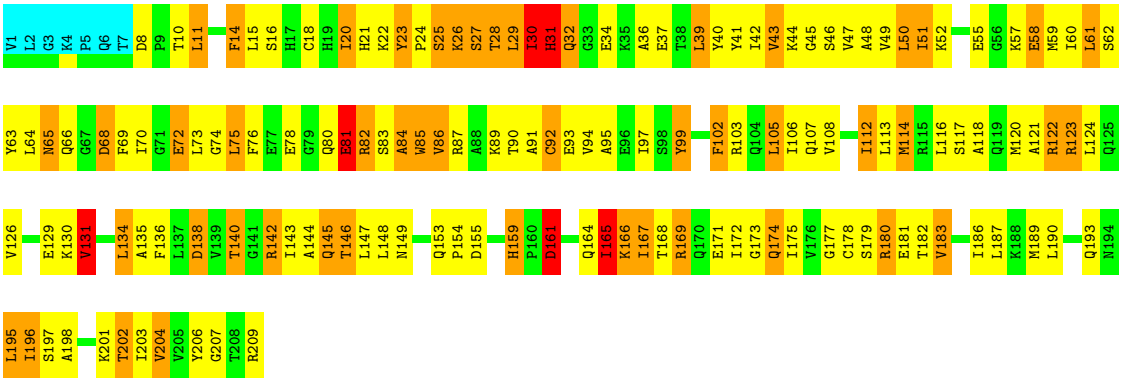


4.2.7 Score per residue for model 7

- Molecule 1: CATABOLITE GENE ACTIVATOR

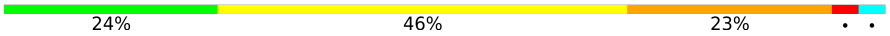
Chain A:

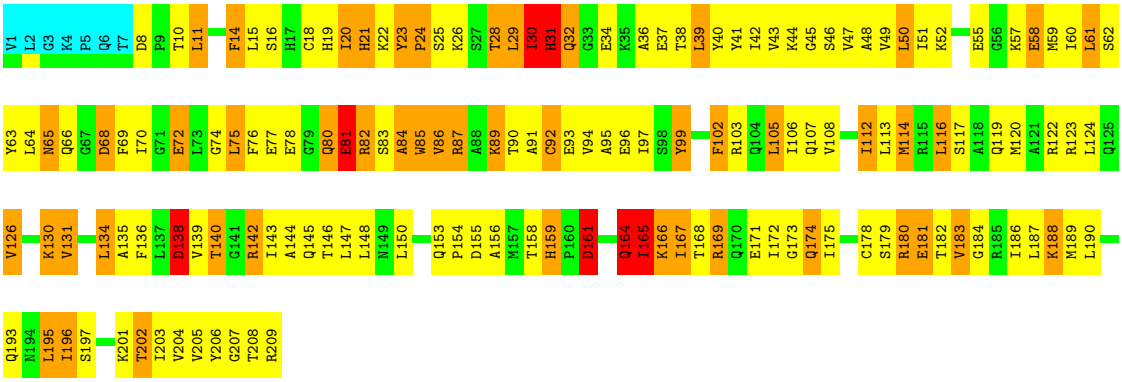




- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B:

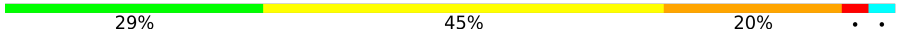


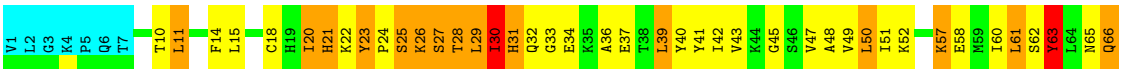


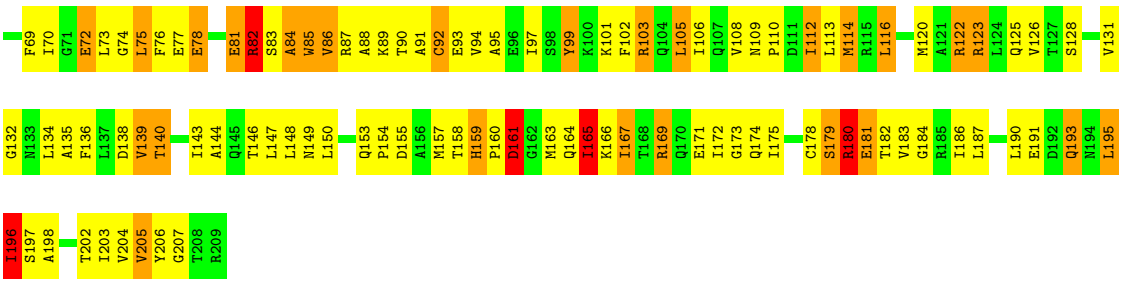
4.2.8 Score per residue for model 8

- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A:

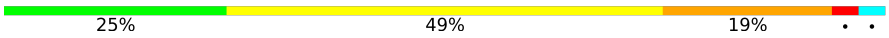


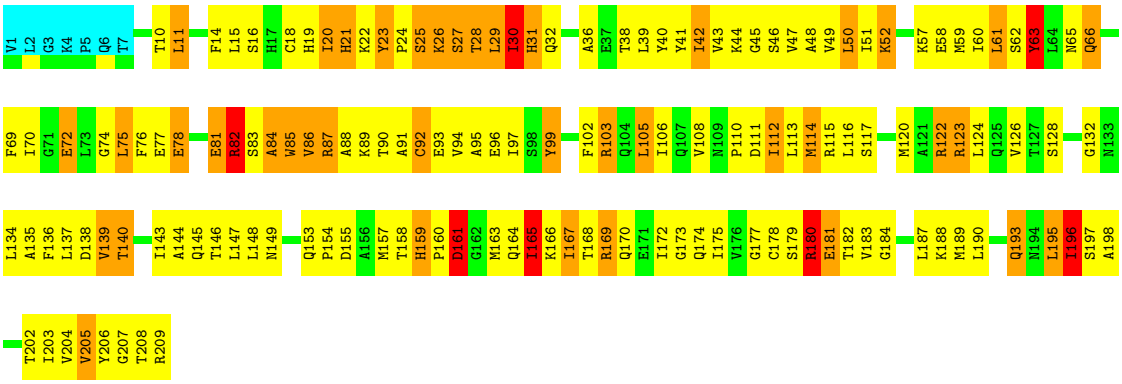




• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B:

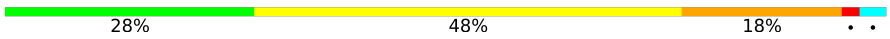


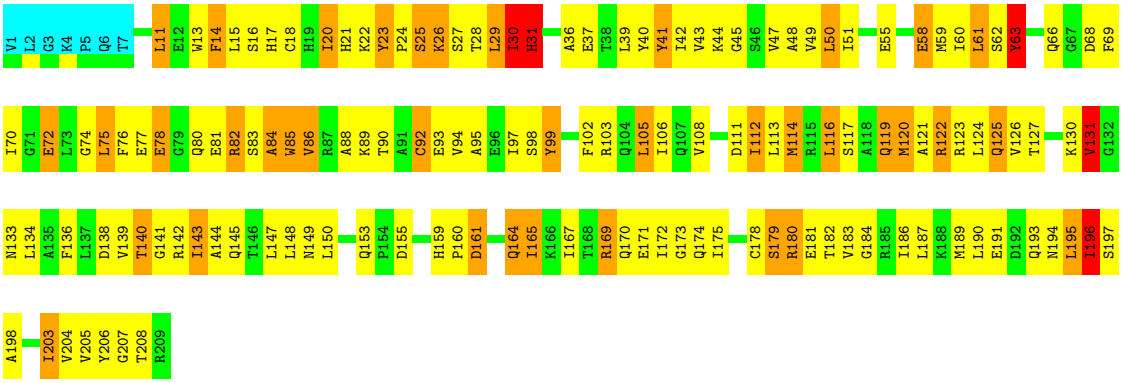


4.2.9 Score per residue for model 9

• Molecule 1: CATABOLITE GENE ACTIVATOR

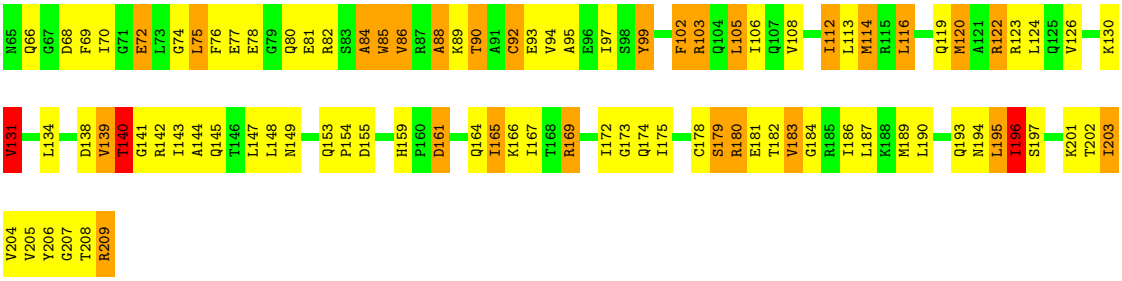
Chain A:





• Molecule 1: CATABOLITE GENE ACTIVATOR

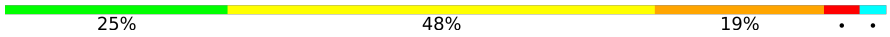
Chain B:

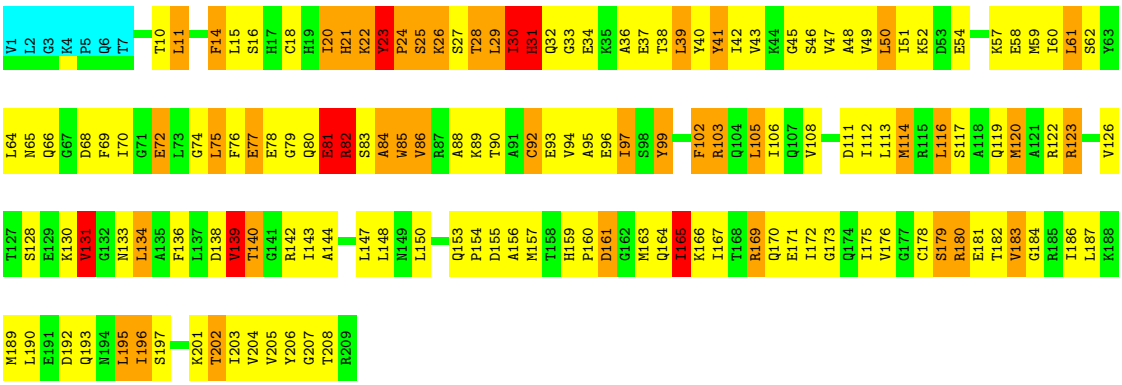


4.2.10 Score per residue for model 10

- Molecule 1: CATABOLITE GENE ACTIVATOR

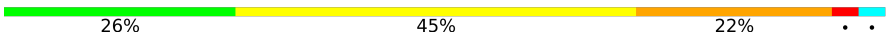
Chain A:

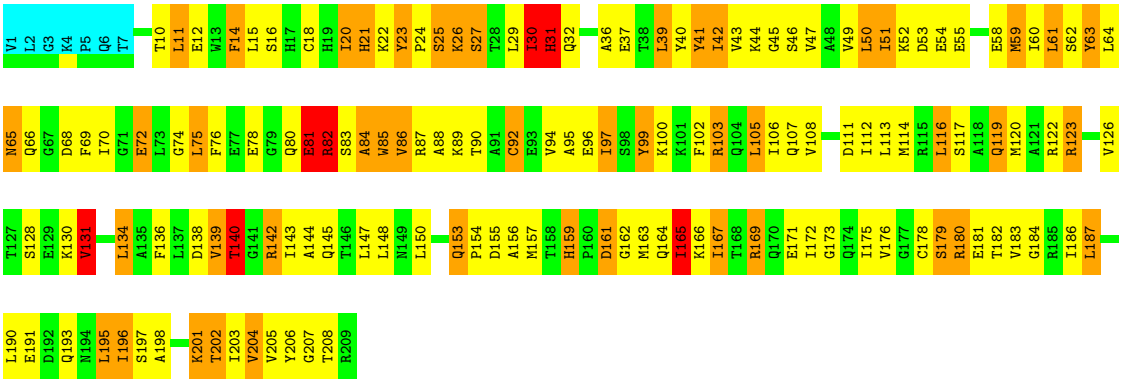




- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B:

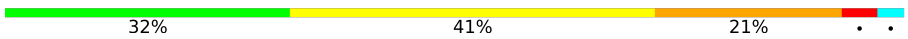


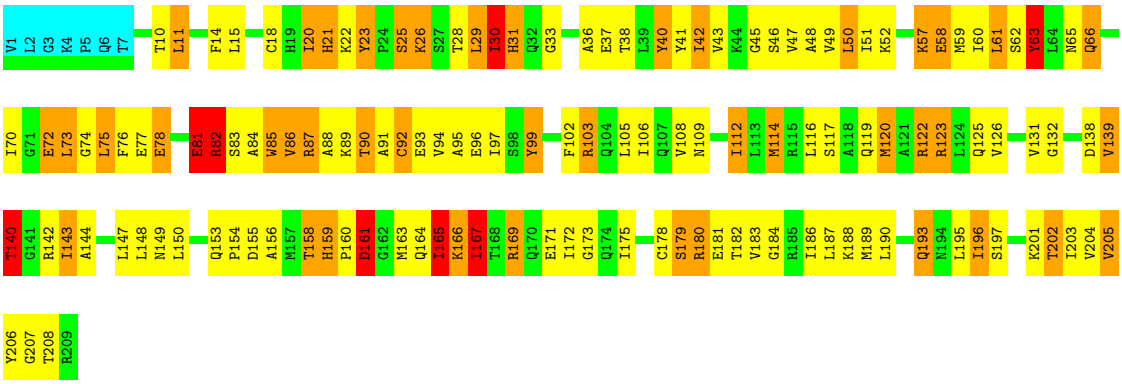


4.2.11 Score per residue for model 11

- Molecule 1: CATABOLITE GENE ACTIVATOR

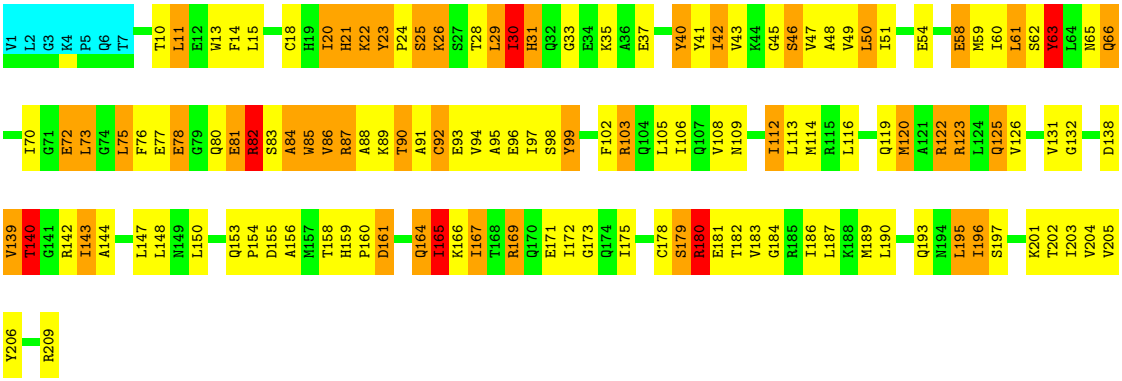
Chain A:





• Molecule 1: CATABOLITE GENE ACTIVATOR

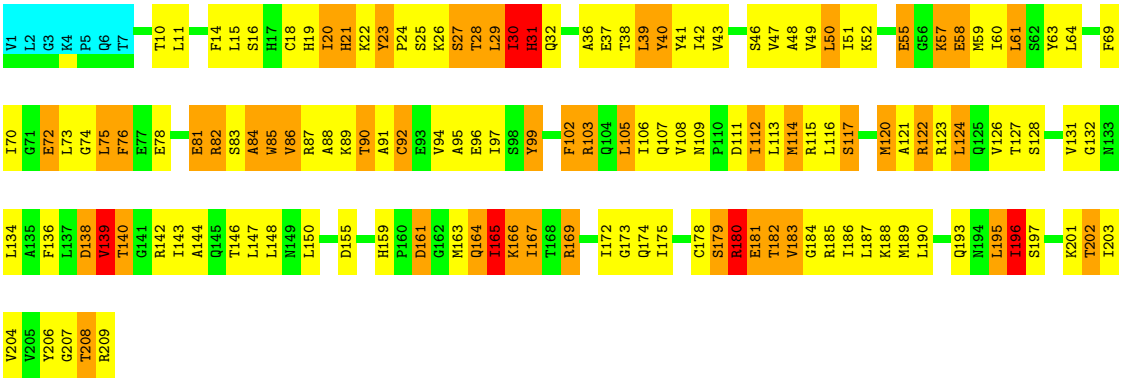
Chain B: 33% 40% 21%



4.2.12 Score per residue for model 12

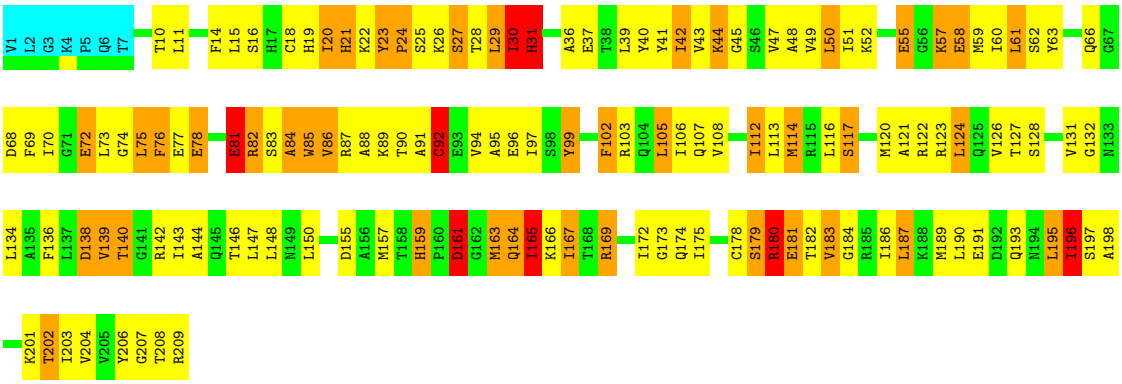
• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 29% 43% 22%



• Molecule 1: CATABOLITE GENE ACTIVATOR

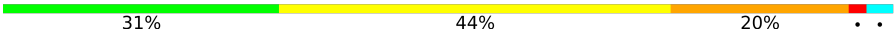
Chain B: 29% 44% 20%

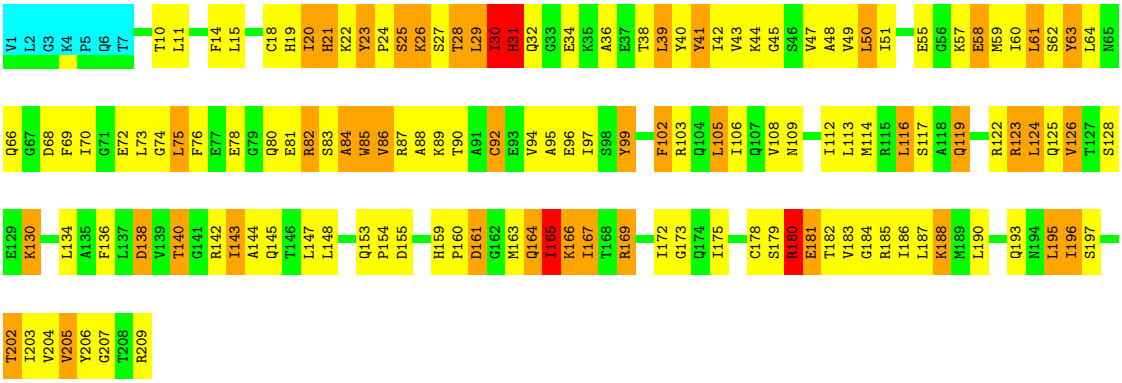


4.2.13 Score per residue for model 13

- Molecule 1: CATABOLITE GENE ACTIVATOR

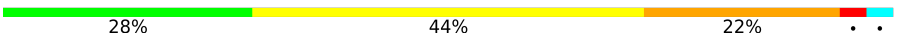
Chain A:

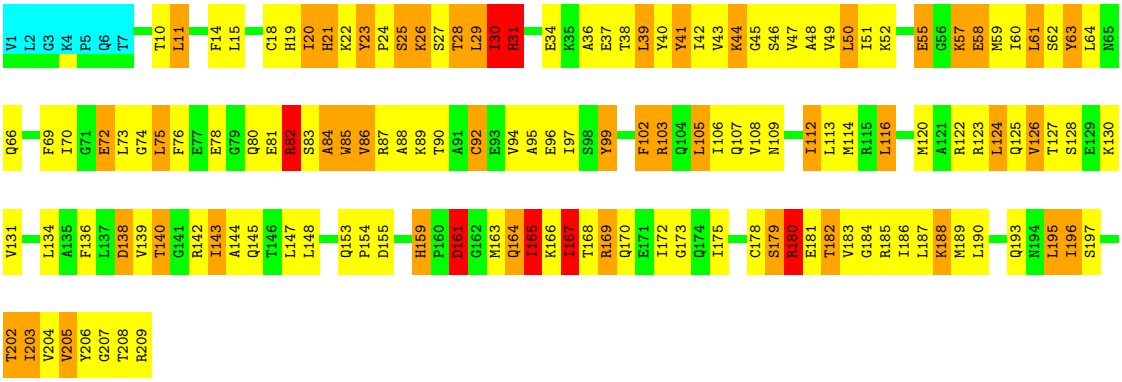




- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B:

