



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 05:47 AM UTC

PDB ID : 2JSS / pdb_00002jss
Title : NMR structure of chaperone Chz1 complexed with histone H2A.Z-H2B
Authors : Zhou, Z.; Feng, H.; Hansen, D.F.; Kato, H.; Luk, E.; Freedberg, D.I.; Kay, L.E.; Wu, C.; Bai, Y.
Deposited on : 2007-07-11

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

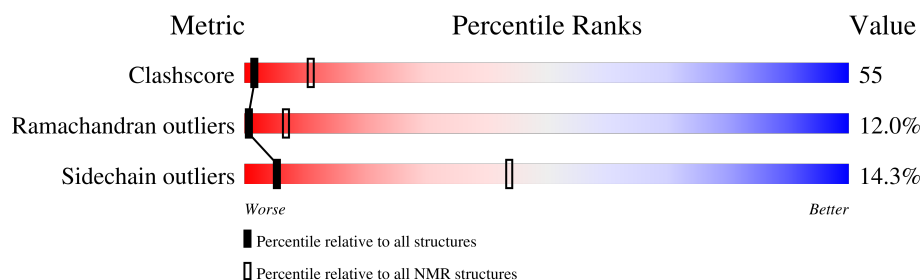
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	192	25% 61% 10% ..
2	B	62	5% 65% 16% 15%

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:3-A:189, B:7-B:47, B:51-B:62 (240)	1.32	5

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4, 7, 10
2	3, 5, 6, 8
Single-model clusters	9

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3977 atoms, of which 2012 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Chimera of Histone H2B.1 and Histone H2A.Z.

Mol	Chain	Residues	Atoms						Trace
1	A	192	Total	C	H	N	O	S	0
			3037	931	1555	273	277	1	

- Molecule 2 is a protein called Uncharacterized protein YER030W.

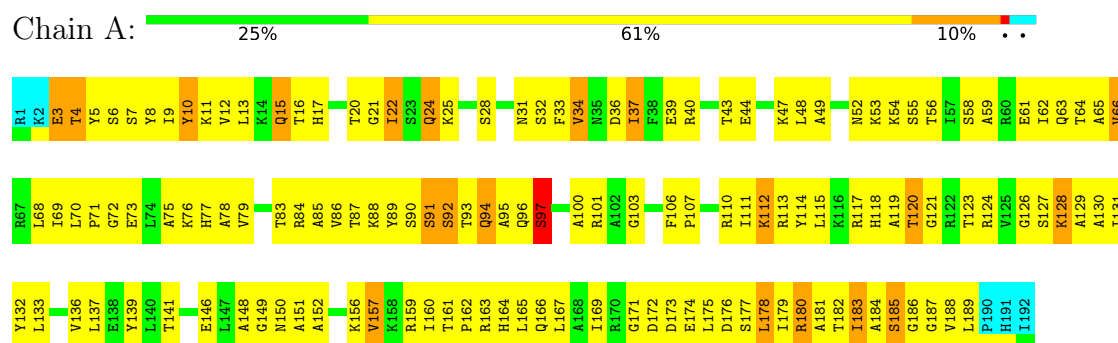
Mol	Chain	Residues	Atoms						Trace
2	B	62	Total	C	H	N	O	S	0
			940	286	457	79	116	2	

4 Residue-property plots

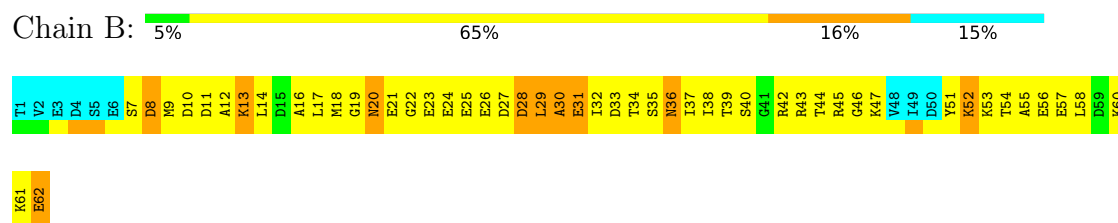
4.1 Average score per residue in the NMR ensemble