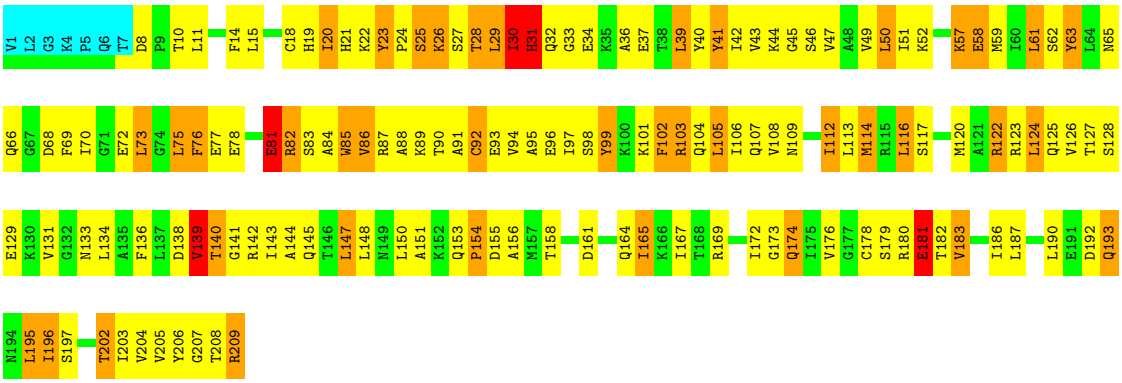




4.2.14 Score per residue for model 14

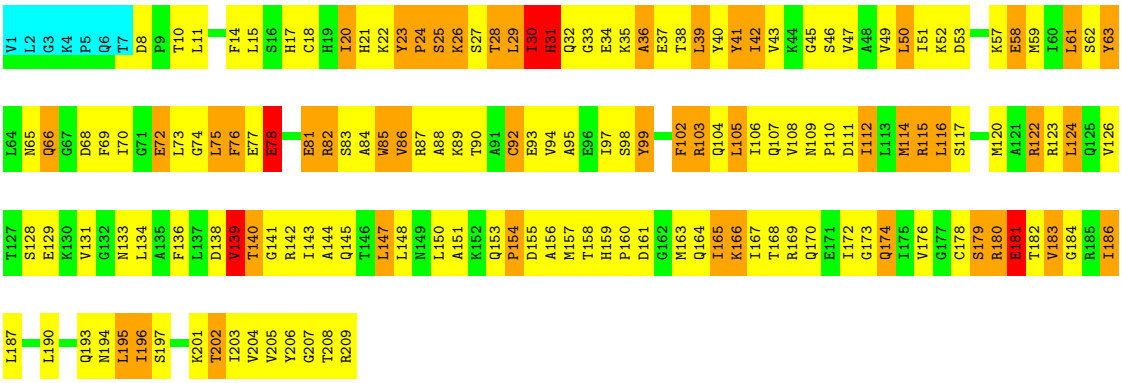
- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 26% 49% 19%



- Molecule 1: CATABOLITE GENE ACTIVATOR

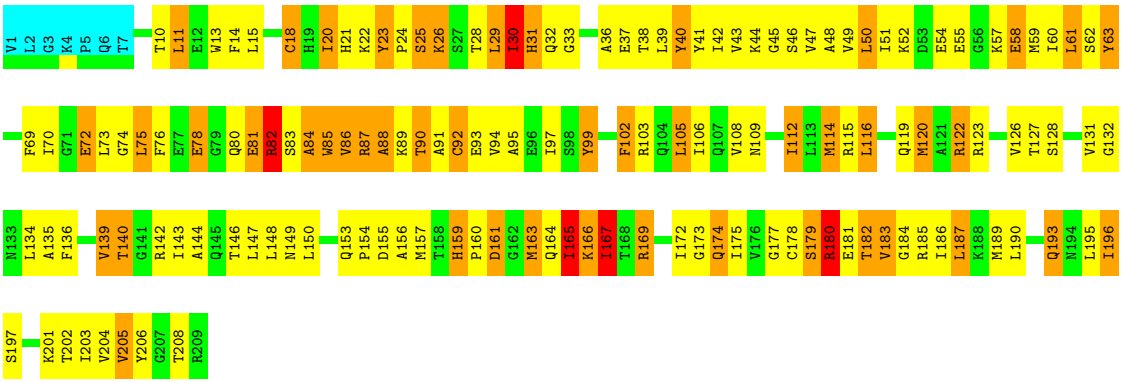
Chain B: 22% 50% 22%



4.2.15 Score per residue for model 15

- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 27% 44% 22%



- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B: 27% 46% 21%

V1 L2 G3 K4 P5 Q6 T7 D8 P9 T10 L11 E12 W13 F14 L15 S16 H17 C18 H19 I20 H21 K22 Y23 P24 S25 K26 S27 T28 L29 I30 H31 Q32 G33 E34 K35 A36 E37 T38 L39 Y40 Y41 I42 V43 K44 G45 S46 V47 A48 V49 L50 I51 K52 D53 K57 E58 M59 I60 L61 S62

Y63 F69 I70 G71 E72 L73 G74 L75 F76 E77 E78 G79 Q80 E81 R82 S83 A84 W85 V86 R87 A88 K89 T90 A91 C92 E93 V94 A95 E96 I97 S98 Y99 F102 R103 Q104 L105 I106 Q107 V108 N109 I112 L113 M114 R115 L116 Q119 M120 A121 R122 R123 V126 T127 S128 E129 K130

V131 G132 N133 L134 A135 F136 V139 T140 G141 R142 I143 L147 L148 N149 L150 Q153 P154 D155 A156 M157 P160 D161 G162 M163 Q164 I165 K166 I167 T168 R169 Q170 E171 I172 G173 Q174 I175 V176 G177 C178 S179 R180 E181 T182 V183 G184 R185 I186 L187 K188 M189 L190 Q193 N194 L195 I196

S197 K201 T202 I203 V204 V205 Y206 G207 T208 R209

4.2.16 Score per residue for model 16

- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 25% 48% 19%

V1 L2 G3 K4 P5 Q6 T7 T10 L11 E12 W13 F14 L15 C18 H19 I20 H21 K22 Y23 P24 S25 K26 S27 T28 L29 I30 H31 K35 A36 L39 Y40 Y41 I42 V43 K44 G45 S46 V47 A48 V49 L50 I51 K52 K57 E58 M59 I60 L61 S62 Y63 L64 N65 F69 I70

G71 E72 L73 G74 L75 F76 E77 E78 G79 Q80 E81 R82 S83 A84 W85 V86 R87 A88 K89 T90 A91 C92 E93 V94 A95 E96 I97 S98 Y99 F102 R103 Q104 L105 I106 Q107 V108 N109 P110 D111 I112 L113 M114 R115 L116 S117 A118 Q119 M120 A121 R122 R123 L124 Q125 V126 T127 S128 E129 K130 V131

L134 A135 F136 L137 D138 V139 T140 G141 R142 I143 A144 Q145 T146 L147 L148 N149 L150 A151 K152 Q153 P154 D155 A156 M157 T158 H159 P160 D161 G162 M163 Q164 I165 K166 I167 T168 R169 Q170 E171 I172 G173 Q174 I175 C178 S179 R180 E181 T182 V183 G184 R185 I186 L187 K188 M189 L190 Q193 N194

L195 I196 S197 K201 T202 I203 V204 V205 Y206 G207 T208 R209

- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B: 29% 44% 21%

V1 L2 G3 K4 P5 Q6 T7 T10 L11 E12 W13 F14 L15 C18 H19 I20 H21 K22 Y23 P24 S25 K26 S27 T28 L29 I30 H31 E34 K35 A36 L39 Y40 Y41 I42 V43 K44 G45 S46 V47 A48 V49 L50 I51 K57 E58 M59 I60 L61 S62 Y63 L64 N65 Q66 F69

I70 G71 E72 L73 G74 L75 F76 E77 E78 G79 Q80 E81 R82 S83 A84 W85 V86 R87 A88 K89 T90 A91 C92 E93 V94 A95 E96 I97 S98 Y99 F102 R103 Q104 L105 I106 Q107 V108 N109 P110 D111 I112 L113 M114 R115 L116 S117 A118 Q119 M120 A121 R122 R123 L124 Q125 V126 T127 S128 V131

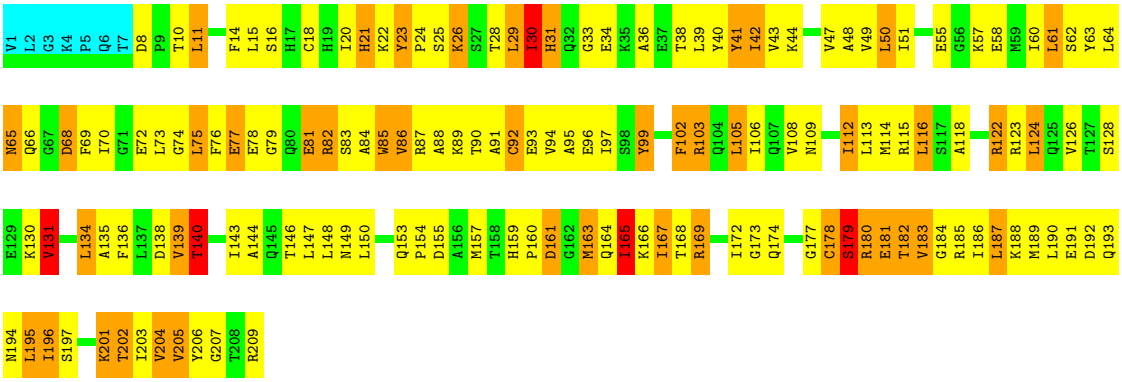
G132 N133 L134 A135 F136 L137 D138 V139 T140 G141 R142 I143 A144 Q145 T146 L147 L148 N149 L150 Q153 P154 D155 A156 M157 T158 H159 P160 D161 G162 M163 Q164 I165 K166 I167 T168 R169 I172 G173 Q174 I175 C178 S179 R180 E181 T182 V183 G184 R185 I186 L187 L190 Q193 N194 L195 I196

S197 T202 I203 V204 V205 Y206 G207 T208 R209

4.2.17 Score per residue for model 17

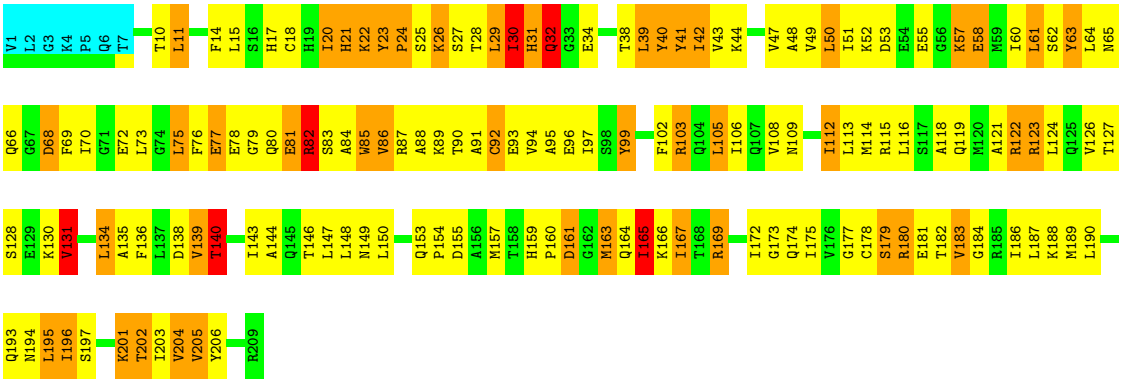
- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 25% 48% 22%



- Molecule 1: CATABOLITE GENE ACTIVATOR

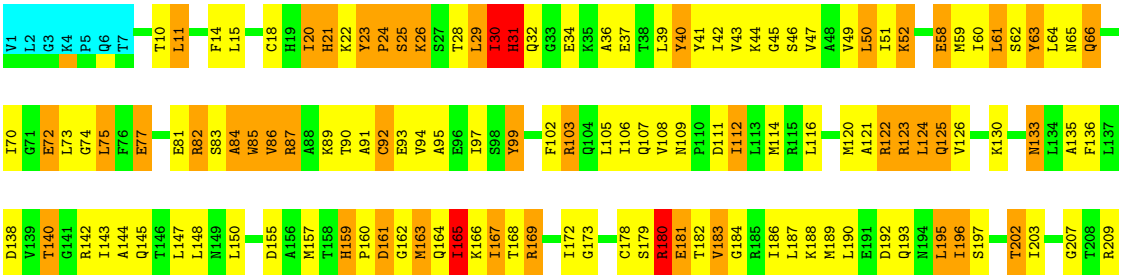
Chain B: 25% 46% 22%



4.2.18 Score per residue for model 18

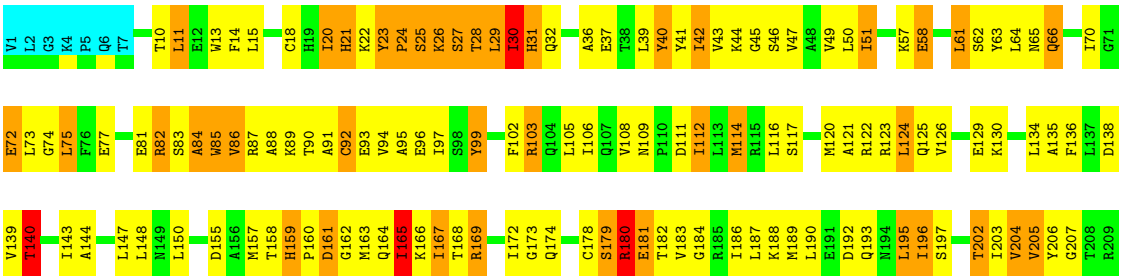
- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 34% 40% 21%



- Molecule 1: CATABOLITE GENE ACTIVATOR

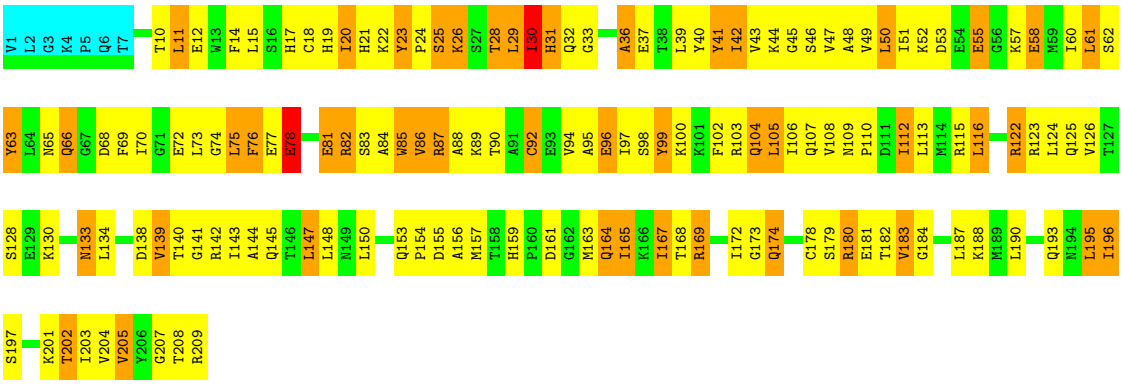
Chain B: 32% 44% 19%



4.2.19 Score per residue for model 19

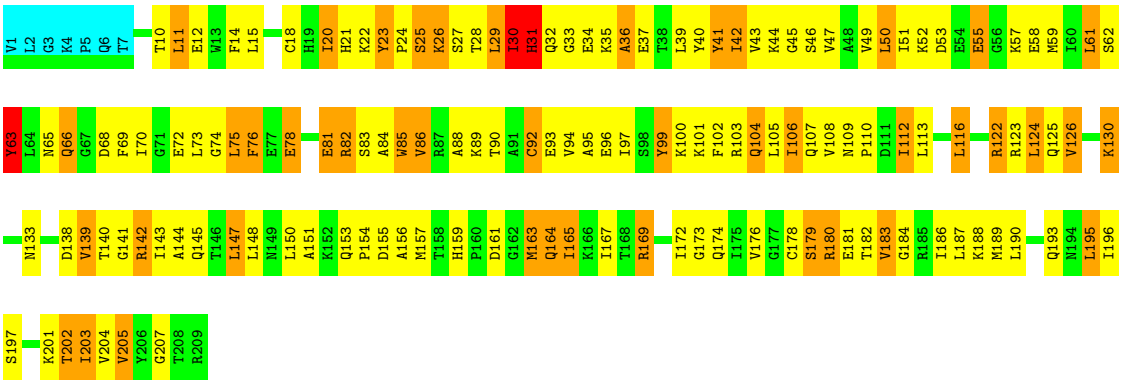
- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 27% 47% 22%



- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B: 28% 46% 21%



4.2.20 Score per residue for model 20

- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 28% 44% 21%

V1 L2 G3 K4 P5 Q6 T7 T10 L11 E12 W13 F14 L15 S16 H17 C18 H19 I20 H21 K22 Y23 P24 S25 K26 S27 T28 L29 I30 H31 Q32 A36 E37 T38 L39 Y40 Y41 I42 V43 K44 G45 S46 V47 A48 V49 L50 I51 K52 E55 G56 K57 E58 M59 I60 L61 S62 Y63

Q66 F69 I70 G71 E72 L73 G74 L75 F76 E77 E78 G79 Q80 E81 R82 S83 A84 W85 V86 R87 A88 K89 T90 A91 C92 E93 V94 A95 E96 I97 S98 Y99 F102 R103 Q104 L105 I106 Q107 V108 N109 I112 L113 M114 R115 L116 S117 A118 Q119 M120 A121 R122 R123 L124 Q125 V126 T127 S128

D138 V139 T140 G141 R142 I143 A144 L147 L148 N149 L150 Q153 P154 D155 A156 M157 T158 H159 P160 D161 G162 M163 Q164 I165 K166 I167 T168 R169 Q170 E171 I172 G173 C178 S179 R180 E181 T182 V183 G184 R185 I186 L187 K188 M189 L190 Q193 N194 L195 I196 S197 K201 T202 I203 V204

V205 Y206 G207 T208 R209

- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B: 26% 44% 22%

V1 L2 G3 K4 P5 Q6 T7 T10 L11 E12 W13 F14 L15 C18 H19 I20 H21 K22 Y23 P24 S25 K26 S27 T28 L29 I30 H31 Q32 G33 E34 K35 A36 E37 T38 L39 Y40 Y41 I42 V43 K44 G45 S46 V47 A48 V49 L50 I51 K52 D53 E54 E55 G56 K57 E58 M59 I60 L61 S62

Y63 Q66 G67 D68 F69 I70 G71 E72 L73 G74 L75 F76 E77 E78 E81 R82 S83 A84 W85 V86 R87 A88 K89 T90 A91 C92 E93 V94 A95 E96 I97 S98 Y99 K100 K101 F102 R103 Q104 L105 I106 Q107 V108 N109 I112 L113 M114 R115 L116 S117 A118 Q119 M120 A121 R122 R123 L124 Q125

V126 T127 S128 E129 K130 V131 L134 A135 D138 V139 T140 G141 R142 I143 A144 L147 L148 N149 L150 Q153 P154 D155 A156 M157 D161 G162 M163 Q164 I165 K166 I167 T168 R169 Q170 E171 I172 G173 Q174 I175 V176 G177 C178 S179 R180 E181 T182 V183 G184 R185 I186 L187 K188 M189 L190

Q193 N194 L195 I196 S197 T202 I203 V204 V205 Y206 G207 T208 R209

5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
HADDOCK-CNS	refinement	
NMRView	structure solution	
ARIA	structure solution	
HADDOCK	structure solution	
CNS	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.61±0.02	0±0/1624 (0.0± 0.0%)	0.98±0.02	2±1/2186 (0.1± 0.0%)
1	B	0.61±0.01	0±0/1624 (0.0± 0.0%)	0.98±0.02	3±1/2186 (0.1± 0.0%)
All	All	0.61	0/64960 (0.0%)	0.98	97/87438 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.7±0.6
1	B	0.0±0.0	0.7±0.7
All	All	0	28

There are no bond-length outliers.