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: Chimera of Histone H2B.1 and Histone H2A.Z



- Molecule 2: Uncharacterized protein YER030W

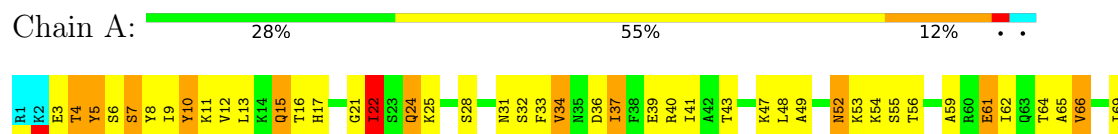


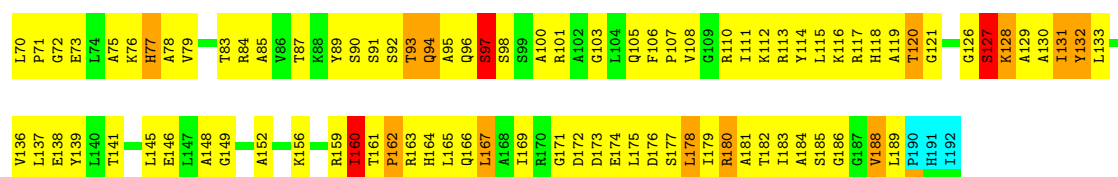
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

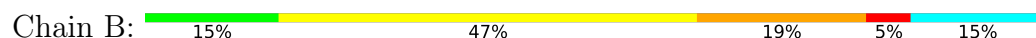
4.2.1 Score per residue for model 1

- Molecule 1: Chimera of Histone H2B.1 and Histone H2A.Z



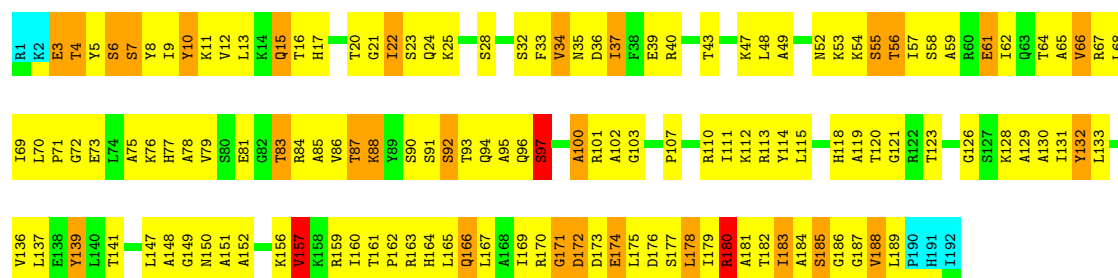


• Molecule 2: Uncharacterized protein YER030W

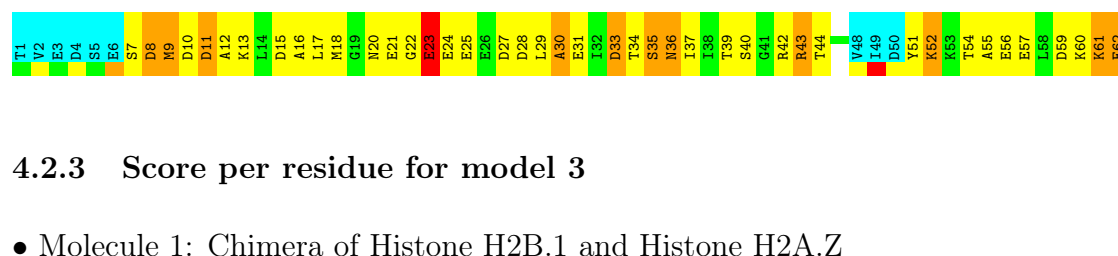
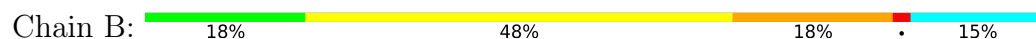


4.2.2 Score per residue for model 2

• Molecule 1: Chimera of Histone H2B.1 and Histone H2A.Z

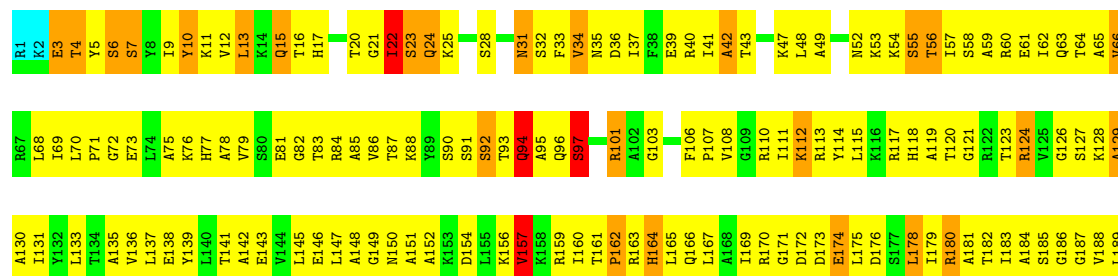


• Molecule 2: Uncharacterized protein YER030W



4.2.3 Score per residue for model 3

• Molecule 1: Chimera of Histone H2B.1 and Histone H2A.Z





- Molecule 2: Uncharacterized protein YER030W

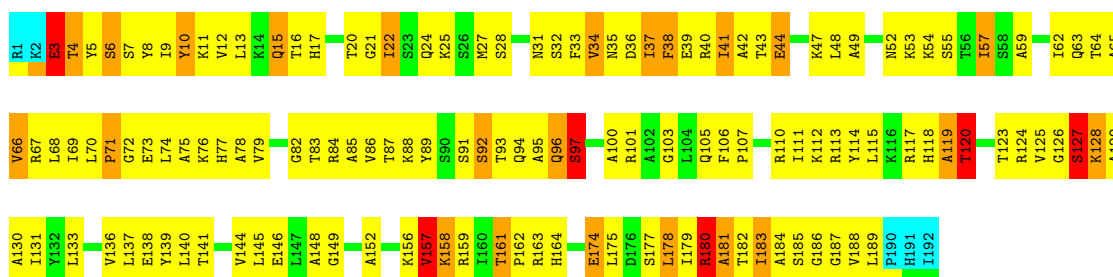
Chain B: 19% 40% 24% 15%



4.2.4 Score per residue for model 4

- Molecule 1: Chimera of Histone H2B.1 and Histone H2A.Z

Chain A: 26% 57% 12% 1%



- Molecule 2: Uncharacterized protein YER030W

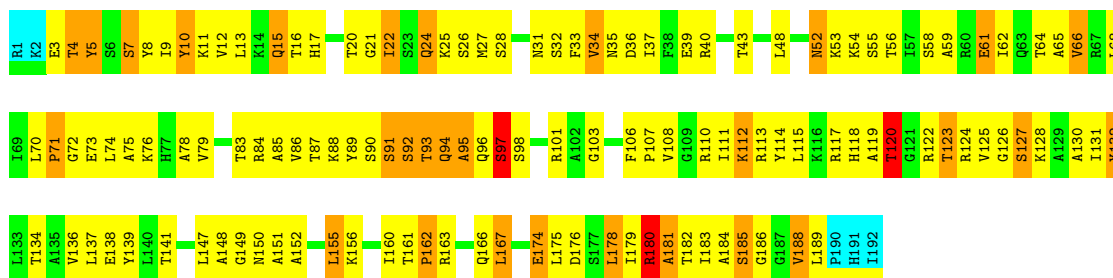
Chain B: 19% 48% 18% 15%



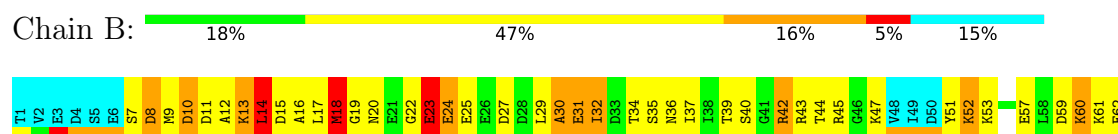
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Chimera of Histone H2B.1 and Histone H2A.Z