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	205	VAL	N-CA-C	-8.55	87.91	111.00	11	15
1	B	205	VAL	N-CA-C	-7.64	90.37	111.00	4	19
1	B	24	PRO	CA-C-N	-6.58	102.71	117.20	12	8
1	A	28	THR	CA-C-N	-6.44	103.04	117.20	4	4
1	A	24	PRO	CA-C-N	-6.39	103.15	117.20	5	6
1	B	63	TYR	CA-C-N	-6.16	103.66	117.20	19	7
1	A	63	TYR	CA-C-N	-6.07	103.85	117.20	19	9
1	B	28	THR	CA-C-N	-6.01	103.98	117.20	4	3
1	B	187	LEU	CB-CA-C	5.63	120.91	110.20	6	8
1	B	138	ASP	N-CA-C	5.54	125.97	111.00	12	3
1	A	187	LEU	CB-CA-C	5.42	120.49	110.20	3	4
1	B	23	TYR	CB-CG-CD1	5.39	124.23	121.00	3	1
1	A	179	SER	CA-C-N	-5.29	105.56	117.20	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	164	GLN	CA-C-N	-5.25	105.64	117.20	7	1
1	A	138	ASP	N-CA-C	5.22	125.08	111.00	12	2
1	B	30	ILE	CA-C-N	-5.15	105.86	117.20	17	1
1	A	31	HIS	N-CA-CB	-5.15	101.33	110.60	7	1
1	A	30	ILE	CA-C-N	-5.13	105.91	117.20	17	1
1	A	30	ILE	N-CA-CB	5.13	122.60	110.80	20	1
1	A	23	TYR	CB-CG-CD1	5.11	124.06	121.00	10	2

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	31	HIS	Mainchain	13
1	B	31	HIS	Mainchain	11
1	B	179	SER	Mainchain	1
1	A	138	ASP	Mainchain	1
1	B	138	ASP	Mainchain	1
1	B	92	CYS	Mainchain	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1599	1642	1636	157±10
1	B	1599	1642	1636	157±11
All	All	63960	65680	65439	6157

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 48.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:VAL:O	1:A:66:GLN:CG	1.08	2.02	17	2
1:A:43:VAL:O	1:A:66:GLN:HG3	1.06	1.47	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:VAL:O	1:B:66:GLN:CG	1.01	2.08	17	2
1:B:18:CYS:SG	1:B:95:ALA:HB1	0.97	2.00	4	20
1:A:190:LEU:HD22	1:A:196:ILE:HG12	0.97	1.32	13	3
1:B:169:ARG:HB3	1:B:187:LEU:HD12	0.96	1.37	20	19
1:A:18:CYS:SG	1:A:95:ALA:HB1	0.96	2.01	18	20
1:B:44:LYS:HA	1:B:66:GLN:HG3	0.94	1.39	17	6
1:A:169:ARG:HB3	1:A:187:LEU:HD12	0.93	1.39	15	20
1:A:153:GLN:OE1	1:A:155:ASP:OD2	0.93	1.87	14	1
1:B:43:VAL:O	1:B:66:GLN:HG3	0.92	1.62	17	2
1:B:153:GLN:OE1	1:B:155:ASP:OD2	0.90	1.89	14	1
1:A:49:VAL:HB	1:A:62:SER:O	0.90	1.65	16	4
1:B:173:GLY:HA2	1:B:178:CYS:O	0.89	1.66	17	19
1:B:49:VAL:HB	1:B:62:SER:O	0.88	1.68	6	3
1:B:51:ILE:O	1:B:58:GLU:HA	0.87	1.68	20	20
1:A:42:ILE:HD11	1:A:46:SER:HA	0.87	1.47	11	8
1:A:135:ALA:HB3	1:B:135:ALA:HB3	0.87	1.45	3	7
1:A:15:LEU:HA	1:A:18:CYS:SG	0.86	2.10	20	20
1:B:22:LYS:HB3	1:B:92:CYS:O	0.86	1.70	12	19
1:A:70:ILE:HG23	1:A:86:VAL:HG21	0.85	1.46	10	15
1:B:40:TYR:O	1:B:70:ILE:HB	0.85	1.71	2	20
1:B:45:GLY:H	1:B:66:GLN:HG2	0.84	1.29	8	8
1:B:42:ILE:HD11	1:B:46:SER:HA	0.84	1.48	11	10
1:A:40:TYR:O	1:A:70:ILE:HB	0.84	1.73	12	20
1:A:45:GLY:H	1:A:66:GLN:HG2	0.84	1.33	19	7
1:A:15:LEU:HB3	1:A:20:ILE:HD11	0.84	1.50	1	14
1:A:190:LEU:HD22	1:A:196:ILE:CG1	0.84	2.03	16	16
1:A:124:LEU:HD21	1:B:124:LEU:HD21	0.83	1.48	18	1
1:A:173:GLY:HA2	1:A:178:CYS:O	0.83	1.72	17	19
1:A:42:ILE:HA	1:A:94:VAL:HG12	0.83	1.50	6	18
1:A:51:ILE:O	1:A:58:GLU:HA	0.83	1.74	14	20
1:B:72:GLU:HB3	1:B:116:LEU:HD11	0.82	1.49	7	16
1:B:44:LYS:HA	1:B:66:GLN:CG	0.82	2.05	17	1
1:B:18:CYS:HA	1:B:97:ILE:HG21	0.82	1.51	11	20
1:A:187:LEU:HD22	1:A:190:LEU:HD11	0.81	1.51	13	14
1:B:42:ILE:HA	1:B:94:VAL:HG12	0.81	1.51	11	18
1:B:42:ILE:HD12	1:B:47:VAL:HG13	0.81	1.50	14	10
1:A:41:TYR:HB3	1:A:95:ALA:HB3	0.81	1.52	8	16
1:B:193:GLN:HA	1:B:196:ILE:O	0.81	1.74	8	20
1:B:147:LEU:HD22	1:B:167:ILE:HD13	0.81	1.52	11	5
1:B:41:TYR:HB3	1:B:95:ALA:HB3	0.81	1.52	13	16
1:A:143:ILE:HG12	1:A:183:VAL:HG22	0.80	1.52	20	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LYS:HA	1:A:66:GLN:HG3	0.80	1.51	17	5
1:A:18:CYS:HA	1:A:97:ILE:HG21	0.80	1.54	8	20
1:B:15:LEU:HB3	1:B:20:ILE:HD11	0.80	1.52	20	11
1:B:164:GLN:HB3	1:B:204:VAL:HG23	0.80	1.51	18	12
1:B:47:VAL:HB	1:B:87:ARG:O	0.80	1.77	15	6
1:B:22:LYS:HG2	1:B:23:TYR:CD1	0.80	2.12	12	19
1:B:37:GLU:HA	1:B:99:TYR:CE2	0.79	2.12	15	14
1:A:20:ILE:HD13	1:A:95:ALA:HB2	0.79	1.52	18	10
1:B:45:GLY:N	1:B:66:GLN:HG2	0.79	1.93	11	8
1:B:196:ILE:HG22	1:B:197:SER:H	0.79	1.38	11	14
1:B:15:LEU:HD22	1:B:20:ILE:HD11	0.78	1.55	17	5
1:B:22:LYS:HG3	1:B:94:VAL:HG22	0.78	1.54	1	17
1:B:20:ILE:HD13	1:B:95:ALA:HB2	0.78	1.55	18	9
1:B:75:LEU:HB2	1:B:99:TYR:CD2	0.78	2.14	17	18
1:A:20:ILE:HG13	1:A:43:VAL:HG21	0.78	1.55	2	1
1:B:146:THR:HG21	1:B:175:ILE:HG21	0.77	1.55	6	9
1:B:43:VAL:O	1:B:66:GLN:HG2	0.77	1.77	17	1
1:A:196:ILE:HG22	1:A:197:SER:H	0.77	1.38	2	13
1:B:44:LYS:CA	1:B:66:GLN:HG3	0.77	2.09	17	1
1:A:51:ILE:HG21	1:B:128:SER:HB3	0.77	1.57	15	9
1:A:128:SER:HB3	1:B:51:ILE:HG21	0.77	1.57	15	11
1:A:193:GLN:HA	1:A:196:ILE:O	0.77	1.80	1	19
1:A:26:LYS:H	1:A:88:ALA:HB3	0.76	1.40	6	7
1:A:48:ALA:HB1	1:A:60:ILE:HD12	0.76	1.55	8	6
1:B:15:LEU:HA	1:B:18:CYS:SG	0.76	2.20	4	20
1:A:190:LEU:HD22	1:A:196:ILE:HG13	0.76	1.56	8	11
1:B:49:VAL:HA	1:B:85:TRP:O	0.76	1.81	4	7
1:A:44:LYS:HG2	1:A:66:GLN:NE2	0.76	1.96	17	2
1:B:22:LYS:HG2	1:B:23:TYR:CE1	0.76	2.15	12	18
1:B:26:LYS:H	1:B:88:ALA:HB3	0.75	1.42	10	8
1:A:47:VAL:HB	1:A:87:ARG:O	0.75	1.81	12	4
1:A:72:GLU:HB3	1:A:116:LEU:HD11	0.75	1.56	3	15
1:A:75:LEU:HB2	1:A:99:TYR:CD2	0.75	2.17	2	19
1:B:167:ILE:HD11	1:B:203:ILE:HD12	0.74	1.59	9	2
1:B:172:ILE:HG13	1:B:187:LEU:HD11	0.74	1.59	19	7
1:A:49:VAL:HA	1:A:85:TRP:O	0.74	1.82	7	9
1:A:147:LEU:HA	1:A:150:LEU:HD12	0.74	1.58	16	13
1:A:77:GLU:HA	1:B:121:ALA:HB1	0.74	1.58	18	3
1:A:164:GLN:HB3	1:A:204:VAL:HG23	0.74	1.57	5	10
1:B:139:VAL:HG23	1:B:176:VAL:HG11	0.74	1.60	20	4
1:A:22:LYS:HG2	1:A:23:TYR:CD1	0.74	2.18	6	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:53:ASP:HB3	1:B:55:GLU:OE2	0.73	1.83	19	1
1:A:123:ARG:O	1:A:126:VAL:HG12	0.73	1.83	14	16
1:B:49:VAL:HG12	1:B:61:LEU:HD11	0.73	1.59	19	17
1:A:106:ILE:HD13	1:A:113:LEU:HD13	0.73	1.60	3	11
1:B:47:VAL:HG22	1:B:64:LEU:HD12	0.73	1.60	6	8
1:B:14:PHE:CD2	1:B:105:LEU:HD21	0.73	2.17	2	13
1:A:37:GLU:HA	1:A:99:TYR:CE2	0.73	2.17	1	14
1:A:45:GLY:N	1:A:66:GLN:HG2	0.73	1.98	11	6
1:A:14:PHE:CD2	1:A:105:LEU:HD21	0.73	2.19	7	12
1:A:11:LEU:O	1:A:15:LEU:HG	0.73	1.83	2	20
1:A:42:ILE:HD12	1:A:47:VAL:HG13	0.73	1.60	14	11
1:A:43:VAL:O	1:A:66:GLN:HG2	0.73	1.82	17	1
1:B:20:ILE:HG12	1:B:43:VAL:HG21	0.72	1.61	4	3
1:B:155:ASP:HB3	1:B:165:ILE:CG2	0.72	2.15	9	7
1:B:14:PHE:HD2	1:B:105:LEU:HD21	0.72	1.44	15	4
1:A:123:ARG:HA	1:A:126:VAL:HG12	0.72	1.61	3	5
1:B:75:LEU:HG	1:B:76:PHE:N	0.72	1.98	6	18
1:B:138:ASP:O	1:B:142:ARG:HB2	0.72	1.85	13	8
1:B:99:TYR:O	1:B:103:ARG:HB3	0.71	1.84	14	16
1:A:138:ASP:O	1:A:142:ARG:HB2	0.71	1.85	13	8
1:B:44:LYS:HE2	1:B:66:GLN:OE1	0.71	1.85	19	2
1:A:24:PRO:HA	1:A:91:ALA:HB2	0.71	1.60	5	12
1:B:11:LEU:O	1:B:15:LEU:HG	0.71	1.84	9	20
1:B:36:ALA:HB3	1:B:74:GLY:HA3	0.71	1.61	4	16
1:B:169:ARG:CB	1:B:187:LEU:HD12	0.71	2.15	11	18
1:A:75:LEU:HG	1:A:76:PHE:N	0.71	1.99	6	19
1:A:76:PHE:CZ	1:B:121:ALA:HB2	0.71	2.20	12	1
1:B:31:HIS:CE1	1:B:50:LEU:HG	0.71	2.21	8	15
1:B:28:THR:HG23	1:B:86:VAL:O	0.71	1.86	19	1
1:A:190:LEU:HD13	1:A:196:ILE:HD11	0.71	1.62	13	2
1:A:172:ILE:HG13	1:A:187:LEU:HD11	0.71	1.63	9	7
1:B:155:ASP:HB3	1:B:165:ILE:HG22	0.71	1.63	6	20
1:A:22:LYS:C	1:A:23:TYR:HD1	0.70	1.89	19	13
1:A:44:LYS:HA	1:A:66:GLN:CG	0.70	2.16	17	2
1:B:84:ALA:O	1:B:85:TRP:HB2	0.70	1.87	9	20
1:B:190:LEU:HD22	1:B:196:ILE:CG1	0.70	2.16	12	16
1:A:22:LYS:HB3	1:A:92:CYS:O	0.70	1.86	14	19
1:A:29:LEU:N	1:A:29:LEU:HD23	0.70	2.01	17	15
1:B:29:LEU:HD23	1:B:29:LEU:N	0.70	2.01	17	17
1:B:69:PHE:CD1	1:B:116:LEU:HD12	0.70	2.22	6	8
1:A:20:ILE:HD13	1:A:43:VAL:HG21	0.70	1.62	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:GLY:O	1:A:145:GLN:HB2	0.70	1.87	1	4
1:B:48:ALA:HB1	1:B:60:ILE:HD12	0.69	1.63	8	4
1:B:46:SER:O	1:B:89:LYS:HB3	0.69	1.87	18	9
1:B:157:MET:O	1:B:163:MET:HA	0.69	1.87	8	12
1:A:169:ARG:CB	1:A:187:LEU:HD12	0.69	2.17	13	17
1:B:187:LEU:HD22	1:B:190:LEU:HD11	0.69	1.62	9	13
1:A:144:ALA:O	1:A:148:LEU:HG	0.69	1.87	19	20
1:B:22:LYS:C	1:B:23:TYR:HD1	0.69	1.90	20	15
1:B:144:ALA:O	1:B:148:LEU:HG	0.69	1.88	1	19
1:A:47:VAL:HG22	1:A:64:LEU:HD12	0.69	1.62	6	10
1:B:72:GLU:HB2	1:B:120:MET:SD	0.69	2.28	12	7
1:A:36:ALA:HB3	1:A:74:GLY:HA3	0.69	1.63	10	18
1:A:22:LYS:HD2	1:A:92:CYS:SG	0.69	2.28	12	9
1:A:69:PHE:CD1	1:A:116:LEU:HD12	0.68	2.24	6	5
1:A:72:GLU:HA	1:A:75:LEU:HD23	0.68	1.65	1	4
1:A:172:ILE:HG22	1:A:183:VAL:HG21	0.68	1.66	10	20
1:A:31:HIS:CD2	1:A:31:HIS:O	0.68	2.46	12	13
1:A:186:ILE:O	1:A:189:MET:HG2	0.68	1.89	11	14
1:A:46:SER:O	1:A:89:LYS:HB3	0.68	1.88	18	10
1:B:11:LEU:HD11	1:B:41:TYR:CE2	0.68	2.24	13	9
1:A:76:PHE:CZ	1:B:117:SER:HB3	0.68	2.24	14	1
1:A:106:ILE:HG22	1:A:112:ILE:CG2	0.67	2.20	3	16
1:A:164:GLN:HA	1:A:203:ILE:O	0.67	1.89	9	15
1:A:122:ARG:HD2	1:B:77:GLU:OE2	0.67	1.89	7	4
1:B:141:GLY:O	1:B:145:GLN:HB2	0.67	1.89	1	4
1:A:103:ARG:O	1:A:106:ILE:HG12	0.67	1.89	19	1
1:A:84:ALA:O	1:A:85:TRP:HB2	0.67	1.88	17	20
1:B:187:LEU:HD23	1:B:190:LEU:HD12	0.67	1.64	10	1
1:A:147:LEU:HD22	1:A:167:ILE:HD13	0.67	1.67	11	5
1:A:18:CYS:HA	1:A:97:ILE:CG2	0.67	2.20	14	20
1:B:28:THR:CA	1:B:29:LEU:HD23	0.67	2.20	4	16
1:A:53:ASP:HB3	1:A:55:GLU:OE2	0.67	1.90	19	1
1:A:22:LYS:HG3	1:A:94:VAL:HG22	0.67	1.64	1	18
1:A:106:ILE:HG22	1:A:112:ILE:HG22	0.67	1.65	3	7
1:A:157:MET:O	1:A:163:MET:HA	0.67	1.88	8	11
1:B:172:ILE:HG22	1:B:183:VAL:HG21	0.67	1.65	20	20
1:A:29:LEU:O	1:A:30:ILE:HG13	0.67	1.90	20	3
1:A:155:ASP:HB3	1:A:165:ILE:HG22	0.66	1.66	10	20
1:A:103:ARG:O	1:A:107:GLN:HB3	0.66	1.90	14	1
1:A:28:THR:HA	1:A:29:LEU:HD23	0.66	1.66	16	9
1:B:29:LEU:CB	1:B:86:VAL:HB	0.66	2.20	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:44:LYS:HD3	1:B:66:GLN:NE2	0.66	2.05	12	1
1:A:186:ILE:HG22	1:A:187:LEU:HD23	0.66	1.67	16	14
1:A:33:GLY:N	1:A:82:ARG:HD3	0.66	2.05	17	5
1:A:117:SER:HA	1:A:120:MET:SD	0.66	2.31	12	1
1:A:69:PHE:CG	1:A:116:LEU:HD12	0.66	2.25	17	15
1:A:121:ALA:HB2	1:B:76:PHE:CZ	0.66	2.26	12	1
1:B:31:HIS:O	1:B:31:HIS:CD2	0.66	2.49	12	17
1:B:24:PRO:HA	1:B:91:ALA:CB	0.66	2.21	3	8
1:A:22:LYS:HG2	1:A:23:TYR:CE1	0.66	2.26	9	18
1:A:11:LEU:HD12	1:A:15:LEU:HG	0.66	1.67	5	3
1:A:171:GLU:HA	1:A:174:GLN:NE2	0.66	2.06	7	1
1:B:44:LYS:HG2	1:B:66:GLN:NE2	0.66	2.05	17	2
1:A:124:LEU:O	1:A:128:SER:HB2	0.66	1.91	14	1
1:B:186:ILE:O	1:B:190:LEU:HG	0.66	1.91	10	13
1:A:41:TYR:HB2	1:A:95:ALA:HB3	0.65	1.68	7	1
1:B:123:ARG:O	1:B:126:VAL:HG12	0.65	1.90	9	16
1:B:196:ILE:HG22	1:B:204:VAL:O	0.65	1.91	4	10
1:B:143:ILE:HG12	1:B:183:VAL:HG22	0.65	1.68	10	5
1:A:11:LEU:HD21	1:A:41:TYR:CE2	0.65	2.26	19	6
1:A:196:ILE:HG22	1:A:204:VAL:O	0.65	1.92	15	4
1:A:197:SER:O	1:A:204:VAL:HB	0.65	1.91	9	4
1:A:44:LYS:CG	1:A:66:GLN:NE2	0.65	2.59	17	1
1:A:28:THR:CA	1:A:29:LEU:HD23	0.65	2.22	4	16
1:B:179:SER:C	1:B:181:GLU:H	0.65	1.93	19	20
1:A:47:VAL:HA	1:A:89:LYS:H	0.65	1.51	14	6
1:B:164:GLN:HA	1:B:203:ILE:O	0.65	1.90	9	15
1:B:143:ILE:O	1:B:147:LEU:HG	0.65	1.91	5	18
1:A:29:LEU:HD23	1:A:29:LEU:N	0.65	2.05	16	2
1:B:103:ARG:O	1:B:106:ILE:HG12	0.65	1.91	19	1
1:A:30:ILE:HD12	1:A:86:VAL:HG21	0.65	1.69	2	3
1:B:186:ILE:HG22	1:B:187:LEU:HD23	0.65	1.68	16	10
1:A:77:GLU:OE2	1:B:122:ARG:HD2	0.65	1.92	9	1
1:B:42:ILE:HD11	1:B:47:VAL:HG13	0.65	1.69	9	1
1:A:31:HIS:CE1	1:A:50:LEU:HG	0.65	2.26	8	15
1:A:39:LEU:HD13	1:A:102:PHE:CZ	0.65	2.27	20	2
1:B:11:LEU:HD21	1:B:41:TYR:CE2	0.65	2.26	2	8
1:A:14:PHE:HD2	1:A:105:LEU:HD21	0.65	1.50	1	5
1:B:18:CYS:HA	1:B:97:ILE:CG2	0.65	2.23	2	20
1:A:144:ALA:HB2	1:A:195:LEU:HD21	0.65	1.66	13	6
1:B:103:ARG:O	1:B:107:GLN:HB3	0.64	1.92	14	3
1:B:44:LYS:CG	1:B:66:GLN:NE2	0.64	2.60	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ILE:O	1:A:21:HIS:HB2	0.64	1.91	20	14
1:A:24:PRO:HA	1:A:91:ALA:CB	0.64	2.22	20	10
1:B:23:TYR:CD1	1:B:23:TYR:N	0.64	2.64	1	19
1:B:24:PRO:HA	1:B:91:ALA:HB2	0.64	1.68	3	12
1:B:47:VAL:HA	1:B:89:LYS:H	0.64	1.52	9	7
1:B:20:ILE:O	1:B:21:HIS:HB2	0.64	1.93	1	15
1:A:179:SER:C	1:A:181:GLU:H	0.64	1.94	8	19
1:A:187:LEU:HD22	1:A:190:LEU:CD1	0.64	2.23	13	16
1:B:20:ILE:HG23	1:B:43:VAL:HG21	0.64	1.68	2	6
1:B:190:LEU:HD13	1:B:196:ILE:HD11	0.64	1.69	9	3
1:B:69:PHE:CG	1:B:116:LEU:HD12	0.64	2.28	13	16
1:A:30:ILE:HD12	1:A:86:VAL:CG2	0.64	2.22	2	8
1:A:69:PHE:CE2	1:A:116:LEU:HA	0.64	2.28	16	7
1:A:166:LYS:HB3	1:A:202:THR:HG22	0.64	1.67	5	1
1:B:31:HIS:CE1	1:B:58:GLU:HB3	0.64	2.27	8	3
1:A:179:SER:HB3	1:A:181:GLU:OE2	0.64	1.93	14	1
1:A:42:ILE:HD11	1:A:47:VAL:HG13	0.64	1.70	12	3
1:A:146:THR:HG21	1:A:175:ILE:HG21	0.64	1.67	6	9
1:A:150:LEU:HD13	1:A:167:ILE:HG12	0.63	1.68	4	8
1:B:47:VAL:O	1:B:63:TYR:HB3	0.63	1.93	9	15
1:B:197:SER:HB2	1:B:206:TYR:CE1	0.63	2.28	17	13
1:A:48:ALA:HB1	1:A:60:ILE:HD13	0.63	1.69	16	9
1:B:106:ILE:HD13	1:B:113:LEU:HD13	0.63	1.70	7	11
1:B:123:ARG:HA	1:B:126:VAL:HG12	0.63	1.70	14	5
1:A:20:ILE:HG12	1:A:43:VAL:HG21	0.63	1.69	10	1
1:A:190:LEU:HD13	1:A:196:ILE:HD12	0.63	1.69	14	15
1:B:23:TYR:N	1:B:23:TYR:HD1	0.63	1.91	1	2
1:B:49:VAL:HG22	1:B:85:TRP:O	0.63	1.93	13	17
1:B:44:LYS:HD2	1:B:66:GLN:CD	0.63	2.14	20	1
1:A:18:CYS:CB	1:A:97:ILE:HG12	0.63	2.24	14	12
1:A:23:TYR:N	1:A:23:TYR:CD1	0.63	2.67	3	7
1:B:48:ALA:HB1	1:B:60:ILE:HD13	0.63	1.70	15	11
1:B:182:THR:O	1:B:185:ARG:HB2	0.63	1.94	5	5
1:B:70:ILE:HG23	1:B:86:VAL:HG21	0.63	1.68	15	12
1:A:143:ILE:O	1:A:147:LEU:HG	0.63	1.93	18	17
1:B:134:LEU:HD22	1:B:174:GLN:O	0.63	1.94	1	12
1:A:44:LYS:CA	1:A:66:GLN:HG3	0.63	2.23	17	3
1:B:69:PHE:CE2	1:B:116:LEU:HA	0.63	2.28	13	6
1:A:11:LEU:HD11	1:A:41:TYR:CE2	0.63	2.28	11	11
1:A:44:LYS:O	1:A:92:CYS:HB3	0.63	1.94	16	5
1:A:82:ARG:HG2	1:A:83:SER:N	0.63	2.09	17	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:LEU:HA	1:A:190:LEU:HG	0.63	1.68	8	19
1:B:41:TYR:HB2	1:B:95:ALA:HB3	0.63	1.70	7	1
1:B:42:ILE:HD11	1:B:46:SER:CA	0.63	2.24	18	8
1:B:20:ILE:CG1	1:B:43:VAL:HG21	0.62	2.24	4	4
1:A:87:ARG:HD3	1:A:88:ALA:O	0.62	1.94	11	1
1:A:49:VAL:HG22	1:A:85:TRP:O	0.62	1.94	6	15
1:B:82:ARG:HG2	1:B:83:SER:N	0.62	2.08	12	13
1:A:99:TYR:O	1:A:103:ARG:HB3	0.62	1.94	2	17
1:B:187:LEU:HA	1:B:190:LEU:HG	0.62	1.69	9	19
1:A:47:VAL:O	1:A:63:TYR:HB3	0.62	1.94	9	14
1:B:103:ARG:O	1:B:106:ILE:HG13	0.62	1.95	18	6
1:B:61:LEU:HD12	1:B:62:SER:N	0.62	2.10	19	1
1:A:72:GLU:HB2	1:A:120:MET:SD	0.62	2.35	1	8
1:B:166:LYS:HG2	1:B:202:THR:HG22	0.62	1.70	9	1
1:B:33:GLY:N	1:B:82:ARG:HD3	0.62	2.10	11	2
1:A:155:ASP:HB3	1:A:165:ILE:CG2	0.62	2.24	9	9
1:A:134:LEU:HD22	1:A:174:GLN:O	0.62	1.94	16	11
1:A:29:LEU:C	1:A:30:ILE:HG13	0.62	2.15	2	18
1:B:31:HIS:CG	1:B:31:HIS:O	0.62	2.53	2	7
1:B:180:ARG:HA	1:B:183:VAL:HG12	0.62	1.72	8	7
1:B:30:ILE:HD12	1:B:86:VAL:CG2	0.61	2.25	1	11
1:B:190:LEU:HD22	1:B:196:ILE:HG13	0.61	1.73	17	13
1:A:197:SER:HB2	1:A:206:TYR:CE1	0.61	2.30	17	13
1:B:39:LEU:HD11	1:B:41:TYR:CE1	0.61	2.31	7	1
1:A:42:ILE:CA	1:A:94:VAL:HG12	0.61	2.23	20	15
1:A:49:VAL:HG12	1:A:61:LEU:HD11	0.61	1.72	10	15
1:B:29:LEU:C	1:B:30:ILE:HG13	0.61	2.15	1	16
1:A:29:LEU:CB	1:A:86:VAL:HB	0.61	2.25	6	1
1:B:190:LEU:HD13	1:B:196:ILE:CD1	0.61	2.26	13	3
1:B:186:ILE:O	1:B:189:MET:HG2	0.61	1.94	11	12
1:A:42:ILE:HD11	1:A:46:SER:CA	0.61	2.25	20	7
1:A:117:SER:HB3	1:B:76:PHE:CZ	0.61	2.30	14	1
1:B:11:LEU:HD12	1:B:15:LEU:HG	0.61	1.72	5	4
1:B:87:ARG:HD3	1:B:88:ALA:O	0.61	1.96	11	1
1:B:49:VAL:CG1	1:B:61:LEU:HD11	0.61	2.26	19	1
1:A:103:ARG:HA	1:A:106:ILE:CG1	0.61	2.26	17	17
1:A:31:HIS:O	1:A:31:HIS:CG	0.61	2.54	2	13
1:B:52:LYS:HA	1:B:57:LYS:O	0.61	1.96	7	9
1:B:147:LEU:CD2	1:B:203:ILE:HG21	0.61	2.26	19	1
1:B:25:SER:O	1:B:26:LYS:HG3	0.61	1.96	10	2
1:A:134:LEU:O	1:A:177:GLY:HA3	0.61	1.96	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:42:ILE:CA	1:B:94:VAL:HG12	0.60	2.26	20	16
1:B:150:LEU:HD13	1:B:167:ILE:HG12	0.60	1.73	3	10
1:B:190:LEU:HD13	1:B:196:ILE:HD12	0.60	1.73	20	15
1:B:147:LEU:HD22	1:B:167:ILE:CD1	0.60	2.26	11	4
1:B:166:LYS:HG3	1:B:202:THR:HG23	0.60	1.73	15	1
1:A:49:VAL:HG12	1:A:61:LEU:CD1	0.60	2.27	10	20
1:A:117:SER:HB2	1:B:76:PHE:CE1	0.60	2.31	4	3
1:A:147:LEU:HD22	1:A:167:ILE:CD1	0.60	2.26	7	5
1:A:77:GLU:HG3	1:A:79:GLY:N	0.60	2.11	20	4
1:A:31:HIS:CG	1:A:31:HIS:O	0.60	2.55	15	5
1:A:131:VAL:HG12	1:B:131:VAL:HG12	0.60	1.73	9	4
1:B:44:LYS:HA	1:B:66:GLN:CD	0.60	2.16	17	1
1:A:20:ILE:HA	1:A:94:VAL:O	0.60	1.97	12	14
1:B:49:VAL:HG12	1:B:61:LEU:CD1	0.60	2.27	9	19
1:B:20:ILE:HD13	1:B:43:VAL:HG21	0.60	1.72	20	2
1:B:103:ARG:HA	1:B:106:ILE:CG1	0.60	2.26	18	19
1:A:143:ILE:CD1	1:A:186:ILE:HD13	0.60	2.27	1	3
1:B:150:LEU:HB3	1:B:165:ILE:HG21	0.60	1.73	11	4
1:A:196:ILE:HG22	1:A:197:SER:N	0.60	2.11	19	12
1:B:28:THR:HA	1:B:29:LEU:HD23	0.60	1.72	1	7
1:B:50:LEU:CB	1:B:60:ILE:HA	0.60	2.26	10	12
1:A:23:TYR:CD1	1:A:23:TYR:N	0.60	2.70	17	11
1:B:147:LEU:HA	1:B:150:LEU:HD12	0.60	1.74	5	12
1:A:72:GLU:HG3	1:A:120:MET:HE2	0.60	1.73	14	1
1:A:44:LYS:HE2	1:A:66:GLN:OE1	0.60	1.95	19	1
1:A:19:HIS:HB3	1:A:96:GLU:O	0.60	1.97	1	7
1:B:41:TYR:O	1:B:43:VAL:HG23	0.60	1.97	11	11
1:B:42:ILE:HD11	1:B:64:LEU:HD12	0.60	1.72	10	2
1:A:48:ALA:CB	1:A:60:ILE:HD12	0.60	2.27	3	4
1:B:59:MET:HE3	1:B:174:GLN:HB2	0.60	1.74	3	3
1:A:41:TYR:CB	1:A:95:ALA:HB3	0.60	2.26	7	6
1:B:89:LYS:CE	1:B:155:ASP:OD1	0.60	2.50	10	1
1:A:37:GLU:HA	1:A:99:TYR:CZ	0.60	2.31	11	4
1:B:28:THR:HA	1:B:87:ARG:HA	0.60	1.71	15	4
1:A:143:ILE:HD13	1:A:186:ILE:HG21	0.59	1.72	8	2
1:A:173:GLY:CA	1:A:178:CYS:O	0.59	2.50	14	3
1:A:180:ARG:O	1:A:184:GLY:HA3	0.59	1.97	19	14
1:B:196:ILE:HG22	1:B:209:ARG:OXT	0.59	1.96	9	1
1:B:44:LYS:O	1:B:92:CYS:HB3	0.59	1.96	16	6
1:B:159:HIS:CE1	1:B:161:ASP:HB3	0.59	2.33	18	5
1:A:51:ILE:HD12	1:A:61:LEU:HB3	0.59	1.74	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:TYR:O	1:A:64:LEU:HD23	0.59	1.97	12	1
1:A:63:TYR:CD2	1:A:89:LYS:HD2	0.59	2.32	18	2
1:A:28:THR:HA	1:A:87:ARG:HA	0.59	1.73	11	4
1:B:179:SER:HB2	1:B:181:GLU:OE2	0.59	1.98	14	1
1:A:53:ASP:HB2	1:A:57:LYS:HG2	0.59	1.74	1	2
1:B:31:HIS:CE1	1:B:58:GLU:HB2	0.59	2.32	1	5
1:B:106:ILE:HG22	1:B:112:ILE:CG2	0.59	2.27	17	14
1:A:122:ARG:NH2	1:B:78:GLU:HB3	0.59	2.13	19	6
1:A:31:HIS:CE1	1:A:58:GLU:HB3	0.59	2.31	8	4
1:A:103:ARG:O	1:A:106:ILE:HG13	0.59	1.97	1	9
1:B:196:ILE:HG22	1:B:197:SER:N	0.59	2.12	19	10
1:A:76:PHE:CE2	1:A:120:MET:HG3	0.59	2.33	12	1
1:B:27:SER:O	1:B:88:ALA:N	0.59	2.32	13	3
1:A:195:LEU:O	1:A:209:ARG:HB3	0.59	1.98	20	1
1:B:134:LEU:O	1:B:177:GLY:HA3	0.59	1.97	4	6
1:B:180:ARG:O	1:B:184:GLY:HA3	0.59	1.98	12	13
1:A:24:PRO:HA	1:A:91:ALA:CA	0.59	2.28	12	10
1:A:77:GLU:OE2	1:B:122:ARG:HA	0.59	1.97	9	1
1:B:50:LEU:HB3	1:B:60:ILE:HG22	0.59	1.75	10	1
1:A:22:LYS:C	1:A:23:TYR:CD1	0.58	2.77	2	19
1:B:22:LYS:HD2	1:B:92:CYS:SG	0.58	2.38	15	13
1:B:47:VAL:HA	1:B:89:LYS:N	0.58	2.12	12	15
1:B:102:PHE:CE1	1:B:106:ILE:HG21	0.58	2.33	12	9
1:A:182:THR:O	1:A:185:ARG:HB2	0.58	1.97	4	6
1:A:27:SER:O	1:A:88:ALA:N	0.58	2.34	13	3
1:A:102:PHE:CE1	1:A:106:ILE:HG21	0.58	2.32	12	9
1:B:169:ARG:CB	1:B:187:LEU:HD13	0.58	2.28	10	1
1:B:51:ILE:HD12	1:B:61:LEU:HB3	0.58	1.72	18	1
1:B:42:ILE:HG21	1:B:45:GLY:O	0.58	1.98	2	1
1:A:23:TYR:N	1:A:23:TYR:HD1	0.58	1.96	3	2
1:B:196:ILE:HG13	1:B:197:SER:N	0.58	2.14	13	1
1:B:99:TYR:HA	1:B:102:PHE:HB3	0.58	1.76	20	14
1:B:69:PHE:CG	1:B:116:LEU:HD13	0.58	2.34	2	1
1:B:172:ILE:CG2	1:B:183:VAL:HG21	0.58	2.28	14	8
1:A:11:LEU:HD11	1:A:41:TYR:HE2	0.58	1.59	5	4
1:A:28:THR:C	1:A:29:LEU:HD23	0.58	2.19	12	14
1:A:123:ARG:CA	1:A:126:VAL:HG12	0.58	2.28	3	2
1:A:31:HIS:O	1:A:31:HIS:CD2	0.58	2.56	10	4
1:B:31:HIS:O	1:B:31:HIS:CG	0.58	2.56	12	11
1:A:102:PHE:CE2	1:A:106:ILE:HG23	0.58	2.33	3	1
1:A:72:GLU:CB	1:A:116:LEU:HD11	0.58	2.28	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ILE:CG1	1:A:43:VAL:HG21	0.58	2.29	2	1
1:B:139:VAL:HA	1:B:176:VAL:CG1	0.58	2.29	3	1
1:A:30:ILE:HG22	1:A:34:GLU:HB2	0.58	1.74	10	3
1:A:143:ILE:HG21	1:A:187:LEU:HD21	0.58	1.75	10	4
1:A:123:ARG:HA	1:A:126:VAL:CG1	0.57	2.29	14	2
1:A:23:TYR:HD1	1:A:23:TYR:N	0.57	1.97	18	6
1:A:41:TYR:O	1:A:43:VAL:HG23	0.57	1.98	11	9
1:A:70:ILE:HD13	1:A:86:VAL:HG11	0.57	1.76	13	14
1:A:186:ILE:O	1:A:190:LEU:HG	0.57	2.00	17	13
1:B:70:ILE:HD13	1:B:86:VAL:HG11	0.57	1.76	20	14
1:A:52:LYS:HA	1:A:57:LYS:O	0.57	1.98	7	12
1:B:28:THR:HA	1:B:29:LEU:HD22	0.57	1.77	13	1
1:A:117:SER:HB2	1:B:76:PHE:CZ	0.57	2.34	4	5
1:B:117:SER:HA	1:B:120:MET:CE	0.57	2.29	4	1
1:B:61:LEU:HD22	1:B:62:SER:HB2	0.57	1.75	10	9
1:A:15:LEU:HD22	1:A:20:ILE:HD11	0.57	1.76	17	3
1:B:169:ARG:CG	1:B:187:LEU:HD12	0.57	2.30	2	2
1:B:190:LEU:CD1	1:B:196:ILE:HD12	0.57	2.29	18	12
1:B:174:GLN:HG2	1:B:175:ILE:N	0.57	2.14	6	3
1:A:28:THR:HB	1:A:87:ARG:HA	0.57	1.76	2	4
1:B:104:GLN:O	1:B:107:GLN:HG2	0.57	2.00	19	1
1:A:53:ASP:HB2	1:A:57:LYS:CG	0.56	2.30	1	1
1:B:187:LEU:HD22	1:B:190:LEU:CD1	0.56	2.30	1	15
1:A:72:GLU:CB	1:A:120:MET:HE1	0.56	2.30	4	2
1:A:41:TYR:O	1:A:43:VAL:HG13	0.56	2.00	19	4
1:B:169:ARG:HB3	1:B:187:LEU:HD13	0.56	1.75	10	1
1:A:172:ILE:CG2	1:A:183:VAL:HG21	0.56	2.30	14	8
1:A:60:ILE:HB	1:A:174:GLN:CD	0.56	2.19	3	4
1:B:197:SER:HB3	1:B:206:TYR:CE1	0.56	2.35	15	6
1:A:22:LYS:H	1:A:93:GLU:HA	0.56	1.59	17	17
1:B:22:LYS:C	1:B:23:TYR:CD1	0.56	2.78	5	19
1:B:166:LYS:HA	1:B:201:LYS:O	0.56	2.01	10	6
1:B:167:ILE:CD1	1:B:203:ILE:HD12	0.56	2.30	10	10
1:B:11:LEU:HD11	1:B:41:TYR:HE2	0.56	1.61	5	1
1:B:114:MET:HA	1:B:117:SER:OG	0.56	2.00	7	7
1:B:144:ALA:HB2	1:B:195:LEU:HD21	0.56	1.77	9	5
1:B:190:LEU:HD22	1:B:196:ILE:HG12	0.56	1.77	13	3
1:B:18:CYS:CB	1:B:97:ILE:HG12	0.56	2.31	6	16
1:B:37:GLU:HA	1:B:99:TYR:CZ	0.56	2.36	11	3
1:B:119:GLN:O	1:B:123:ARG:HD3	0.56	2.00	7	9
1:A:113:LEU:HD12	1:A:116:LEU:HD23	0.56	1.76	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:39:LEU:HD11	1:B:41:TYR:HE1	0.56	1.61	7	1
1:A:147:LEU:CD2	1:A:203:ILE:HG21	0.56	2.30	19	2
1:A:49:VAL:N	1:A:62:SER:O	0.56	2.39	14	13
1:A:118:ALA:O	1:A:122:ARG:HB2	0.56	2.01	2	4
1:B:173:GLY:CA	1:B:178:CYS:O	0.56	2.54	14	3
1:B:65:ASN:O	1:B:68:ASP:HB2	0.56	2.01	7	4
1:B:20:ILE:HG13	1:B:95:ALA:HB2	0.56	1.76	4	1
1:B:42:ILE:HG22	1:B:68:ASP:H	0.56	1.59	12	2
1:A:89:LYS:CE	1:A:155:ASP:OD1	0.56	2.53	10	1
1:B:22:LYS:CG	1:B:94:VAL:HG22	0.56	2.30	1	1
1:B:49:VAL:N	1:B:62:SER:O	0.56	2.39	14	14
1:B:149:ASN:O	1:B:153:GLN:HG3	0.56	2.00	8	2
1:B:53:ASP:HB2	1:B:57:LYS:CG	0.56	2.31	1	1
1:B:167:ILE:HD12	1:B:203:ILE:HD12	0.56	1.76	11	2
1:A:187:LEU:CD2	1:A:190:LEU:HD11	0.56	2.31	8	4
1:B:197:SER:O	1:B:204:VAL:HB	0.56	2.01	9	3
1:B:166:LYS:HG2	1:B:202:THR:HG23	0.56	1.77	13	1
1:B:208:THR:O	1:B:209:ARG:HB2	0.56	2.01	14	1
1:A:43:VAL:C	1:A:66:GLN:HG3	0.56	2.19	17	1
1:A:149:ASN:O	1:A:153:GLN:HG3	0.55	2.01	8	2
1:B:63:TYR:CD2	1:B:89:LYS:HD2	0.55	2.35	8	2
1:A:29:LEU:HD12	1:A:40:TYR:CD1	0.55	2.36	10	1
1:B:183:VAL:HG13	1:B:187:LEU:HD12	0.55	1.77	10	1
1:B:20:ILE:HA	1:B:94:VAL:O	0.55	2.01	1	16
1:B:167:ILE:HD11	1:B:203:ILE:CD1	0.55	2.29	9	1
1:B:53:ASP:OD1	1:B:57:LYS:HB3	0.55	2.02	14	1
1:A:169:ARG:HB2	1:A:180:ARG:HB3	0.55	1.78	2	14
1:B:18:CYS:HB3	1:B:97:ILE:HG12	0.55	1.78	14	14
1:B:169:ARG:HB2	1:B:180:ARG:HB3	0.55	1.78	7	11
1:A:51:ILE:HA	1:A:84:ALA:HB1	0.55	1.76	15	3
1:A:60:ILE:O	1:A:174:GLN:HG3	0.55	2.01	3	3
1:B:198:ALA:HB2	1:B:203:ILE:HG12	0.55	1.78	12	4
1:B:180:ARG:O	1:B:184:GLY:CA	0.55	2.55	13	16
1:B:45:GLY:HA3	1:B:92:CYS:CB	0.55	2.31	16	5