Chain A: 30% 51% 15% 1%

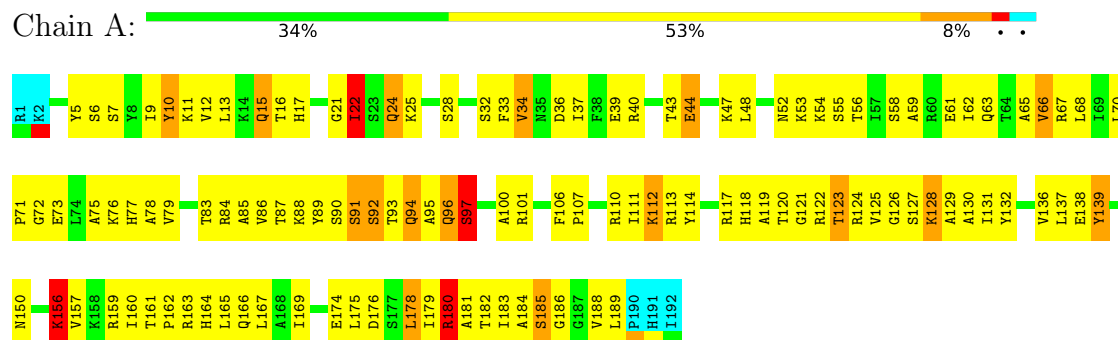


- Molecule 2: Uncharacterized protein YER030W

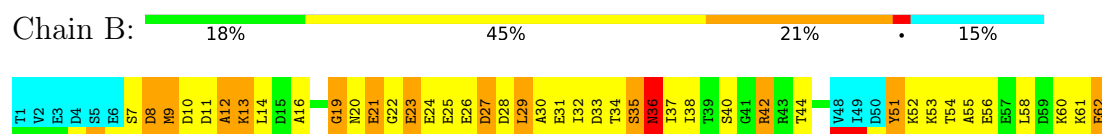


4.2.6 Score per residue for model 6

- Molecule 1: Chimera of Histone H2B.1 and Histone H2A.Z



- Molecule 2: Uncharacterized protein YER030W

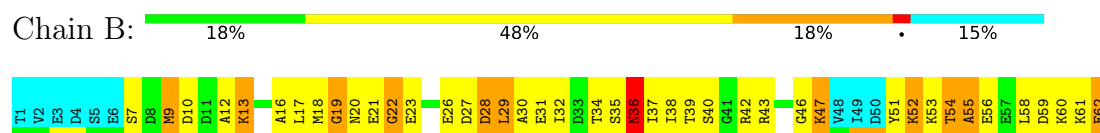


4.2.7 Score per residue for model 7

- Molecule 1: Chimera of Histone H2B.1 and Histone H2A.Z

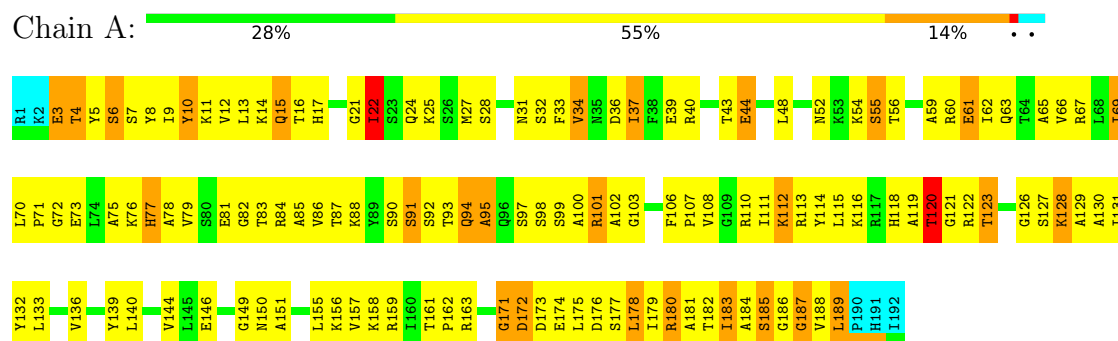


- Molecule 2: Uncharacterized protein YER030W

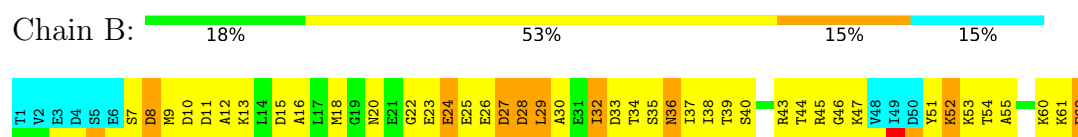


4.2.8 Score per residue for model 8

- Molecule 1: Chimera of Histone H2B.1 and Histone H2A.Z

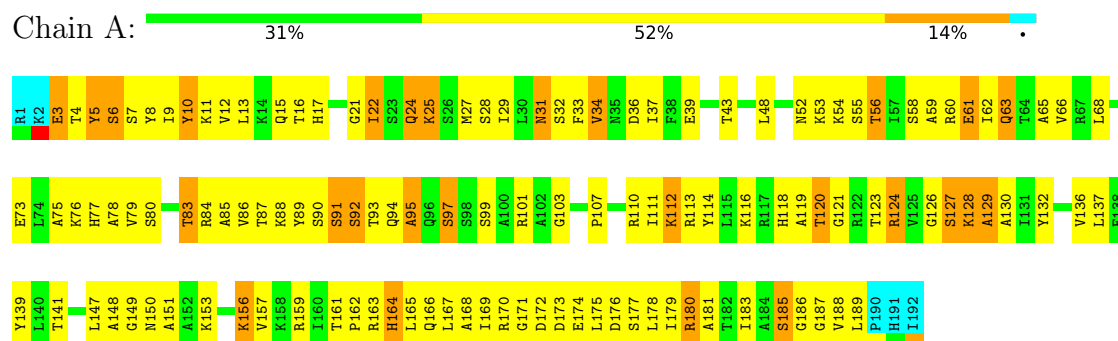


- Molecule 2: Uncharacterized protein YER030W