1:A:8:ASP:O	1:A:12:GLU:HB2	0.55	2.01	4	1
1:A:29:LEU:HD12	1:A:70:ILE:HG21	0.55	1.78	11	8
1:B:28:THR:C	1:B:29:LEU:HD23	0.55	2.22	12	14
1:A:47:VAL:HA	1:A:89:LYS:N	0.55	2.16	17	14
1:B:190:LEU:CD2	1:B:195:LEU:HB3	0.55	2.31	13	10
1:B:29:LEU:O	1:B:30:ILE:HG13	0.55	2.01	6	5
1:A:114:MET:HA	1:A:117:SER:OG	0.55	2.02	12	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:41:TYR:CB	1:B:95:ALA:HB3	0.55	2.31	15	8
1:A:121:ALA:HB1	1:B:77:GLU:HA	0.55	1.76	18	4
1:B:124:LEU:HA	1:B:128:SER:HB2	0.55	1.79	14	1
1:B:143:ILE:HG23	1:B:172:ILE:HG21	0.55	1.77	16	13
1:A:171:GLU:O	1:A:175:ILE:HG13	0.55	2.02	10	4
1:B:143:ILE:HD13	1:B:186:ILE:HG12	0.55	1.79	10	2
1:A:76:PHE:HD2	1:A:120:MET:SD	0.55	2.25	16	7
1:A:164:GLN:HB3	1:A:204:VAL:CG2	0.55	2.32	20	7
1:B:189:MET:SD	1:B:195:LEU:HD13	0.55	2.42	7	3
1:B:11:LEU:O	1:B:14:PHE:HB3	0.54	2.02	7	5
1:B:143:ILE:HD12	1:B:143:ILE:H	0.54	1.62	10	1
1:A:24:PRO:HA	1:A:91:ALA:HA	0.54	1.78	12	7
1:A:42:ILE:CD1	1:A:47:VAL:HG13	0.54	2.32	8	6
1:A:139:VAL:HG23	1:A:176:VAL:HG11	0.54	1.78	14	3
1:B:20:ILE:HD13	1:B:95:ALA:CB	0.54	2.32	13	6
1:A:39:LEU:HB2	1:A:75:LEU:HD22	0.54	1.78	13	1
1:A:99:TYR:HA	1:A:102:PHE:HB3	0.54	1.79	20	11
1:A:20:ILE:HD13	1:A:95:ALA:CB	0.54	2.31	16	8
1:A:159:HIS:CE1	1:A:161:ASP:HB3	0.54	2.37	18	4
1:A:42:ILE:HD13	1:A:46:SER:HA	0.54	1.79	2	1
1:A:105:LEU:HG	1:A:106:ILE:N	0.54	2.17	14	8
1:A:52:LYS:O	1:B:129:GLU:HA	0.54	2.03	6	3
1:B:14:PHE:CD2	1:B:102:PHE:CE2	0.54	2.95	8	8
1:B:80:GLN:O	1:B:81:GLU:HB2	0.54	2.03	7	8
1:A:28:THR:HA	1:A:29:LEU:HD22	0.54	1.79	10	2
1:A:61:LEU:HD13	1:A:62:SER:N	0.54	2.18	14	8
1:B:72:GLU:O	1:B:76:PHE:HB3	0.54	2.03	4	4
1:A:20:ILE:HG23	1:A:43:VAL:HG21	0.54	1.80	6	9
1:B:8:ASP:O	1:B:12:GLU:HB2	0.54	2.03	3	2
1:A:142:ARG:O	1:A:145:GLN:HB3	0.54	2.03	5	4
1:B:105:LEU:HG	1:B:106:ILE:N	0.54	2.17	14	7
1:B:132:GLY:HA2	1:B:135:ALA:HB3	0.54	1.79	5	1
1:A:81:GLU:O	1:A:82:ARG:HD2	0.54	2.02	14	1
1:B:151:ALA:HA	1:B:156:ALA:HB2	0.54	1.78	19	2
1:B:150:LEU:CD1	1:B:167:ILE:HG12	0.54	2.33	15	4
1:A:138:ASP:OD2	1:A:142:ARG:HD3	0.54	2.03	11	1
1:B:19:HIS:HB3	1:B:96:GLU:O	0.54	2.02	1	9
1:B:113:LEU:HD12	1:B:116:LEU:HD23	0.54	1.78	2	1
1:B:39:LEU:HD22	1:B:102:PHE:CD1	0.54	2.38	13	7
1:A:195:LEU:O	1:A:209:ARG:HG3	0.54	2.02	12	4
1:B:134:LEU:HD13	1:B:174:GLN:O	0.54	2.03	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:29:LEU:HB3	1:B:40:TYR:CZ	0.54	2.38	13	1
1:A:180:ARG:O	1:A:184:GLY:CA	0.53	2.56	10	17
1:A:197:SER:CB	1:A:206:TYR:CE1	0.53	2.91	1	17
1:B:41:TYR:O	1:B:94:VAL:HA	0.53	2.02	11	7
1:B:197:SER:CB	1:B:206:TYR:CE1	0.53	2.91	1	16
1:B:22:LYS:H	1:B:93:GLU:HA	0.53	1.62	17	17
1:B:45:GLY:HA3	1:B:92:CYS:HB3	0.53	1.80	10	15
1:B:123:ARG:HA	1:B:126:VAL:CG1	0.53	2.34	14	2
1:B:77:GLU:HG3	1:B:79:GLY:N	0.53	2.19	5	5
1:A:11:LEU:O	1:A:14:PHE:HB3	0.53	2.03	7	3
1:B:72:GLU:CB	1:B:116:LEU:HD11	0.53	2.33	18	4
1:A:167:ILE:HD11	1:A:203:ILE:CD1	0.53	2.33	9	1
1:B:20:ILE:HG13	1:B:43:VAL:HG21	0.53	1.79	15	1
1:B:24:PRO:HA	1:B:91:ALA:CA	0.53	2.33	20	9
1:A:59:MET:HE3	1:A:174:GLN:HB2	0.53	1.79	3	4
1:A:183:VAL:O	1:A:187:LEU:HG	0.53	2.04	4	3
1:A:18:CYS:HB3	1:A:97:ILE:HG12	0.53	1.80	17	14
1:A:129:GLU:HA	1:B:52:LYS:O	0.53	2.03	6	2
1:A:190:LEU:CD1	1:A:196:ILE:HD12	0.53	2.34	11	14
1:B:156:ALA:HA	1:B:164:GLN:O	0.53	2.02	20	4
1:A:29:LEU:HD23	1:A:86:VAL:HB	0.53	1.79	13	1
1:A:45:GLY:HA3	1:A:92:CYS:HB3	0.53	1.81	10	15
1:B:24:PRO:HA	1:B:91:ALA:HA	0.53	1.80	12	9
1:B:49:VAL:HG13	1:B:85:TRP:HA	0.53	1.80	19	5
1:A:174:GLN:HG2	1:A:175:ILE:N	0.53	2.18	6	2
1:B:164:GLN:HG3	1:B:202:THR:HG22	0.53	1.81	19	2
1:B:143:ILE:HG21	1:B:187:LEU:HD21	0.53	1.79	20	4
1:A:80:GLN:O	1:A:81:GLU:HB2	0.53	2.03	5	8
1:A:143:ILE:HG23	1:A:172:ILE:HG21	0.53	1.80	4	14
1:A:180:ARG:HA	1:A:183:VAL:HG12	0.53	1.80	20	6
1:A:198:ALA:HB2	1:A:203:ILE:HG12	0.53	1.80	8	3
1:B:171:GLU:HB3	1:B:175:ILE:HD12	0.53	1.79	7	1
1:A:106:ILE:HG22	1:A:112:ILE:HG21	0.53	1.81	7	7
1:A:31:HIS:HA	1:A:82:ARG:HG3	0.53	1.80	17	6
1:B:42:ILE:HG12	1:B:42:ILE:O	0.53	2.02	5	1
1:A:134:LEU:HB3	1:A:175:ILE:O	0.53	2.04	9	1
1:A:41:TYR:O	1:A:94:VAL:HA	0.53	2.03	11	6
1:A:45:GLY:HA3	1:A:92:CYS:CB	0.53	2.34	16	7
1:B:42:ILE:O	1:B:67:GLY:HA2	0.53	2.03	2	1
1:B:41:TYR:O	1:B:43:VAL:HG13	0.53	2.04	5	3
1:B:32:GLN:H	1:B:82:ARG:HG3	0.53	1.64	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LEU:HD22	1:A:29:LEU:N	0.53	2.19	10	2
1:B:123:ARG:HD3	1:B:123:ARG:N	0.53	2.19	20	1
1:A:119:GLN:O	1:A:123:ARG:HD3	0.52	2.05	2	8
1:B:183:VAL:HG13	1:B:187:LEU:CD1	0.52	2.34	10	1
1:B:126:VAL:O	1:B:130:LYS:HB2	0.52	2.04	13	1
1:B:11:LEU:HD11	1:B:41:TYR:OH	0.52	2.04	19	1
1:A:48:ALA:HB1	1:A:60:ILE:HG21	0.52	1.81	4	1
1:B:23:TYR:O	1:B:91:ALA:HA	0.52	2.05	1	8
1:B:165:ILE:O	1:B:165:ILE:HD12	0.52	2.04	20	2
1:B:22:LYS:CB	1:B:92:CYS:O	0.52	2.51	12	1
1:B:179:SER:C	1:B:181:GLU:N	0.52	2.61	14	19
1:B:23:TYR:HD1	1:B:23:TYR:N	0.52	2.03	18	5
1:A:196:ILE:CD1	1:A:203:ILE:HG23	0.52	2.35	13	1
1:B:139:VAL:HG22	1:B:143:ILE:HD11	0.52	1.81	20	1
1:B:138:ASP:O	1:B:138:ASP:CG	0.52	2.48	12	3
1:A:39:LEU:HD11	1:A:41:TYR:CE1	0.52	2.39	7	1
1:A:73:LEU:HD23	1:A:120:MET:SD	0.52	2.44	11	1
1:A:100:LYS:O	1:A:103:ARG:HG2	0.52	2.04	19	1
1:A:22:LYS:N	1:A:93:GLU:HA	0.52	2.19	2	10
1:B:30:ILE:O	1:B:86:VAL:HG23	0.52	2.05	2	1
1:A:29:LEU:CD1	1:A:70:ILE:HG21	0.52	2.34	19	6
1:B:20:ILE:HD12	1:B:43:VAL:HG21	0.52	1.81	9	2
1:A:121:ALA:CB	1:B:77:GLU:HA	0.52	2.35	18	1
1:A:138:ASP:CG	1:A:138:ASP:O	0.52	2.48	20	1
1:B:23:TYR:CB	1:B:24:PRO:HD2	0.52	2.34	10	7
1:B:25:SER:HB3	1:B:90:THR:N	0.52	2.20	4	2
1:B:106:ILE:HG22	1:B:112:ILE:HG22	0.52	1.80	17	6
1:B:32:GLN:N	1:B:82:ARG:HG3	0.52	2.19	17	3
1:A:29:LEU:N	1:A:29:LEU:CD2	0.52	2.73	18	15
1:B:60:ILE:HB	1:B:174:GLN:CD	0.52	2.25	7	5
1:B:76:PHE:HD2	1:B:120:MET:SD	0.52	2.28	11	6
1:B:76:PHE:CD2	1:B:120:MET:SD	0.52	3.03	12	3
1:A:166:LYS:HG3	1:A:201:LYS:HB3	0.52	1.82	4	1
1:A:14:PHE:CD1	1:A:14:PHE:C	0.52	2.83	10	6
1:B:134:LEU:HD22	1:B:176:VAL:HA	0.52	1.80	10	1
1:B:196:ILE:CD1	1:B:203:ILE:HG23	0.52	2.34	13	1
1:A:124:LEU:HA	1:A:128:SER:HB2	0.52	1.82	14	1
1:B:173:GLY:HA3	1:B:178:CYS:O	0.52	2.05	14	1
1:A:49:VAL:HG13	1:A:85:TRP:HA	0.52	1.81	19	5
1:A:138:ASP:O	1:A:140:THR:N	0.52	2.43	8	10
1:A:23:TYR:HD2	1:A:27:SER:CB	0.52	2.17	14	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:ASN:O	1:A:68:ASP:HB2	0.52	2.05	7	3
1:A:15:LEU:HD21	1:A:41:TYR:CE2	0.52	2.40	10	2
1:A:142:ARG:O	1:A:145:GLN:HB2	0.52	2.04	13	1
1:A:124:LEU:HG	1:B:124:LEU:HD23	0.52	1.81	20	1
1:B:138:ASP:O	1:B:140:THR:N	0.51	2.44	10	11
1:A:135:ALA:HA	1:B:135:ALA:HA	0.51	1.83	5	1
1:B:48:ALA:O	1:B:87:ARG:HB3	0.51	2.05	15	2
1:B:102:PHE:CE2	1:B:106:ILE:HG23	0.51	2.40	17	2
1:A:44:LYS:HA	1:A:66:GLN:CD	0.51	2.24	17	1
1:B:29:LEU:N	1:B:29:LEU:CD2	0.51	2.72	1	12
1:A:162:GLY:HA3	1:A:204:VAL:CG2	0.51	2.35	2	1
1:A:197:SER:HB3	1:A:206:TYR:CE1	0.51	2.40	13	3
1:A:178:CYS:SG	1:A:183:VAL:HB	0.51	2.44	17	1
1:A:14:PHE:CD2	1:A:102:PHE:CE2	0.51	2.97	3	7
1:A:96:GLU:O	1:A:96:GLU:HG3	0.51	2.05	17	4
1:B:36:ALA:CB	1:B:74:GLY:HA3	0.51	2.34	7	10
1:A:51:ILE:HD12	1:B:128:SER:HA	0.51	1.81	4	1
1:A:42:ILE:HG12	1:A:42:ILE:O	0.51	2.05	5	1
1:B:50:LEU:HB2	1:B:59:MET:O	0.51	2.05	11	6
1:A:47:VAL:HA	1:A:89:LYS:CB	0.51	2.35	12	4
1:B:22:LYS:NZ	1:B:29:LEU:HD11	0.51	2.21	13	1
1:A:33:GLY:HA2	1:A:82:ARG:HB3	0.51	1.82	19	2
1:B:179:SER:O	1:B:181:GLU:N	0.51	2.32	1	10
1:A:36:ALA:CB	1:A:74:GLY:HA3	0.51	2.35	7	12
1:B:51:ILE:HA	1:B:84:ALA:HB1	0.51	1.81	2	5
1:B:47:VAL:HA	1:B:89:LYS:CB	0.51	2.35	12	3
1:B:43:VAL:C	1:B:66:GLN:HG3	0.51	2.23	17	1
1:B:193:GLN:HG2	1:B:197:SER:OG	0.51	2.05	19	1
1:B:106:ILE:HG22	1:B:112:ILE:HG21	0.51	1.82	2	8
1:B:30:ILE:HD12	1:B:86:VAL:HG23	0.51	1.81	4	4
1:A:165:ILE:HD12	1:A:165:ILE:O	0.51	2.05	20	2
1:A:50:LEU:CB	1:A:60:ILE:HA	0.51	2.36	15	9
1:B:183:VAL:O	1:B:187:LEU:HG	0.51	2.05	4	4
1:B:63:TYR:OH	1:B:175:ILE:HD11	0.51	2.05	13	1
1:B:139:VAL:CG2	1:B:183:VAL:HG23	0.51	2.36	20	2
1:B:25:SER:O	1:B:26:LYS:CB	0.51	2.59	19	15
1:B:47:VAL:CG2	1:B:64:LEU:HD12	0.51	2.35	6	3
1:B:146:THR:O	1:B:149:ASN:HB3	0.51	2.06	17	2
1:B:167:ILE:HG13	1:B:203:ILE:HD12	0.51	1.81	14	1
1:B:187:LEU:N	1:B:187:LEU:HD23	0.51	2.20	1	4
1:A:22:LYS:HB3	1:A:92:CYS:C	0.51	2.26	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:30:ILE:HG22	1:B:34:GLU:HB2	0.51	1.83	13	2
1:A:72:GLU:HB2	1:A:120:MET:CE	0.51	2.36	5	2
1:A:47:VAL:CG2	1:A:64:LEU:HD12	0.51	2.35	6	1
1:A:22:LYS:HE2	1:A:27:SER:OG	0.51	2.06	10	1
1:B:14:PHE:CE1	1:B:41:TYR:CD2	0.51	2.99	17	3
1:A:208:THR:O	1:A:209:ARG:HB2	0.51	2.05	19	2
1:A:11:LEU:HD11	1:A:41:TYR:OH	0.51	2.06	19	1
1:A:153:GLN:HB3	1:A:154:PRO:HD2	0.51	1.83	15	15
1:B:45:GLY:HA3	1:B:92:CYS:HA	0.51	1.83	20	8
1:A:78:GLU:HB3	1:B:122:ARG:NH2	0.51	2.21	19	4
1:A:102:PHE:CZ	1:A:106:ILE:HG21	0.51	2.41	15	7
1:A:109:ASN:OD1	1:A:112:ILE:HG13	0.51	2.06	19	2
1:B:109:ASN:CG	1:B:112:ILE:HG13	0.51	2.25	14	1
1:B:14:PHE:CD1	1:B:14:PHE:C	0.51	2.85	7	5
1:B:31:HIS:HA	1:B:82:ARG:HG3	0.51	1.83	15	5
1:A:139:VAL:CG2	1:A:183:VAL:HG23	0.51	2.36	4	4
1:A:61:LEU:HD22	1:A:62:SER:HB2	0.51	1.81	10	6
1:B:82:ARG:CG	1:B:83:SER:N	0.50	2.73	12	17
1:B:164:GLN:HB3	1:B:204:VAL:CG2	0.50	2.36	1	6
1:B:14:PHE:CD1	1:B:15:LEU:HD23	0.50	2.42	19	6
1:B:166:LYS:CA	1:B:202:THR:HA	0.50	2.36	4	7
1:B:29:LEU:HB2	1:B:86:VAL:HB	0.50	1.83	10	2
1:A:169:ARG:HG3	1:A:180:ARG:HB3	0.50	1.83	20	1
1:A:150:LEU:CD1	1:A:167:ILE:HG12	0.50	2.35	4	7
1:A:179:SER:C	1:A:181:GLU:N	0.50	2.65	13	19
1:B:60:ILE:HG21	1:B:63:TYR:CE2	0.50	2.41	1	9
1:A:60:ILE:HD11	1:A:87:ARG:NH1	0.50	2.21	2	1
1:A:166:LYS:O	1:A:166:LYS:HD3	0.50	2.06	7	1
1:B:29:LEU:HD22	1:B:29:LEU:N	0.50	2.20	13	1
1:A:82:ARG:CG	1:A:83:SER:N	0.50	2.74	5	18
1:B:123:ARG:CA	1:B:126:VAL:HG12	0.50	2.36	3	4
1:A:205:VAL:HG12	1:A:209:ARG:OXT	0.50	2.07	5	2
1:A:191:GLU:HG2	1:A:198:ALA:O	0.50	2.06	9	1
1:A:166:LYS:HG2	1:A:202:THR:HG23	0.50	1.83	20	2
1:A:29:LEU:HB3	1:A:40:TYR:CZ	0.50	2.41	13	1
1:A:106:ILE:CD1	1:A:113:LEU:HD22	0.50	2.36	19	1
1:B:121:ALA:O	1:B:124:LEU:HB2	0.50	2.06	18	3
1:A:50:LEU:HB2	1:A:59:MET:C	0.50	2.27	15	11
1:B:73:LEU:HD23	1:B:120:MET:SD	0.50	2.46	11	1
1:A:77:GLU:HA	1:B:121:ALA:CB	0.50	2.34	18	1
1:A:103:ARG:HA	1:A:106:ILE:HG12	0.50	1.83	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:18:CYS:HB3	1:B:97:ILE:CD1	0.50	2.37	20	8
1:A:69:PHE:CD1	1:A:116:LEU:HD13	0.50	2.41	2	1
1:B:60:ILE:O	1:B:174:GLN:HG3	0.50	2.07	15	4
1:A:146:THR:HG21	1:A:175:ILE:HG23	0.50	1.84	7	1
1:B:143:ILE:HG12	1:B:183:VAL:CG2	0.50	2.36	11	1
1:B:50:LEU:HB2	1:B:59:MET:C	0.50	2.27	20	14
1:B:72:GLU:HA	1:B:75:LEU:HD23	0.50	1.82	8	6
1:A:23:TYR:CB	1:A:24:PRO:HD2	0.50	2.36	10	7
1:B:42:ILE:CD1	1:B:46:SER:HA	0.50	2.35	4	3
1:B:146:THR:HG21	1:B:175:ILE:HG23	0.50	1.81	7	1
1:A:11:LEU:HD23	1:A:14:PHE:HB3	0.50	1.84	9	4
1:A:166:LYS:HB3	1:A:202:THR:HA	0.50	1.82	20	2
1:A:164:GLN:HB2	1:A:202:THR:HG22	0.50	1.84	12	1
1:B:81:GLU:O	1:B:82:ARG:HD2	0.50	2.06	14	1
1:A:75:LEU:CB	1:A:99:TYR:CD2	0.50	2.95	11	9
1:A:196:ILE:CG2	1:A:197:SER:H	0.50	2.17	18	7
1:A:42:ILE:HG12	1:A:94:VAL:HG12	0.50	1.84	2	1
1:B:187:LEU:CD2	1:B:190:LEU:HD11	0.50	2.35	9	4
1:A:129:GLU:O	1:A:130:LYS:HG2	0.50	2.07	6	1
1:B:23:TYR:CD2	1:B:27:SER:HB3	0.50	2.42	6	2
1:A:187:LEU:HA	1:A:190:LEU:CG	0.50	2.37	8	1
1:B:11:LEU:HD23	1:B:14:PHE:HB3	0.50	1.84	19	2
1:A:143:ILE:H	1:A:143:ILE:HD12	0.50	1.64	10	1
1:A:124:LEU:HG	1:B:124:LEU:CD2	0.50	2.37	20	3
1:A:104:GLN:O	1:A:107:GLN:HG2	0.50	2.06	19	1
1:B:33:GLY:HA2	1:B:82:ARG:HB3	0.50	1.83	19	1
1:A:42:ILE:CD1	1:A:46:SER:HA	0.50	2.36	5	3
1:B:50:LEU:HB3	1:B:60:ILE:HA	0.50	1.83	10	2
1:A:89:LYS:HE2	1:A:155:ASP:OD1	0.50	2.07	10	1
1:B:55:GLU:OE1	1:B:57:LYS:HB2	0.50	2.06	20	3
1:A:186:ILE:HA	1:A:189:MET:HG2	0.50	1.84	17	1
1:B:166:LYS:HA	1:B:202:THR:HA	0.49	1.84	6	13
1:A:169:ARG:HB2	1:A:180:ARG:CB	0.49	2.37	11	7
1:B:103:ARG:HA	1:B:106:ILE:HG12	0.49	1.83	4	7
1:A:11:LEU:HD12	1:A:15:LEU:CG	0.49	2.38	4	2
1:A:196:ILE:HG12	1:A:209:ARG:OXT	0.49	2.07	7	2
1:B:171:GLU:O	1:B:175:ILE:HG13	0.49	2.07	10	2
1:A:11:LEU:C	1:A:13:TRP:H	0.49	2.10	20	1
1:A:50:LEU:HB2	1:A:59:MET:O	0.49	2.08	11	5
1:B:196:ILE:CG2	1:B:197:SER:H	0.49	2.16	6	6
1:B:47:VAL:HG21	1:B:86:VAL:HG12	0.49	1.83	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:HIS:CE1	1:A:58:GLU:HB2	0.49	2.42	4	4
1:A:128:SER:HB3	1:B:51:ILE:CG2	0.49	2.35	5	5
1:B:109:ASN:OD1	1:B:112:ILE:HG13	0.49	2.07	19	2
1:A:60:ILE:HG21	1:A:63:TYR:CE2	0.49	2.43	16	4
1:A:15:LEU:HA	1:A:18:CYS:HG	0.49	1.66	5	2
1:B:61:LEU:HD13	1:B:62:SER:N	0.49	2.22	15	6
1:B:50:LEU:HA	1:B:61:LEU:HD12	0.49	1.84	11	1
1:B:147:LEU:O	1:B:150:LEU:HB2	0.49	2.07	20	3
1:A:25:SER:O	1:A:26:LYS:CB	0.49	2.60	19	17
1:A:164:GLN:HG3	1:A:202:THR:HG22	0.49	1.83	14	3
1:A:166:LYS:HA	1:A:202:THR:HA	0.49	1.83	12	11
1:B:102:PHE:CZ	1:B:106:ILE:HG21	0.49	2.43	9	7
1:B:29:LEU:HD12	1:B:70:ILE:HG21	0.49	1.84	11	10
1:B:143:ILE:HD12	1:B:186:ILE:HB	0.49	1.84	18	2
1:A:24:PRO:CA	1:A:91:ALA:HB2	0.49	2.34	5	1
1:B:50:LEU:HB3	1:B:60:ILE:HD13	0.49	1.84	17	3
1:A:164:GLN:C	1:A:165:ILE:HG13	0.49	2.28	12	10
1:B:42:ILE:CD1	1:B:47:VAL:HG13	0.49	2.37	13	5
1:B:22:LYS:HB3	1:B:92:CYS:C	0.49	2.28	14	4
1:B:23:TYR:HD2	1:B:27:SER:CB	0.49	2.20	14	3
1:B:117:SER:HA	1:B:120:MET:HE3	0.49	1.85	4	1
1:A:144:ALA:HB2	1:A:195:LEU:CD2	0.49	2.37	18	4
1:A:120:MET:O	1:A:123:ARG:HB2	0.49	2.07	16	2
1:A:50:LEU:HB3	1:A:60:ILE:HD13	0.49	1.84	6	3
1:A:49:VAL:CA	1:A:85:TRP:O	0.49	2.59	16	2
1:A:41:TYR:HD1	1:A:68:ASP:O	0.49	1.91	10	2
1:B:169:ARG:HG3	1:B:180:ARG:HB2	0.49	1.85	10	1
1:A:190:LEU:HD13	1:A:196:ILE:CD1	0.49	2.37	13	2
1:B:103:ARG:HA	1:B:106:ILE:HG13	0.49	1.85	13	9
1:B:64:LEU:HB3	1:B:68:ASP:CB	0.49	2.37	2	2
1:A:146:THR:HG21	1:A:175:ILE:CG2	0.49	2.37	7	1
1:A:117:SER:HB3	1:B:76:PHE:CE2	0.49	2.43	14	1
1:B:22:LYS:NZ	1:B:88:ALA:HB2	0.49	2.23	18	2
1:B:101:LYS:O	1:B:104:GLN:HG2	0.49	2.08	19	1
1:A:135:ALA:HB1	1:B:135:ALA:HB1	0.49	1.84	1	2
1:B:75:LEU:CB	1:B:99:TYR:CD2	0.49	2.95	6	11
1:A:41:TYR:CD1	1:A:41:TYR:C	0.49	2.85	13	6
1:B:138:ASP:O	1:B:142:ARG:CB	0.49	2.60	7	1
1:B:143:ILE:CD1	1:B:183:VAL:HA	0.49	2.37	18	1
1:A:40:TYR:HB2	1:A:70:ILE:HB	0.49	1.83	20	1
1:A:135:ALA:CB	1:B:135:ALA:HB3	0.49	2.36	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:TYR:CE1	1:A:69:PHE:HD1	0.49	2.26	7	1
1:A:14:PHE:O	1:A:17:HIS:HB2	0.49	2.08	9	1
1:A:69:PHE:CG	1:A:116:LEU:HD13	0.48	2.43	2	1
1:A:167:ILE:HG22	1:A:171:GLU:HG3	0.48	1.84	8	1
1:B:22:LYS:CG	1:B:23:TYR:CD1	0.48	2.96	16	1
1:A:184:GLY:O	1:A:188:LYS:HB2	0.48	2.08	6	5
1:B:22:LYS:N	1:B:93:GLU:HA	0.48	2.23	2	11
1:B:99:TYR:CD1	1:B:99:TYR:C	0.48	2.86	20	12
1:A:81:GLU:O	1:A:82:ARG:HD3	0.48	2.09	2	3
1:A:32:GLN:N	1:A:82:ARG:HG3	0.48	2.23	6	3
1:B:15:LEU:HD21	1:B:41:TYR:HE2	0.48	1.68	10	1
1:A:166:LYS:C	1:A:167:ILE:HG13	0.48	2.28	15	2
1:A:37:GLU:O	1:A:99:TYR:CD1	0.48	2.66	19	1
1:A:14:PHE:CD1	1:A:15:LEU:HD23	0.48	2.43	19	7
1:A:102:PHE:CE2	1:A:106:ILE:CG2	0.48	2.96	3	4
1:B:96:GLU:HG3	1:B:96:GLU:O	0.48	2.09	17	3
1:A:157:MET:O	1:A:163:MET:HB3	0.48	2.08	3	1
1:B:143:ILE:CG2	1:B:187:LEU:HD21	0.48	2.38	5	4
1:A:47:VAL:CG1	1:A:88:ALA:HA	0.48	2.38	12	1
1:B:180:ARG:HD2	1:B:181:GLU:OE2	0.48	2.07	12	1
1:B:31:HIS:HB2	1:B:84:ALA:HA	0.48	1.84	14	1
1:A:54:GLU:HB2	1:B:133:ASN:OD1	0.48	2.07	1	1
1:A:39:LEU:HD22	1:A:102:PHE:CD1	0.48	2.43	20	6
1:A:51:ILE:HG21	1:B:128:SER:HB2	0.48	1.85	3	1
1:B:140:THR:O	1:B:142:ARG:N	0.48	2.46	3	1
1:B:11:LEU:HD23	1:B:14:PHE:CG	0.48	2.44	9	1
1:A:33:GLY:N	1:A:82:ARG:HD2	0.48	2.24	10	1
1:B:18:CYS:HA	1:B:97:ILE:HG23	0.48	1.84	10	1
1:B:76:PHE:CD1	1:B:120:MET:HE1	0.48	2.44	14	1
1:B:143:ILE:HD13	1:B:186:ILE:CG1	0.48	2.38	20	1
1:B:143:ILE:HD13	1:B:186:ILE:HG13	0.48	1.85	1	1
1:A:121:ALA:O	1:A:124:LEU:HB2	0.48	2.07	18	2
1:B:156:ALA:HA	1:B:165:ILE:HG23	0.48	1.84	20	2
1:B:169:ARG:CA	1:B:187:LEU:HD12	0.48	2.38	11	1
1:B:143:ILE:HD13	1:B:183:VAL:HA	0.48	1.85	18	2
1:A:130:LYS:HG3	1:A:133:ASN:OD1	0.48	2.08	19	1
1:A:18:CYS:HA	1:A:97:ILE:HG23	0.48	1.84	10	3
1:A:34:GLU:OE2	1:A:82:ARG:HB2	0.48	2.08	17	5
1:A:103:ARG:HA	1:A:106:ILE:HG13	0.48	1.84	13	8
1:A:103:ARG:O	1:A:107:GLN:HG2	0.48	2.09	18	1
1:B:164:GLN:C	1:B:165:ILE:HG13	0.48	2.29	12	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:TYR:O	1:A:91:ALA:HA	0.48	2.08	5	7
1:B:39:LEU:HG	1:B:40:TYR:N	0.48	2.24	3	3
1:B:118:ALA:O	1:B:122:ARG:HB2	0.48	2.08	2	4
1:B:187:LEU:HD23	1:B:187:LEU:N	0.48	2.24	2	4
1:B:48:ALA:CB	1:B:60:ILE:HD12	0.48	2.37	8	3
1:A:156:ALA:HA	1:A:165:ILE:HG23	0.48	1.85	20	4
1:A:166:LYS:HB3	1:A:202:THR:HG23	0.48	1.86	10	1
1:A:124:LEU:HA	1:A:128:SER:CB	0.48	2.38	14	1
1:A:147:LEU:CD2	1:A:167:ILE:HD11	0.48	2.39	19	2
1:A:169:ARG:HG3	1:A:180:ARG:CB	0.48	2.39	20	1
1:A:190:LEU:CD2	1:A:195:LEU:HB3	0.48	2.39	14	6
1:A:122:ARG:CZ	1:B:78:GLU:HB3	0.48	2.38	20	3
1:A:143:ILE:CG2	1:A:187:LEU:HD21	0.48	2.38	8	2
1:B:77:GLU:O	1:B:78:GLU:HB2	0.48	2.09	14	1
1:A:99:TYR:CD1	1:A:99:TYR:C	0.48	2.87	3	11
1:A:124:LEU:HG	1:B:124:LEU:HG	0.48	1.86	13	4
1:A:109:ASN:CB	1:A:112:ILE:HG13	0.48	2.39	11	2
1:B:106:ILE:HD13	1:B:113:LEU:HD22	0.48	1.85	15	3
1:A:173:GLY:HA3	1:A:178:CYS:O	0.48	2.09	14	1
1:A:42:ILE:HB	1:A:68:ASP:O	0.47	2.09	2	1
1:A:166:LYS:HA	1:A:201:LYS:O	0.47	2.10	10	4
1:A:11:LEU:HD23	1:A:14:PHE:CG	0.47	2.44	14	4
1:B:143:ILE:CG1	1:B:183:VAL:HG22	0.47	2.38	10	1
1:B:117:SER:HA	1:B:120:MET:HE2	0.47	1.86	12	1
1:A:109:ASN:CG	1:A:112:ILE:HG13	0.47	2.29	14	1
1:A:54:GLU:OE1	1:B:130:LYS:HE3	0.47	2.09	15	1
1:B:51:ILE:CD1	1:B:61:LEU:HB3	0.47	2.39	18	1
1:A:45:GLY:HA3	1:A:92:CYS:HA	0.47	1.85	20	6
1:A:147:LEU:O	1:A:150:LEU:HB2	0.47	2.09	20	4
1:B:33:GLY:H	1:B:82:ARG:HB2	0.47	1.68	14	1
1:B:143:ILE:HD12	1:B:186:ILE:CB	0.47	2.39	18	2
1:B:8:ASP:O	1:B:12:GLU:HG2	0.47	2.09	1	1
1:B:14:PHE:CE1	1:B:41:TYR:HD2	0.47	2.27	2	1
1:B:28:THR:HB	1:B:87:ARG:HA	0.47	1.86	7	4
1:A:23:TYR:CD2	1:A:27:SER:HB3	0.47	2.44	6	1
1:A:51:ILE:HD13	1:A:51:ILE:H	0.47	1.69	7	1
1:B:69:PHE:CB	1:B:116:LEU:HD12	0.47	2.39	9	3
1:B:138:ASP:OD2	1:B:142:ARG:HD3	0.47	2.09	11	1
1:A:109:ASN:HB2	1:A:112:ILE:HG13	0.47	1.86	13	11
1:A:27:SER:N	1:A:88:ALA:HB3	0.47	2.25	14	4
1:B:166:LYS:HB3	1:B:202:THR:HG23	0.47	1.87	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:134:LEU:HB3	1:B:175:ILE:O	0.47	2.09	9	1
1:A:76:PHE:CE1	1:B:117:SER:HB2	0.47	2.45	10	1
1:B:75:LEU:CB	1:B:99:TYR:HD2	0.47	2.22	20	2
1:B:33:GLY:HA2	1:B:82:ARG:CB	0.47	2.39	14	1
1:B:102:PHE:O	1:B:106:ILE:HG23	0.47	2.08	19	1
1:B:153:GLN:HB3	1:B:154:PRO:HD2	0.47	1.85	17	15
1:A:123:ARG:HD3	1:A:123:ARG:N	0.47	2.23	7	1
1:A:190:LEU:HD23	1:A:195:LEU:HB3	0.47	1.85	19	2
1:B:147:LEU:HD21	1:B:203:ILE:HG21	0.47	1.86	14	1
1:A:179:SER:O	1:A:181:GLU:N	0.47	2.48	13	8
1:B:169:ARG:HB2	1:B:180:ARG:CB	0.47	2.39	11	5
1:A:27:SER:H	1:A:88:ALA:HB3	0.47	1.70	14	3
1:A:14:PHE:CE1	1:A:41:TYR:HD2	0.47	2.27	2	3
1:B:69:PHE:CD1	1:B:116:LEU:HD13	0.47	2.45	2	1
1:A:76:PHE:CD2	1:A:120:MET:SD	0.47	3.08	16	5
1:A:157:MET:O	1:A:163:MET:CA	0.47	2.63	8	1
1:A:150:LEU:HB3	1:A:165:ILE:HG21	0.47	1.86	9	3
1:A:64:LEU:HD13	1:A:68:ASP:HB3	0.47	1.84	10	1
1:B:122:ARG:O	1:B:125:GLN:HG2	0.47	2.08	11	1
1:A:46:SER:HB2	1:A:64:LEU:O	0.47	2.09	12	1
1:A:141:GLY:O	1:A:145:GLN:CB	0.47	2.63	14	1
1:B:147:LEU:CD2	1:B:167:ILE:HD11	0.47	2.40	14	1
1:B:76:PHE:CE2	1:B:120:MET:HE3	0.47	2.45	2	1
1:A:20:ILE:HD12	1:A:43:VAL:HG21	0.47	1.86	11	3
1:A:22:LYS:NZ	1:A:88:ALA:HB2	0.47	2.25	9	3
1:A:167:ILE:HD11	1:A:203:ILE:HD12	0.47	1.86	9	1
1:A:164:GLN:OE1	1:A:202:THR:HB	0.47	2.10	19	1
1:A:61:LEU:C	1:A:61:LEU:HD22	0.47	2.30	12	9
1:B:15:LEU:HA	1:B:18:CYS:HG	0.47	1.69	8	4
1:A:60:ILE:HB	1:A:174:GLN:NE2	0.47	2.25	3	2
1:A:180:ARG:HD2	1:A:181:GLU:OE1	0.47	2.10	4	3
1:A:14:PHE:CE1	1:A:41:TYR:CD2	0.47	3.03	1	6
1:B:45:GLY:HA3	1:B:92:CYS:CA	0.47	2.39	16	3
1:B:60:ILE:HB	1:B:174:GLN:NE2	0.47	2.25	6	4
1:B:157:MET:O	1:B:163:MET:HB3	0.47	2.09	3	1
1:B:47:VAL:HB	1:B:88:ALA:HA	0.47	1.85	5	2
1:B:130:LYS:HA	1:B:133:ASN:OD1	0.47	2.09	5	3
1:A:128:SER:O	1:B:51:ILE:HG13	0.47	2.10	10	1
1:B:33:GLY:N	1:B:82:ARG:HB2	0.47	2.25	14	1
1:B:124:LEU:O	1:B:128:SER:HB2	0.47	2.10	14	1
1:A:51:ILE:CG2	1:B:128:SER:HB3	0.46	2.38	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LEU:HD13	1:A:41:TYR:OH	0.46	2.11	10	3
1:B:109:ASN:CB	1:B:112:ILE:HG13	0.46	2.40	11	3
1:A:77:GLU:OE1	1:B:122:ARG:HD2	0.46	2.10	14	1
1:A:143:ILE:CD1	1:A:183:VAL:HG22	0.46	2.41	16	2
1:B:102:PHE:CE2	1:B:106:ILE:HG22	0.46	2.45	19	1
1:B:76:PHE:CE2	1:B:116:LEU:HG	0.46	2.45	2	1
1:A:166:LYS:CA	1:A:202:THR:HA	0.46	2.40	4	4
1:B:178:CYS:SG	1:B:182:THR:HB	0.46	2.50	5	1
1:B:64:LEU:HA	1:B:123:ARG:NH2	0.46	2.24	17	2
1:B:102:PHE:CE2	1:B:106:ILE:CG2	0.46	2.99	15	3
1:B:23:TYR:HB3	1:B:24:PRO:HD2	0.46	1.86	13	1
1:B:99:TYR:HD1	1:B:100:LYS:N	0.46	2.08	20	1
1:B:61:LEU:C	1:B:61:LEU:HD22	0.46	2.30	12	5
1:A:25:SER:HB3	1:A:90:THR:N	0.46	2.24	19	2
1:B:41:TYR:CE1	1:B:69:PHE:HD1	0.46	2.29	7	1
1:A:143:ILE:HG23	1:A:172:ILE:CG2	0.46	2.40	8	1
1:A:28:THR:CA	1:A:29:LEU:HD22	0.46	2.40	10	1
1:B:25:SER:O	1:B:26:LYS:CG	0.46	2.63	10	1
1:A:72:GLU:O	1:A:76:PHE:HB3	0.46	2.10	12	1
1:A:76:PHE:CE1	1:A:113:LEU:HD21	0.46	2.45	17	1
1:A:39:LEU:HD22	1:A:102:PHE:CE1	0.46	2.45	20	1
1:B:22:LYS:HG3	1:B:94:VAL:CG2	0.46	2.39	19	2
1:B:30:ILE:HD12	1:B:86:VAL:HG21	0.46	1.86	1	1
1:A:32:GLN:HA	1:A:32:GLN:OE1	0.46	2.09	4	1
1:B:142:ARG:O	1:B:145:GLN:HB3	0.46	2.10	4	4
1:A:18:CYS:HB3	1:A:97:ILE:CD1	0.46	2.41	13	5
1:B:103:ARG:C	1:B:106:ILE:HG13	0.46	2.31	18	1
1:A:167:ILE:CD1	1:A:203:ILE:HD12	0.46	2.40	6	6
1:A:64:LEU:HA	1:A:123:ARG:NH2	0.46	2.26	10	3
1:A:133:ASN:HD21	1:A:142:ARG:NH2	0.46	2.09	2	1
1:A:14:PHE:CE2	1:A:102:PHE:CE1	0.46	3.04	10	2
1:A:15:LEU:HD22	1:A:20:ILE:CD1	0.46	2.40	11	2
1:A:96:GLU:O	1:A:97:ILE:HG23	0.46	2.11	11	2
1:A:155:ASP:CB	1:A:165:ILE:HG22	0.46	2.41	15	2