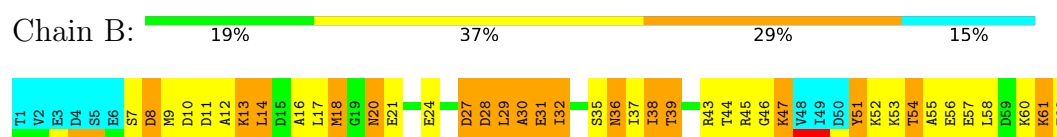


4.2.9 Score per residue for model 9

- Molecule 1: Chimera of Histone H2B.1 and Histone H2A.Z

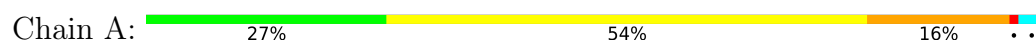


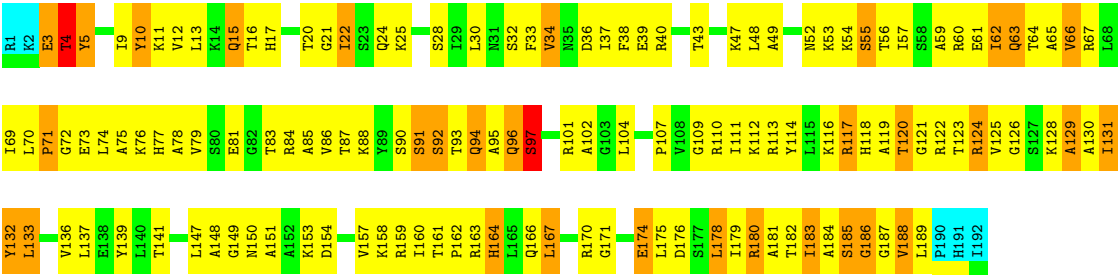
- Molecule 2: Uncharacterized protein YER030W



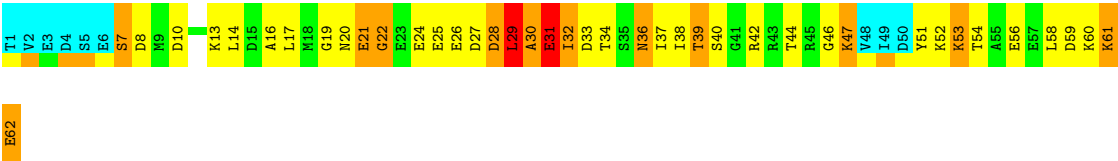
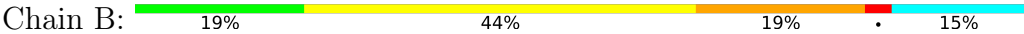
4.2.10 Score per residue for model 10

- Molecule 1: Chimera of Histone H2B.1 and Histone H2A.Z





● Molecule 2: Uncharacterized protein YER030W



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing, molecular dynamics*.

Of the 50 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy and no violations*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	2.16
X-PLOR NIH	refinement	2.16

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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	0.92±0.01	0±0/1456 (0.0± 0.0%)	1.09±0.01	1±1/1966 (0.0± 0.0%)
2	B	0.91±0.02	0±0/414 (0.0± 0.0%)	1.01±0.02	0±0/550 (0.0± 0.1%)
All	All	0.91	0/18700 (0.0%)	1.07	10/25160 (0.0%)

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	186	GLY	N-CA-C	-5.79	108.30	114.67	10	1
1	A	164	HIS	CA-CB-CG	-5.58	108.22	113.80	3	1
1	A	77	HIS	CA-CB-CG	-5.34	108.46	113.80	2	2
1	A	134	THR	N-CA-C	-5.30	106.32	112.89	7	1
1	A	100	ALA	N-CA-C	-5.23	108.66	114.62	4	3
2	B	17	LEU	N-CA-C	-5.13	106.72	112.87	2	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1437	1502	1502	156±11
2	B	414	394	394	57±8
All	All	18510	18960	18960	2052