1:A:28:THR:CB	1:A:87:ARG:HA	0.46	2.41	17	2
1:B:196:ILE:CG2	1:B:197:SER:N	0.46	2.78	19	3
1:B:27:SER:N	1:B:88:ALA:HB3	0.46	2.26	9	5
1:B:50:LEU:HD23	1:B:50:LEU:O	0.46	2.11	5	1
1:A:78:GLU:HB3	1:B:122:ARG:CZ	0.46	2.40	9	1
1:B:187:LEU:HA	1:B:190:LEU:CG	0.46	2.41	9	1
1:A:34:GLU:O	1:A:82:ARG:HA	0.46	2.11	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:44:LYS:CE	1:B:66:GLN:OE1	0.46	2.59	19	1
1:A:41:TYR:CE2	1:A:69:PHE:CE1	0.46	3.04	16	4
1:B:109:ASN:HB2	1:B:112:ILE:HG13	0.46	1.87	18	9
1:A:122:ARG:HA	1:B:77:GLU:OE2	0.46	2.11	8	1
1:B:143:ILE:O	1:B:147:LEU:HD12	0.46	2.11	19	1
1:B:61:LEU:HD22	1:B:61:LEU:C	0.46	2.31	5	6
1:A:70:ILE:CG2	1:A:86:VAL:HG21	0.46	2.32	10	1
1:B:96:GLU:O	1:B:97:ILE:HG23	0.46	2.11	11	2
1:A:146:THR:O	1:A:149:ASN:HB2	0.46	2.11	16	1
1:B:155:ASP:CB	1:B:165:ILE:HG22	0.46	2.41	20	1
1:A:127:THR:O	1:A:131:VAL:HG23	0.46	2.11	6	2
1:A:64:LEU:HB3	1:A:68:ASP:CB	0.46	2.41	2	2
1:A:138:ASP:O	1:A:138:ASP:CG	0.46	2.54	6	2
1:A:113:LEU:HD21	1:B:114:MET:HG2	0.46	1.88	9	1
1:B:22:LYS:HZ3	1:B:88:ALA:HB2	0.46	1.71	19	1
1:A:76:PHE:CE2	1:A:116:LEU:HG	0.46	2.46	2	1
1:B:60:ILE:HD11	1:B:87:ARG:NH1	0.46	2.26	2	1
1:A:76:PHE:HD2	1:A:120:MET:CE	0.46	2.24	7	1
1:B:29:LEU:CD1	1:B:70:ILE:HG21	0.46	2.41	9	3
1:A:30:ILE:O	1:A:86:VAL:HG23	0.45	2.11	2	1
1:B:150:LEU:HD13	1:B:165:ILE:HD13	0.45	1.88	5	1
1:A:187:LEU:N	1:A:187:LEU:HD23	0.45	2.26	13	3
1:A:139:VAL:HG21	1:A:183:VAL:HG23	0.45	1.88	10	1
1:A:128:SER:HB3	1:B:128:SER:HB3	0.45	1.87	14	1
1:A:53:ASP:CB	1:A:57:LYS:HG2	0.45	2.42	19	2
1:B:184:GLY:O	1:B:188:LYS:HB2	0.45	2.11	13	2
1:B:89:LYS:NZ	1:B:155:ASP:OD2	0.45	2.48	10	1
1:B:90:THR:O	1:B:91:ALA:C	0.45	2.55	11	2
1:A:11:LEU:HD21	1:A:41:TYR:CZ	0.45	2.46	16	2
1:A:116:LEU:HG	1:A:120:MET:CE	0.45	2.41	18	1
1:B:47:VAL:HA	1:B:89:LYS:HB3	0.45	1.87	18	1
1:A:31:HIS:CE1	1:A:58:GLU:CB	0.45	3.00	20	5
1:A:114:MET:HG2	1:B:113:LEU:HD21	0.45	1.88	9	2
1:A:125:GLN:O	1:A:125:GLN:HG3	0.45	2.10	9	1
1:A:22:LYS:HZ1	1:A:29:LEU:HD22	0.45	1.71	12	1
1:A:76:PHE:CE2	1:A:120:MET:HE3	0.45	2.46	2	1
1:B:117:SER:HA	1:B:120:MET:SD	0.45	2.51	4	1
1:A:46:SER:HB2	1:A:64:LEU:C	0.45	2.32	12	1
1:B:193:GLN:CA	1:B:196:ILE:O	0.45	2.59	12	1
1:B:147:LEU:HD13	1:B:203:ILE:HG21	0.45	1.87	18	1
1:B:76:PHE:CE2	1:B:120:MET:SD	0.45	3.10	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:LEU:HD22	1:A:167:ILE:HD11	0.45	1.89	13	1
1:A:169:ARG:CG	1:A:187:LEU:HD12	0.45	2.42	5	3
1:A:124:LEU:CD2	1:B:124:LEU:HG	0.45	2.42	4	1
1:A:164:GLN:CB	1:A:204:VAL:HG23	0.45	2.42	4	1
1:B:209:ARG:HG3	1:B:209:ARG:OXT	0.45	2.12	8	1
1:A:97:ILE:HD12	1:A:102:PHE:HB2	0.45	1.89	10	2
1:B:142:ARG:O	1:B:145:GLN:HB2	0.45	2.12	13	1
1:B:196:ILE:CG1	1:B:197:SER:N	0.45	2.79	13	1
1:A:123:ARG:C	1:A:126:VAL:HG12	0.45	2.30	14	1
1:A:124:LEU:CA	1:A:128:SER:HB2	0.45	2.42	14	1
1:B:33:GLY:CA	1:B:82:ARG:HB2	0.45	2.41	14	1
1:B:53:ASP:CB	1:B:57:LYS:HG2	0.45	2.41	1	1
1:A:47:VAL:HB	1:A:88:ALA:HA	0.45	1.87	5	2
1:A:61:LEU:HD22	1:A:61:LEU:C	0.45	2.32	5	4
1:A:131:VAL:HG12	1:A:132:GLY:N	0.45	2.26	6	1
1:B:27:SER:H	1:B:88:ALA:HB3	0.45	1.70	14	2
1:A:81:GLU:O	1:A:83:SER:N	0.45	2.50	11	2
1:A:187:LEU:HD23	1:A:187:LEU:N	0.45	2.26	16	8
1:A:119:GLN:OE1	1:A:119:GLN:HA	0.45	2.12	6	1
1:A:103:ARG:O	1:A:107:GLN:HB2	0.45	2.12	12	2
1:B:14:PHE:CE2	1:B:102:PHE:CE1	0.45	3.05	10	1
1:A:14:PHE:HD1	1:A:15:LEU:HD23	0.45	1.72	14	3
1:A:48:ALA:CB	1:A:60:ILE:HD13	0.45	2.40	15	2
1:A:180:ARG:NH1	1:A:181:GLU:HA	0.45	2.27	17	1
1:B:40:TYR:N	1:B:40:TYR:CD2	0.45	2.84	20	2
1:A:47:VAL:HG21	1:A:86:VAL:HG12	0.45	1.89	17	2
1:B:195:LEU:O	1:B:209:ARG:HG3	0.45	2.12	7	3
1:B:39:LEU:HD13	1:B:102:PHE:CZ	0.45	2.46	9	1
1:B:15:LEU:HD21	1:B:41:TYR:CE2	0.45	2.46	10	1
1:A:23:TYR:HB3	1:A:24:PRO:HD2	0.45	1.87	13	1
1:B:39:LEU:HB2	1:B:75:LEU:HD22	0.45	1.89	13	1
1:B:144:ALA:HB2	1:B:195:LEU:CD2	0.45	2.42	18	2
1:A:196:ILE:CG2	1:A:197:SER:N	0.45	2.80	19	2
1:A:11:LEU:O	1:A:15:LEU:N	0.45	2.50	5	8
1:B:139:VAL:HG23	1:B:176:VAL:CG1	0.45	2.42	5	1
1:A:51:ILE:HG21	1:B:128:SER:CB	0.45	2.41	10	1
1:B:47:VAL:HG21	1:B:70:ILE:HD11	0.45	1.88	12	1
1:A:63:TYR:OH	1:A:175:ILE:HD11	0.45	2.12	13	1
1:A:190:LEU:CD1	1:A:203:ILE:HD13	0.44	2.42	14	2
1:B:157:MET:O	1:B:163:MET:CA	0.44	2.62	8	1
1:A:143:ILE:CG1	1:A:183:VAL:HG22	0.44	2.38	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:20:ILE:HG21	1:B:43:VAL:HG21	0.44	1.89	10	1
1:A:134:LEU:HD21	1:A:174:GLN:O	0.44	2.12	14	2
1:A:20:ILE:CD1	1:A:95:ALA:HB2	0.44	2.40	16	1
1:B:190:LEU:CD1	1:B:203:ILE:HD13	0.44	2.41	16	1
1:B:27:SER:O	1:B:88:ALA:HB2	0.44	2.12	18	1
1:B:14:PHE:HD1	1:B:15:LEU:HD23	0.44	1.72	20	3
1:A:172:ILE:HB	1:A:183:VAL:HG11	0.44	1.88	3	1
1:A:143:ILE:HD12	1:A:186:ILE:HB	0.44	1.89	4	2
1:A:32:GLN:O	1:A:34:GLU:HG3	0.44	2.12	7	2
1:B:106:ILE:HD12	1:B:113:LEU:HB2	0.44	1.87	5	2
1:A:135:ALA:HB3	1:B:135:ALA:CB	0.44	2.40	6	1
1:B:41:TYR:CE2	1:B:69:PHE:CE1	0.44	3.04	17	3
1:B:120:MET:O	1:B:123:ARG:HB2	0.44	2.11	11	1
1:A:31:HIS:HB2	1:A:84:ALA:HA	0.44	1.87	14	1
1:A:147:LEU:HD21	1:A:203:ILE:HG21	0.44	1.89	14	1
1:A:49:VAL:CB	1:A:62:SER:O	0.44	2.54	16	1
1:A:52:LYS:O	1:B:129:GLU:HG2	0.44	2.12	18	1
1:B:51:ILE:HD13	1:B:51:ILE:H	0.44	1.72	18	1
1:A:102:PHE:CE2	1:A:106:ILE:HG22	0.44	2.47	19	1
1:A:76:PHE:CZ	1:B:117:SER:HB2	0.44	2.46	7	4
1:A:196:ILE:HD12	1:A:203:ILE:HG23	0.44	1.88	13	2
1:A:20:ILE:O	1:A:21:HIS:CB	0.44	2.65	16	8
1:B:189:MET:CG	1:B:195:LEU:HB2	0.44	2.42	1	1
1:A:23:TYR:CD2	1:A:27:SER:CB	0.44	3.00	2	2
1:A:128:SER:HA	1:B:51:ILE:HD12	0.44	1.90	4	1
1:A:143:ILE:HD13	1:A:183:VAL:HG22	0.44	1.90	13	2
1:B:103:ARG:O	1:B:107:GLN:HB2	0.44	2.13	12	4
1:B:72:GLU:HB2	1:B:120:MET:CE	0.44	2.43	7	3
1:A:47:VAL:HG21	1:A:70:ILE:HD11	0.44	1.90	7	1
1:A:143:ILE:CD1	1:A:186:ILE:HG13	0.44	2.41	10	1
1:B:42:ILE:HD11	1:B:64:LEU:CD1	0.44	2.43	10	1
1:A:104:GLN:O	1:A:108:VAL:HB	0.44	2.13	20	1
1:A:204:VAL:O	1:A:204:VAL:HG12	0.44	2.12	20	1
1:A:128:SER:HB2	1:B:51:ILE:HG21	0.44	1.90	3	1
1:A:149:ASN:O	1:A:153:GLN:HG2	0.44	2.12	4	1
1:A:166:LYS:HB3	1:A:202:THR:CG2	0.44	2.40	5	1
1:A:90:THR:O	1:A:91:ALA:C	0.44	2.56	11	3
1:B:20:ILE:CD1	1:B:43:VAL:HG21	0.44	2.43	11	1
1:B:106:ILE:HB	1:B:113:LEU:HB2	0.44	1.89	15	1
1:B:159:HIS:O	1:B:161:ASP:N	0.44	2.49	8	5
1:B:39:LEU:O	1:B:96:GLU:HA	0.44	2.13	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:76:PHE:HD2	1:B:120:MET:CE	0.44	2.25	7	1
1:A:110:PRO:HB3	1:B:110:PRO:HB3	0.44	1.90	19	2
1:B:11:LEU:HD21	1:B:41:TYR:CZ	0.44	2.47	20	2
1:A:195:LEU:HA	1:A:209:ARG:NH2	0.44	2.27	16	1
1:A:189:MET:SD	1:A:195:LEU:HD13	0.44	2.53	18	1
1:A:51:ILE:HG23	1:A:61:LEU:CD1	0.44	2.42	7	1
1:A:134:LEU:HD13	1:A:174:GLN:O	0.44	2.12	7	1
1:A:72:GLU:CG	1:A:120:MET:HE2	0.44	2.41	14	1
1:B:11:LEU:O	1:B:15:LEU:N	0.44	2.48	11	5
1:B:41:TYR:CD1	1:B:41:TYR:C	0.44	2.91	6	2
1:A:138:ASP:O	1:A:142:ARG:CB	0.44	2.65	7	1
1:B:169:ARG:HA	1:B:187:LEU:HD12	0.44	1.88	11	1
1:A:40:TYR:CD2	1:A:40:TYR:N	0.44	2.85	12	1
1:A:47:VAL:H	1:A:64:LEU:HB2	0.44	1.72	12	1
1:B:169:ARG:HG3	1:B:180:ARG:CB	0.44	2.43	15	1
1:B:169:ARG:HD3	1:B:180:ARG:HB3	0.44	1.90	17	1
1:A:105:LEU:HD11	1:A:112:ILE:HD12	0.44	1.89	19	1
1:B:100:LYS:O	1:B:103:ARG:HG2	0.44	2.13	19	1
1:B:106:ILE:HD12	1:B:113:LEU:HD22	0.44	1.88	19	1
1:A:40:TYR:O	1:A:70:ILE:N	0.44	2.51	20	1
1:A:30:ILE:HD12	1:A:86:VAL:HG23	0.43	1.90	4	4
1:A:191:GLU:O	1:A:191:GLU:HG2	0.43	2.13	17	2
1:B:159:HIS:HD2	1:B:162:GLY:O	0.43	1.96	18	2
1:A:143:ILE:HG12	1:A:183:VAL:CG2	0.43	2.40	11	1
1:A:113:LEU:O	1:A:116:LEU:HB3	0.43	2.12	12	1
1:B:111:ASP:O	1:B:115:ARG:HB3	0.43	2.13	14	1
1:B:9:PRO:O	1:B:13:TRP:HB2	0.43	2.13	15	1
1:B:166:LYS:HB2	1:B:202:THR:HA	0.43	1.90	18	1
1:B:106:ILE:CD1	1:B:113:LEU:HD22	0.43	2.44	19	1
1:A:18:CYS:HG	1:A:95:ALA:HB1	0.43	1.73	3	2
1:B:156:ALA:HB1	1:B:163:MET:SD	0.43	2.52	5	1
1:B:196:ILE:HG12	1:B:209:ARG:OXT	0.43	2.12	7	1
1:A:55:GLU:OE1	1:A:57:LYS:HB2	0.43	2.13	20	2
1:A:18:CYS:SG	1:A:19:HIS:N	0.43	2.92	19	1
1:B:99:TYR:C	1:B:99:TYR:HD1	0.43	2.17	5	6
1:A:42:ILE:HG12	1:A:94:VAL:CG1	0.43	2.42	2	1
1:B:46:SER:O	1:B:90:THR:HG23	0.43	2.14	2	1
1:A:39:LEU:HG	1:A:40:TYR:N	0.43	2.27	3	4
1:A:139:VAL:HA	1:A:176:VAL:CG1	0.43	2.43	3	1
1:A:146:THR:O	1:A:149:ASN:HB3	0.43	2.13	6	3
1:A:143:ILE:HD12	1:A:186:ILE:CB	0.43	2.43	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:142:ARG:HB3	1:B:176:VAL:HG13	0.43	1.90	19	1
1:B:23:TYR:CD2	1:B:27:SER:CB	0.43	3.01	2	1
1:B:34:GLU:OE2	1:B:82:ARG:HB2	0.43	2.13	3	3
1:B:11:LEU:HD13	1:B:41:TYR:OH	0.43	2.13	9	1
1:A:126:VAL:O	1:A:130:LYS:HB2	0.43	2.14	13	1
1:A:30:ILE:HG21	1:A:36:ALA:HA	0.43	1.90	14	1
1:A:151:ALA:HA	1:A:156:ALA:HB2	0.43	1.90	14	1
1:A:143:ILE:HD13	1:A:183:VAL:HA	0.43	1.90	17	2
1:A:99:TYR:C	1:A:99:TYR:HD1	0.43	2.17	3	6
1:B:180:ARG:HD2	1:B:181:GLU:OE1	0.43	2.14	7	2
1:B:25:SER:O	1:B:26:LYS:HB2	0.43	2.14	11	2
1:B:35:LYS:HA	1:B:81:GLU:HA	0.43	1.89	19	3
1:B:153:GLN:CB	1:B:154:PRO:HD2	0.43	2.44	3	2
1:A:132:GLY:HA2	1:A:135:ALA:HB3	0.43	1.89	5	1
1:A:11:LEU:HA	1:A:14:PHE:HB3	0.43	1.90	6	3
1:A:190:LEU:O	1:A:197:SER:HA	0.43	2.12	19	2
1:A:69:PHE:CB	1:A:116:LEU:HD12	0.43	2.44	9	3
1:A:187:LEU:O	1:A:190:LEU:HG	0.43	2.13	9	1
1:B:27:SER:O	1:B:29:LEU:CD2	0.43	2.65	18	2
1:A:127:THR:O	1:A:127:THR:HG22	0.43	2.14	14	1
1:B:159:HIS:CG	1:B:160:PRO:HD2	0.43	2.49	14	1
1:B:48:ALA:CB	1:B:60:ILE:HD13	0.43	2.42	15	1
1:B:53:ASP:HB2	1:B:57:LYS:HB2	0.43	1.91	15	1
1:A:143:ILE:HD12	1:A:186:ILE:HD13	0.43	1.90	17	1
1:A:33:GLY:H	1:A:82:ARG:HB2	0.43	1.73	14	1
1:A:156:ALA:HA	1:A:164:GLN:O	0.43	2.13	19	1
1:B:53:ASP:HB2	1:B:57:LYS:HG2	0.43	1.89	1	1
1:B:143:ILE:HD13	1:B:183:VAL:HG22	0.43	1.90	7	2
1:B:32:GLN:O	1:B:34:GLU:HG3	0.43	2.14	7	1
1:B:22:LYS:HB2	1:B:94:VAL:HG22	0.43	1.89	12	1
1:B:18:CYS:HB3	1:B:97:ILE:CG1	0.43	2.42	14	3
1:B:49:VAL:HG13	1:B:85:TRP:O	0.43	2.14	15	1
1:A:130:LYS:O	1:A:130:LYS:HG2	0.43	2.14	19	1
1:B:166:LYS:CB	1:B:202:THR:HA	0.43	2.43	20	1
1:A:30:ILE:CG2	1:A:34:GLU:HB2	0.43	2.44	2	1
1:B:23:TYR:CD2	1:B:27:SER:HB2	0.43	2.49	2	1
1:B:137:LEU:HG	1:B:178:CYS:SG	0.43	2.53	4	1
1:A:158:THR:HA	1:A:163:MET:HB3	0.43	1.91	5	2
1:A:50:LEU:HA	1:A:61:LEU:HD12	0.43	1.91	11	2
1:A:47:VAL:HG12	1:A:88:ALA:HA	0.43	1.91	12	1
1:A:196:ILE:HG22	1:A:209:ARG:O	0.43	2.13	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:30:ILE:CG2	1:B:34:GLU:HB2	0.43	2.43	17	2
1:A:147:LEU:CG	1:A:167:ILE:HD11	0.43	2.44	14	1
1:A:169:ARG:HB3	1:A:187:LEU:CD1	0.43	2.40	16	1
1:B:178:CYS:SG	1:B:183:VAL:HB	0.43	2.54	17	1
1:B:11:LEU:HA	1:B:14:PHE:HB3	0.43	1.91	20	2
1:A:153:GLN:C	1:A:155:ASP:H	0.43	2.16	8	1
1:B:14:PHE:O	1:B:17:HIS:HB2	0.43	2.13	9	1
1:A:33:GLY:HA2	1:A:82:ARG:NH1	0.43	2.29	11	1
1:B:20:ILE:O	1:B:21:HIS:CB	0.43	2.67	15	1
1:A:139:VAL:HG22	1:A:143:ILE:HD11	0.43	1.91	20	1
1:B:70:ILE:CD1	1:B:86:VAL:HG11	0.42	2.44	5	1
1:A:32:GLN:OE1	1:A:32:GLN:HA	0.42	2.14	6	1
1:A:137:LEU:HG	1:A:178:CYS:SG	0.42	2.54	6	1
1:A:159:HIS:O	1:A:161:ASP:N	0.42	2.51	16	4
1:B:34:GLU:O	1:B:82:ARG:HA	0.42	2.14	14	1
1:B:51:ILE:HD12	1:B:61:LEU:CB	0.42	2.43	18	1
1:B:31:HIS:CA	1:B:82:ARG:HG3	0.42	2.44	8	1
1:A:114:MET:O	1:A:117:SER:HB2	0.42	2.14	14	1
1:A:25:SER:O	1:A:26:LYS:HG3	0.42	2.13	6	1
1:A:102:PHE:CD2	1:A:103:ARG:N	0.42	2.87	17	2
1:A:190:LEU:CD2	1:A:196:ILE:HG12	0.42	2.23	13	1
1:B:114:MET:O	1:B:117:SER:HB2	0.42	2.13	14	1
1:B:44:LYS:HD3	1:B:66:GLN:HB3	0.42	1.91	18	1
1:A:52:LYS:HG3	1:A:58:GLU:HB3	0.42	1.90	1	1
1:A:103:ARG:C	1:A:106:ILE:HG13	0.42	2.34	18	3
1:B:168:THR:HB	1:B:170:GLN:OE1	0.42	2.14	15	4
1:A:20:ILE:HG23	1:A:43:VAL:CG2	0.42	2.45	7	2
1:B:41:TYR:O	1:B:95:ALA:N	0.42	2.49	14	2
1:A:150:LEU:C	1:A:152:LYS:N	0.42	2.73	16	1
1:A:31:HIS:CA	1:A:82:ARG:HG3	0.42	2.45	3	1
1:A:42:ILE:CB	1:A:94:VAL:HG12	0.42	2.45	5	1
1:A:114:MET:CE	1:B:113:LEU:HD21	0.42	2.44	15	2
1:B:42:ILE:O	1:B:42:ILE:HG23	0.42	2.14	8	2
1:B:60:ILE:HD11	1:B:87:ARG:HD3	0.42	1.91	8	1
1:B:153:GLN:C	1:B:155:ASP:H	0.42	2.17	8	1
1:A:11:LEU:HD22	1:A:41:TYR:HE2	0.42	1.74	13	2
1:A:150:LEU:HD13	1:A:165:ILE:HD13	0.42	1.92	14	2
1:B:169:ARG:HA	1:B:172:ILE:HG12	0.42	1.92	15	1
1:A:166:LYS:CB	1:A:202:THR:HA	0.42	2.45	16	2
1:A:122:ARG:O	1:A:125:GLN:HG2	0.42	2.14	18	1
1:A:18:CYS:HB2	1:A:97:ILE:HG12	0.42	1.90	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:ALA:HB1	1:A:60:ILE:HG23	0.42	1.90	19	1
1:B:37:GLU:O	1:B:99:TYR:CD1	0.42	2.72	19	1
1:A:99:TYR:HA	1:A:102:PHE:CD2	0.42	2.50	20	1
1:A:121:ALA:HA	1:A:124:LEU:HB2	0.42	1.91	4	1
1:B:81:GLU:O	1:B:83:SER:N	0.42	2.52	10	3
1:B:143:ILE:CD1	1:B:186:ILE:HD13	0.42	2.44	11	1
1:A:75:LEU:CG	1:A:76:PHE:N	0.42	2.81	14	1
1:A:172:ILE:O	1:A:176:VAL:HG23	0.42	2.14	14	1
1:B:143:ILE:HD12	1:B:186:ILE:HD12	0.42	1.91	14	1
1:A:196:ILE:HD12	1:A:203:ILE:CG2	0.42	2.45	16	1
1:A:169:ARG:HD3	1:A:180:ARG:HB3	0.42	1.92	17	2
1:B:14:PHE:HE2	1:B:102:PHE:CE1	0.42	2.32	10	2
1:B:21:HIS:HA	1:B:93:GLU:OE1	0.42	2.14	5	1
1:B:167:ILE:HD12	1:B:167:ILE:O	0.42	2.14	9	1
1:B:179:SER:HB3	1:B:180:ARG:H	0.42	1.46	14	1
1:B:59:MET:HB3	1:B:174:GLN:HG2	0.42	1.91	20	1
1:B:31:HIS:CE1	1:B:58:GLU:CB	0.42	3.03	2	4
1:B:81:GLU:O	1:B:82:ARG:HD3	0.42	2.15	12	4
1:B:77:GLU:O	1:B:78:GLU:CB	0.42	2.68	4	2
1:B:139:VAL:HG21	1:B:178:CYS:SG	0.42	2.55	5	1
1:B:76:PHE:CD1	1:B:113:LEU:HD11	0.42	2.50	6	1
1:A:14:PHE:CE2	1:A:102:PHE:CD1	0.42	3.08	7	2
1:A:51:ILE:CD1	1:A:61:LEU:HB3	0.42	2.45	7	1
1:B:41:TYR:HD1	1:B:68:ASP:O	0.42	1.98	10	2
1:A:41:TYR:CD1	1:A:68:ASP:O	0.42	2.73	13	1
1:B:189:MET:SD	1:B:195:LEU:HB2	0.42	2.55	13	1
1:A:47:VAL:C	1:A:89:LYS:HB2	0.42	2.34	14	1
1:A:147:LEU:HG	1:A:167:ILE:HD11	0.42	1.90	14	1
1:A:42:ILE:HD11	1:A:64:LEU:CD1	0.42	2.44	17	1
1:A:57:LYS:O	1:A:57:LYS:HG3	0.42	2.14	19	1
1:B:143:ILE:CD1	1:B:186:ILE:HG13	0.42	2.45	1	1
1:B:113:LEU:HG	1:B:113:LEU:O	0.42	2.14	5	1
1:B:172:ILE:HG22	1:B:183:VAL:CG2	0.42	2.44	10	1
1:B:166:LYS:O	1:B:167:ILE:HG23	0.42	2.15	13	1
1:B:190:LEU:HD22	1:B:196:ILE:CB	0.42	2.45	16	1
1:A:39:LEU:O	1:A:96:GLU:HA	0.42	2.15	20	1
1:A:22:LYS:HB2	1:A:94:VAL:N	0.42	2.30	2	2
1:A:129:GLU:O	1:A:130:LYS:HG3	0.42	2.15	7	1
1:B:14:PHE:CE2	1:B:102:PHE:CD1	0.42	3.08	7	1
1:B:147:LEU:HD22	1:B:167:ILE:HD11	0.42	1.92	13	1
1:A:40:TYR:HB2	1:A:70:ILE:CG2	0.42	2.45	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:143:ILE:CD1	1:B:183:VAL:HG22	0.42	2.45	16	1
1:B:42:ILE:HD11	1:B:64:LEU:CB	0.42	2.45	17	1
1:B:116:LEU:HG	1:B:120:MET:CE	0.42	2.44	18	1
1:B:119:GLN:OE1	1:B:119:GLN:HA	0.42	2.14	20	1
1:A:73:LEU:HD21	1:B:124:LEU:CD1	0.41	2.45	2	1
1:B:22:LYS:HB2	1:B:94:VAL:N	0.41	2.30	2	1
1:B:15:LEU:HB3	1:B:20:ILE:CD1	0.41	2.45	15	1
1:B:25:SER:HB3	1:B:90:THR:CA	0.41	2.44	9	2
1:A:196:ILE:HG21	1:A:203:ILE:HG23	0.41	1.91	11	1
1:A:180:ARG:HD2	1:A:181:GLU:OE2	0.41	2.15	12	1
1:B:169:ARG:HD2	1:B:170:GLN:N	0.41	2.31	14	1
1:B:31:HIS:O	1:B:32:GLN:HB2	0.41	2.14	17	1
1:A:124:LEU:CD1	1:B:73:LEU:HD21	0.41	2.45	4	2
1:A:8:ASP:CG	1:A:115:ARG:HH12	0.41	2.19	5	1
1:A:50:LEU:HD23	1:A:50:LEU:O	0.41	2.15	5	1
1:B:205:VAL:HG12	1:B:209:ARG:O	0.41	2.15	5	1
1:A:73:LEU:HA	1:A:77:GLU:HB2	0.41	1.92	8	1
1:A:134:LEU:HD22	1:A:176:VAL:HA	0.41	1.92	10	1
1:B:103:ARG:O	1:B:107:GLN:HG3	0.41	2.15	13	2
1:A:77:GLU:O	1:A:78:GLU:CB	0.41	2.68	11	1
1:B:196:ILE:HG21	1:B:203:ILE:HG23	0.41	1.92	11	1
1:A:11:LEU:HD23	1:A:14:PHE:CB	0.41	2.45	13	2
1:B:123:ARG:C	1:B:126:VAL:HG12	0.41	2.35	14	1
1:A:85:TRP:CZ2	1:A:123:ARG:HG2	0.41	2.51	16	1
1:A:159:HIS:HD2	1:A:162:GLY:O	0.41	1.98	18	1
1:A:72:GLU:HG2	1:A:116:LEU:HD11	0.41	1.91	4	1
1:A:41:TYR:HB3	1:A:95:ALA:CB	0.41	2.37	8	1
1:A:15:LEU:HD21	1:A:41:TYR:HE2	0.41	1.74	10	1
1:B:40:TYR:CD2	1:B:40:TYR:N	0.41	2.89	12	1
1:A:45:GLY:HA3	1:A:92:CYS:CA	0.41	2.46	18	1
1:A:106:ILE:HD12	1:A:113:LEU:HD22	0.41	1.90	19	1
1:B:166:LYS:C	1:B:167:ILE:HG13	0.41	2.35	20	1
1:B:127:THR:O	1:B:131:VAL:HG22	0.41	2.15	6	1
1:A:14:PHE:HE2	1:A:97:ILE:HD11	0.41	1.75	8	1
1:A:14:PHE:HE2	1:A:102:PHE:CE1	0.41	2.34	13	2
1:B:23:TYR:CB	1:B:24:PRO:CD	0.41	2.99	10	1
1:B:52:LYS:HG2	1:B:58:GLU:HB3	0.41	1.91	10	1
1:B:164:GLN:CB	1:B:204:VAL:HG23	0.41	2.41	10	1
1:B:134:LEU:HD21	1:B:174:GLN:O	0.41	2.15	14	1
1:B:147:LEU:HD22	1:B:196:ILE:HD13	0.41	1.91	19	1
1:B:73:LEU:HG	1:B:85:TRP:CD2	0.41	2.51	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:149:ASN:O	1:B:153:GLN:HG2	0.41	2.16	4	1
1:A:8:ASP:O	1:A:12:GLU:HG3	0.41	2.15	5	1
1:A:198:ALA:CB	1:A:203:ILE:HG12	0.41	2.46	8	1
1:B:15:LEU:HD22	1:B:20:ILE:CD1	0.41	2.46	11	1
1:B:47:VAL:CG1	1:B:88:ALA:HA	0.41	2.46	12	1
1:A:72:GLU:HG2	1:A:73:LEU:N	0.41	2.31	14	1
1:B:190:LEU:HD23	1:B:195:LEU:HB3	0.41	1.91	14	1
1:A:184:GLY:O	1:A:185:ARG:C	0.41	2.59	15	1
1:A:102:PHE:O	1:A:106:ILE:HG23	0.41	2.15	19	2
1:B:180:ARG:HA	1:B:183:VAL:CG1	0.41	2.45	1	1
1:B:166:LYS:HB3	1:B:202:THR:HA	0.41	1.92	16	2
1:A:189:MET:SD	1:A:195:LEU:HB2	0.41	2.56	6	1
1:A:41:TYR:CE1	1:A:69:PHE:CD1	0.41	3.08	7	1
1:A:70:ILE:CD1	1:A:86:VAL:HG11	0.41	2.46	20	3
1:A:82:ARG:NE	1:A:83:SER:H	0.41	2.13	11	1
1:A:27:SER:O	1:A:29:LEU:CD2	0.41	2.69	16	2
1:B:42:ILE:HG22	1:B:68:ASP:N	0.41	2.29	12	1
1:B:42:ILE:CG2	1:B:94:VAL:HG12	0.41	2.46	17	1
1:A:147:LEU:HD13	1:A:203:ILE:HG21	0.41	1.92	18	1
1:A:75:LEU:HB3	1:A:99:TYR:CD2	0.41	2.51	20	1
1:B:139:VAL:HG21	1:B:183:VAL:HG23	0.41	1.91	20	1
1:B:172:ILE:HB	1:B:183:VAL:HG11	0.41	1.92	3	1
1:A:50:LEU:HB3	1:A:60:ILE:HA	0.41	1.93	6	1
1:B:113:LEU:O	1:B:116:LEU:HB3	0.41	2.15	12	1
1:A:196:ILE:HG13	1:A:197:SER:N	0.41	2.30	13	1
1:A:179:SER:O	1:A:183:VAL:HB	0.41	2.16	16	1
1:A:169:ARG:HA	1:A:172:ILE:CG1	0.41	2.46	17	1
1:B:205:VAL:O	1:B:205:VAL:HG23	0.41	2.16	19	1
1:B:127:THR:HG22	1:B:131:VAL:HG13	0.41	1.92	20	1
1:B:183:VAL:HG13	1:B:187:LEU:HG	0.41	1.92	1	1
1:A:61:LEU:HD22	1:A:62:SER:HB3	0.41	1.92	2	1
1:A:164:GLN:HB3	1:A:204:VAL:HB	0.41	1.93	2	1
1:B:23:TYR:CE2	1:B:27:SER:HB2	0.41	2.51	2	1
1:B:140:THR:C	1:B:142:ARG:N	0.41	2.74	3	1
1:B:186:ILE:HA	1:B:189:MET:HG2	0.41	1.93	4	3
1:A:167:ILE:HD12	1:A:167:ILE:O	0.41	2.15	10	2
1:A:77:GLU:O	1:A:78:GLU:HB2	0.41	2.15	6	1
1:A:59:MET:CE	1:A:175:ILE:HA	0.41	2.46	10	1
1:B:186:ILE:HG23	1:B:195:LEU:HD13	0.41	1.92	12	1
1:A:22:LYS:HE2	1:A:88:ALA:HB2	0.41	1.93	13	1
1:B:102:PHE:CD2	1:B:103:ARG:N	0.41	2.89	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:SER:O	1:A:26:LYS:HB2	0.41	2.15	15	2
1:B:170:GLN:O	1:B:174:GLN:HB2	0.41	2.16	14	1
1:B:179:SER:OG	1:B:181:GLU:HB2	0.41	2.15	17	1
1:A:138:ASP:OD1	1:A:142:ARG:HD3	0.41	2.16	18	1
1:A:124:LEU:HB2	1:B:124:LEU:HG	0.41	1.92	19	1
1:A:23:TYR:CD2	1:A:27:SER:HB2	0.41	2.51	2	3
1:B:198:ALA:CB	1:B:203:ILE:HG12	0.41	2.46	8	1
1:A:42:ILE:HG23	1:A:42:ILE:O	0.41	2.16	15	1
1:B:73:LEU:HD13	1:B:77:GLU:HB2	0.41	1.93	15	1
1:B:166:LYS:CG	1:B:202:THR:HG23	0.41	2.44	15	1
1:A:18:CYS:CA	1:A:97:ILE:CG2	0.41	2.98	16	2
1:B:35:LYS:HA	1:B:81:GLU:CA	0.41	2.46	19	1
1:A:78:GLU:HB3	1:B:122:ARG:NH1	0.40	2.31	2	1
1:A:14:PHE:HE2	1:A:102:PHE:CD1	0.40	2.34	7	1
1:A:73:LEU:HD13	1:A:77:GLU:HG3	0.40	1.93	8	1
1:B:198:ALA:HA	1:B:203:ILE:HA	0.40	1.91	10	1
1:B:182:THR:O	1:B:186:ILE:HD12	0.40	2.16	13	1
1:B:147:LEU:HD21	1:B:167:ILE:HD11	0.40	1.93	14	1
1:A:124:LEU:CD2	1:B:124:LEU:HD21	0.40	2.33	18	1
1:B:186:ILE:O	1:B:189:MET:HB2	0.40	2.16	19	1
1:B:169:ARG:HG3	1:B:180:ARG:HB3	0.40	1.92	20	1
1:A:42:ILE:O	1:A:67:GLY:HA2	0.40	2.16	2	1
1:B:32:GLN:OE1	1:B:32:GLN:HA	0.40	2.16	4	1
1:A:22:LYS:HZ1	1:A:29:LEU:HD21	0.40	1.75	6	1
1:A:83:SER:O	1:A:84:ALA:HB3	0.40	2.16	6	2
1:B:14:PHE:HE2	1:B:102:PHE:CD1	0.40	2.33	7	1
1:B:53:ASP:HB2	1:B:57:LYS:HB3	0.40	1.94	9	1
1:B:59:MET:O	1:B:59:MET:HG2	0.40	2.16	10	1
1:A:31:HIS:HE2	1:A:58:GLU:HB2	0.40	1.76	11	1
1:B:153:GLN:HB2	1:B:154:PRO:HD2	0.40	1.92	14	1
1:A:169:ARG:HA	1:A:172:ILE:HG12	0.40	1.92	17	1
1:B:11:LEU:HD21	1:B:41:TYR:OH	0.40	2.16	17	1
1:A:205:VAL:HG23	1:A:205:VAL:O	0.40	2.15	19	1
1:B:14:PHE:CE2	1:B:97:ILE:HD11	0.40	2.52	19	1
1:B:34:GLU:O	1:B:82:ARG:N	0.40	2.54	20	1
1:B:83:SER:O	1:B:84:ALA:HB3	0.40	2.16	4	1
1:A:34:GLU:O	1:A:82:ARG:N	0.40	2.53	5	1
1:B:147:LEU:HD12	1:B:196:ILE:CD1	0.40	2.47	6	1
1:A:42:ILE:O	1:A:42:ILE:HG23	0.40	2.16	8	1
1:B:72:GLU:CB	1:B:120:MET:SD	0.40	3.07	12	1
1:B:158:THR:HA	1:B:163:MET:HB3	0.40	1.93	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:73:LEU:HG	1:B:85:TRP:CE3	0.40	2.51	2	1
1:B:129:GLU:O	1:B:130:LYS:HG3	0.40	2.15	3	1
1:A:189:MET:CG	1:A:195:LEU:HB2	0.40	2.46	5	1
1:B:42:ILE:CB	1:B:94:VAL:HG12	0.40	2.47	5	1
1:A:171:GLU:HB3	1:A:175:ILE:HD12	0.40	1.92	7	1
1:B:187:LEU:HD23	1:B:203:ILE:HD11	0.40	1.92	10	1
1:B:31:HIS:NE2	1:B:58:GLU:HB2	0.40	2.32	11	1
1:B:99:TYR:C	1:B:99:TYR:CD1	0.40	2.95	11	1
1:A:18:CYS:HB3	1:A:97:ILE:CG1	0.40	2.46	13	1
1:B:110:PRO:O	1:B:114:MET:HB2	0.40	2.17	14	1
1:B:172:ILE:HG21	1:B:183:VAL:CG2	0.40	2.46	14	1
1:B:179:SER:O	1:B:183:VAL:HB	0.40	2.16	18	1
1:B:143:ILE:HG23	1:B:172:ILE:CG2	0.40	2.46	1	1
1:A:49:VAL:O	1:A:61:LEU:HD13	0.40	2.15	4	1
1:B:138:ASP:OD2	1:B:138:ASP:C	0.40	2.60	6	1
1:A:41:TYR:CZ	1:A:69:PHE:CE1	0.40	3.09	7	1
1:B:22:LYS:HZ1	1:B:29:LEU:CD1	0.40	2.29	9	1
1:B:72:GLU:OE2	1:B:72:GLU:N	0.40	2.53	10	1
1:A:124:LEU:HD23	1:B:124:LEU:HD23	0.40	1.91	12	1
1:A:147:LEU:HD21	1:A:167:ILE:HD11	0.40	1.93	14	1
1:A:153:GLN:HB2	1:A:154:PRO:HD2	0.40	1.93	14	1
1:B:141:GLY:O	1:B:145:GLN:CB	0.40	2.67	14	1
1:B:184:GLY:O	1:B:185:ARG:C	0.40	2.59	15	1
1:A:72:GLU:OE2	1:A:72:GLU:N	0.40	2.54	17	1
1:B:53:ASP:N	1:B:57:LYS:O	0.40	2.54	17	1
1:A:143:ILE:CD1	1:A:183:VAL:HA	0.40	2.46	18	1
1:B:49:VAL:HG13	1:B:85:TRP:CA	0.40	2.46	19	1
1:A:99:TYR:C	1:A:99:TYR:CD1	0.40	2.95	20	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	201/209 (96%)	157±4 (78±2%)	26±4 (13±2%)	18±2 (9±1%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	201/209 (96%)	158±3 (79±2%)	25±3 (13±2%)	18±2 (9±1%)	1 12
All	All	8040/8360 (96%)	6296 (78%)	1032 (13%)	712 (9%)	1 12