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 55.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:37:ILE:N	2:B:37:ILE:HD13	0.82	1.89	1	1
1:A:167:LEU:HD12	1:A:167:LEU:O	0.82	1.75	7	2
1:A:156:LYS:HZ1	1:A:163:ARG:HH22	0.82	1.18	2	1
1:A:178:LEU:O	1:A:178:LEU:HD12	0.81	1.75	5	4
1:A:178:LEU:HD12	1:A:178:LEU:O	0.79	1.78	3	4
1:A:156:LYS:O	1:A:157:VAL:HG13	0.78	1.78	3	4
2:B:29:LEU:N	2:B:29:LEU:HD22	0.78	1.93	3	1
1:A:75:ALA:O	1:A:79:VAL:HG23	0.75	1.81	8	4
1:A:130:ALA:O	1:A:134:THR:HG23	0.74	1.82	7	2
1:A:104:LEU:N	1:A:104:LEU:HD22	0.73	1.98	10	1
2:B:29:LEU:HD13	2:B:29:LEU:H	0.72	1.43	3	1
1:A:33:PHE:O	1:A:37:ILE:HG22	0.72	1.84	6	10
2:B:14:LEU:H	2:B:14:LEU:HD22	0.72	1.44	3	1
1:A:54:LYS:O	1:A:56:THR:N	0.71	2.23	3	6
1:A:167:LEU:C	1:A:167:LEU:HD12	0.69	2.12	9	1
1:A:79:VAL:O	1:A:83:THR:HG23	0.69	1.87	1	3
2:B:36:ASN:N	2:B:36:ASN:HD22	0.69	1.86	2	1
1:A:48:LEU:HD12	1:A:48:LEU:C	0.69	2.12	4	5
1:A:48:LEU:C	1:A:48:LEU:HD12	0.69	2.13	1	5
1:A:77:HIS:CE1	2:B:38:ILE:HD11	0.68	2.23	8	1
1:A:186:GLY:O	1:A:188:VAL:N	0.67	2.24	4	6
1:A:115:LEU:O	1:A:123:THR:HG21	0.67	1.89	5	1
1:A:112:LYS:HZ1	2:B:16:ALA:HB2	0.67	1.49	6	1
2:B:29:LEU:N	2:B:29:LEU:HD12	0.67	2.05	2	2
2:B:54:THR:HG23	2:B:55:ALA:N	0.67	2.05	6	3
1:A:132:TYR:O	1:A:136:VAL:HG13	0.66	1.89	5	3
2:B:36:ASN:HD22	2:B:36:ASN:H	0.66	1.33	4	3
1:A:188:VAL:HG23	1:A:188:VAL:O	0.65	1.90	2	1
2:B:14:LEU:H	2:B:14:LEU:HD23	0.65	1.50	5	1
1:A:112:LYS:NZ	2:B:16:ALA:HB2	0.65	2.07	6	2
2:B:29:LEU:HD12	2:B:29:LEU:N	0.64	2.06	1	1
1:A:125:VAL:HG12	1:A:125:VAL:O	0.64	1.90	6	1
1:A:178:LEU:HD12	1:A:178:LEU:C	0.64	2.18	7	5
2:B:37:ILE:N	2:B:37:ILE:CD1	0.64	2.61	1	3
1:A:179:ILE:O	1:A:181:ALA:N	0.63	2.30	2	9
1:A:179:ILE:HG22	1:A:179:ILE:O	0.63	1.92	10	3
1:A:166:GLN:NE2	1:A:189:LEU:HD11	0.63	2.09	6	1
1:A:115:LEU:HD11	1:A:133:LEU:CD1	0.63	2.23	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:36:ASN:ND2	2:B:36:ASN:H	0.63	1.92	9	2
2:B:36:ASN:ND2	2:B:36:ASN:N	0.62	2.47	1	3
1:A:24:GLN:NE2	1:A:24:GLN:H	0.62	1.92	9	4
2:B:27:ASP:OD1	2:B:27:ASP:N	0.62	2.32	3	4
1:A:179:ILE:O	1:A:179:ILE:HG22	0.62	1.95	2	2
1:A:24:GLN:H	1:A:24:GLN:NE2	0.62	1.92	3	2
1:A:89:TYR:CE1	1:A:101:ARG:NH1	0.62	2.68	5	1
1:A:17:HIS:NE2	1:A:150:ASN:ND2	0.62	2.47	6	5
1:A:175:LEU:O	1:A:179:ILE:N	0.62	2.33	8	10
1:A:112:LYS:HZ3	2:B:16:ALA:HB2	0.61	1.54	7	1
1:A:17:HIS:CE1	1:A:150:ASN:ND2	0.61	2.68	10	4
2:B:37:ILE:N	2:B:37:ILE:HD12	0.61	2.10	10	2
1:A:87:THR:O	1:A:91:SER:N	0.61	2.32	4	10
2:B:12:ALA:O	2:B:16:ALA:HB3	0.61	1.96	8	5
1:A:179:ILE:C	1:A:181:ALA:H	0.61	2.03	10	5
1:A:112:LYS:HZ2	2:B:15:ASP:N	0.61	1.93	5	1
2:B:32:ILE:HG23	2:B:32:ILE:O	0.61	1.96	4	1
1:A:166:GLN:NE2	1:A:186:GLY:H	0.61	1.94	10	2
1:A:11:LYS:O	1:A:15:GLN:NE2	0.61	2.34	9	4
1:A:167:LEU:HD12	1:A:167:LEU:C	0.61	2.21	5	2
1:A:157:VAL:O	1:A:159:ARG:N	0.60	2.34	10	7
1:A:78:ALA:HB1	1:A:136:VAL:HG12	0.60	1.71	8	6
2:B:44:THR:HG22	2:B:45:ARG:N	0.60	2.11	1	1
1:A:83:THR:O	1:A:86:VAL:N	0.59	2.35	10	9
1:A:166:GLN:O	1:A:170:ARG:N	0.59	2.35	2	1
1:A:140:LEU:O	1:A:144:VAL:HG23	0.59	1.96	8	2
2:B:35:SER:C	2:B:37:ILE:H	0.59	2.05	6	5
2:B:51:TYR:O	2:B:53:LYS:N	0.59	2.34	3	5
2:B:36:ASN:N	2:B:36:ASN:ND2	0.59	2.49	2	3
1:A:5:TYR:CD2	1:A:110:ARG:NH2	0.59	2.70	8	1
1:A:156:LYS:HZ3	1:A:164:HIS:CD2	0.59	2.14	6	1
1:A:39:GLU:O	1:A:43:THR:N	0.59	2.36	6	10
2:B:61:LYS:N	2:B:61:LYS:CD	0.59	2.66	1	1
1:A:56:THR:HG23	1:A:56:THR:O	0.58	1.98	10	1
1:A:77:HIS:NE2	2:B:38:ILE:HD11	0.58	2.13	4	1
2:B:17:LEU:N	2:B:17:LEU:HD12	0.58	2.13	4	1
1:A:123:THR:HG23	1:A:123:THR:O	0.58	1.98	5	1
1:A:63:GLN:HE21	1:A:64:THR:N	0.58	1.97	10	1
1:A:77:HIS:CE1	2:B:40:SER:H	0.58	2.15	6	2
1:A:110:ARG:O	1:A:114:TYR:CD1	0.58	2.56	8	7
1:A:139:TYR:C	1:A:139:TYR:CD1	0.58	2.81	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:LEU:O	1:A:171:GLY:N	0.58	2.36	3	3
1:A:157:VAL:C	1:A:159:ARG:H	0.58	2.05	10	6
1:A:59:ALA:N	1:A:128:LYS:O	0.58	2.36	10	10
1:A:17:HIS:CE1	1:A:150:ASN:HD21	0.58	2.16	9	3
1:A:119:ALA:C	1:A:120:THR:HG22	0.58	2.24	5	2
1:A:104:LEU:N	1:A:104:LEU:CD2	0.58	2.67	10	1
1:A:119:ALA:C	1:A:120:THR:HG23	0.58	2.23	2	3
2:B:29:LEU:O	2:B:30:ALA:HB3	0.58	1.98	7	1
1:A:24:GLN:NE2	1:A:25:LYS:H	0.58	1.96	8	3
1:A:160:ILE:HG22	1:A:161:THR:N	0.58	2.14	2	5
1:A:17:HIS:CD2	1:A:150:ASN:HD21	0.58	2.17	10	1
1:A:9:ILE:O	1:A:12:VAL:N	0.58	2.37	10	10
1:A:112:LYS:HZ2	2:B:15:ASP:C	0.58	2.05	1	2
1:A:92:SER:OG	1:A:93:THR:N	0.58	2.37	