All 81 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	HIS	20
1	A	26	LYS	20
1	A	30	ILE	20
1	A	31	HIS	20
1	A	81	GLU	20
1	A	85	TRP	20
1	A	161	ASP	20
1	A	196	ILE	20
1	B	21	HIS	20
1	B	26	LYS	20
1	B	30	ILE	20
1	B	31	HIS	20
1	B	81	GLU	20
1	B	85	TRP	20
1	B	161	ASP	20
1	A	78	GLU	19
1	B	78	GLU	19
1	B	196	ILE	19
1	B	180	ARG	18
1	A	165	ILE	17
1	A	180	ARG	17
1	B	84	ALA	17
1	B	139	VAL	17
1	A	139	VAL	16
1	A	207	GLY	16
1	A	84	ALA	15
1	B	165	ILE	15
1	B	140	THR	15
1	A	140	THR	14
1	B	207	GLY	14
1	A	160	PRO	13
1	B	66	GLN	11
1	B	160	PRO	11
1	B	82	ARG	10
1	A	66	GLN	9

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Mol	Chain	Res	Type	Models (Total)
1	B	132	GLY	8
1	A	82	ARG	8
1	A	132	GLY	7
1	B	42	ILE	7
1	A	131	VAL	5
1	A	143	ILE	4
1	A	32	GLN	4
1	B	32	GLN	4
1	B	131	VAL	4
1	A	42	ILE	4
1	A	201	LYS	3
1	B	143	ILE	3
1	B	130	LYS	3
1	A	167	ILE	3
1	B	128	SER	2
1	B	185	ARG	2
1	A	88	ALA	2
1	B	88	ALA	2
1	A	130	LYS	2
1	B	167	ILE	2
1	A	181	GLU	2
1	B	36	ALA	2
1	B	99	TYR	2
1	B	135	ALA	2
1	A	179	SER	2
1	A	45	GLY	1
1	A	128	SER	1
1	A	138	ASP	1
1	B	141	GLY	1
1	A	185	ARG	1
1	A	28	THR	1
1	B	28	THR	1
1	B	201	LYS	1
1	B	137	LEU	1
1	A	136	PHE	1
1	B	136	PHE	1
1	A	208	THR	1
1	B	208	THR	1
1	A	154	PRO	1
1	B	154	PRO	1
1	B	181	GLU	1
1	B	179	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	133	ASN	1
1	A	36	ALA	1
1	A	83	SER	1
1	B	53	ASP	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	174/180 (97%)	115±4 (66±2%)	59±4 (34±2%)	1 11
1	B	174/180 (97%)	114±4 (66±2%)	60±4 (34±2%)	1 10
All	All	6960/7200 (97%)	4589 (66%)	2371 (34%)	1 10

All 270 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	23	TYR	20
1	A	25	SER	20
1	A	30	ILE	20
1	A	50	LEU	20
1	A	61	LEU	20
1	A	75	LEU	20
1	A	82	ARG	20
1	A	86	VAL	20
1	A	92	CYS	20
1	A	99	TYR	20
1	A	105	LEU	20
1	A	108	VAL	20
1	A	122	ARG	20
1	A	165	ILE	20
1	A	182	THR	20
1	B	23	TYR	20
1	B	25	SER	20
1	B	30	ILE	20
1	B	50	LEU	20
1	B	61	LEU	20

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Mol	Chain	Res	Type	Models (Total)
1	B	75	LEU	20
1	B	82	ARG	20
1	B	86	VAL	20
1	B	92	CYS	20
1	B	99	TYR	20
1	B	105	LEU	20
1	B	108	VAL	20
1	B	122	ARG	20
1	B	165	ILE	20
1	B	182	THR	20
1	A	10	THR	19
1	A	29	LEU	19
1	A	39	LEU	19
1	A	90	THR	19
1	A	114	MET	19
1	A	140	THR	19
1	A	169	ARG	19
1	B	10	THR	19
1	B	20	ILE	19
1	B	39	LEU	19
1	B	90	THR	19
1	B	114	MET	19
1	B	139	VAL	19
1	B	140	THR	19
1	B	169	ARG	19
1	B	202	THR	19
1	A	20	ILE	18
1	A	159	HIS	18
1	A	202	THR	18
1	B	29	LEU	18
1	B	72	GLU	18
1	B	112	ILE	18
1	B	167	ILE	18
1	B	195	LEU	18
1	A	72	GLU	17
1	A	112	ILE	17
1	A	195	LEU	17
1	B	63	TYR	17
1	A	167	ILE	16
1	B	124	LEU	16
1	B	159	HIS	16
1	B	179	SER	16

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Mol	Chain	Res	Type	Models (Total)
1	A	58	GLU	15
1	A	63	TYR	15
1	A	161	ASP	15
1	B	58	GLU	15
1	B	123	ARG	15
1	A	65	ASN	14
1	A	73	LEU	14
1	A	183	VAL	14
1	B	161	ASP	14
1	A	123	ARG	14
1	A	11	LEU	13
1	A	124	LEU	13
1	A	136	PHE	13
1	B	11	LEU	13
1	B	55	GLU	13
1	A	103	ARG	13
1	A	139	VAL	13
1	A	180	ARG	13
1	B	131	VAL	13
1	A	116	LEU	12
1	B	81	GLU	12
1	B	116	LEU	12
1	B	136	PHE	12
1	A	131	VAL	12
1	B	103	ARG	12
1	A	55	GLU	11
1	A	208	THR	11
1	B	27	SER	11
1	B	41	TYR	11
1	B	65	ASN	11
1	B	102	PHE	11
1	B	183	VAL	11
1	B	208	THR	11
1	A	57	LYS	11
1	A	87	ARG	11
1	A	102	PHE	11
1	A	81	GLU	11
1	B	180	ARG	11
1	A	125	GLN	10
1	A	142	ARG	10
1	A	179	SER	10
1	B	73	LEU	10

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Mol	Chain	Res	Type	Models (Total)
1	B	142	ARG	10
1	A	16	SER	10
1	A	41	TYR	10
1	B	87	ARG	9
1	B	163	MET	9
1	B	168	THR	9
1	B	174	GLN	9
1	A	166	LYS	9
1	A	201	LYS	9
1	B	16	SER	9
1	B	57	LYS	9
1	B	68	ASP	9
1	B	126	VAL	9
1	B	201	LYS	9
1	A	181	GLU	9
1	A	174	GLN	8
1	A	204	VAL	8
1	B	120	MET	8
1	A	32	GLN	8
1	B	32	GLN	8
1	B	204	VAL	8
1	B	205	VAL	8
1	A	188	LYS	8
1	B	166	LYS	8
1	B	188	LYS	8
1	A	120	MET	7
1	A	130	LYS	7
1	A	168	THR	7
1	B	13	TRP	7
1	A	27	SER	7
1	A	28	THR	7
1	A	126	VAL	7
1	B	80	GLN	7
1	A	164	GLN	7
1	B	28	THR	7
1	B	158	THR	7
1	A	68	ASP	7
1	B	134	LEU	7
1	A	38	THR	7
1	A	111	ASP	6
1	A	163	MET	6
1	A	193	GLN	6

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Mol	Chain	Res	Type	Models (Total)
1	B	40	TYR	6
1	B	125	GLN	6
1	A	31	HIS	6
1	B	31	HIS	6
1	B	44	LYS	6
1	B	194	ASN	6
1	A	205	VAL	6
1	A	77	GLU	6
1	B	130	LYS	6
1	A	133	ASN	6
1	B	38	THR	6
1	B	181	GLU	6
1	A	119	GLN	5
1	B	22	LYS	5
1	B	119	GLN	5
1	A	44	LYS	5
1	B	12	GLU	5
1	B	42	ILE	5
1	A	192	ASP	5
1	B	77	GLU	5
1	B	111	ASP	5
1	A	98	SER	5
1	A	134	LEU	5
1	B	164	GLN	5
1	A	115	ARG	5
1	A	13	TRP	4
1	B	193	GLN	4
1	A	12	GLU	4
1	A	117	SER	4
1	A	194	ASN	4
1	B	98	SER	4
1	B	127	THR	4
1	B	191	GLU	4
1	A	8	ASP	4
1	A	80	GLN	4
1	A	14	PHE	4
1	A	170	GLN	4
1	B	14	PHE	4
1	A	158	THR	4
1	A	196	ILE	4
1	B	115	ARG	4
1	A	40	TYR	4

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Mol	Chain	Res	Type	Models (Total)
1	B	170	GLN	3
1	B	209	ARG	3
1	A	101	LYS	3
1	B	145	GLN	3
1	B	153	GLN	3
1	B	192	ASP	3
1	A	145	GLN	3
1	B	8	ASP	3
1	B	53	ASP	3
1	A	78	GLU	3
1	B	196	ILE	3
1	A	127	THR	3
1	B	203	ILE	3
1	A	76	PHE	3
1	B	76	PHE	3
1	B	78	GLU	3
1	B	189	MET	2
1	A	18	CYS	2
1	A	209	ARG	2
1	A	22	LYS	2
1	A	52	LYS	2
1	B	52	LYS	2
1	A	89	LYS	2
1	B	46	SER	2
1	B	185	ARG	2
1	A	42	ILE	2
1	B	106	ILE	2
1	A	149	ASN	2
1	B	51	ILE	2
1	B	54	GLU	2
1	A	138	ASP	2
1	B	138	ASP	2
1	A	104	GLN	2
1	A	147	LEU	2
1	B	17	HIS	2
1	B	104	GLN	2
1	B	147	LEU	2
1	A	53	ASP	1
1	B	18	CYS	1
1	B	107	GLN	1
1	A	199	HIS	1
1	A	60	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	85	TRP	1
1	B	85	TRP	1
1	B	93	GLU	1
1	A	107	GLN	1
1	A	37	GLU	1
1	A	93	GLU	1
1	A	137	LEU	1
1	B	37	GLU	1
1	B	199	HIS	1
1	A	43	VAL	1
1	A	51	ILE	1
1	A	146	THR	1
1	B	89	LYS	1
1	A	143	ILE	1
1	A	171	GLU	1
1	A	203	ILE	1
1	A	24	PRO	1
1	A	54	GLU	1
1	A	97	ILE	1
1	B	59	MET	1
1	B	97	ILE	1
1	B	100	LYS	1
1	B	117	SER	1
1	A	185	ARG	1
1	A	129	GLU	1
1	A	186	ILE	1
1	B	24	PRO	1
1	B	129	GLU	1
1	B	133	ASN	1
1	B	186	ILE	1
1	B	149	ASN	1
1	A	35	LYS	1
1	A	178	CYS	1
1	B	96	GLU	1
1	A	17	HIS	1
1	A	96	GLU	1
1	B	34	GLU	1
1	B	83	SER	1
1	A	46	SER	1
1	A	153	GLN	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided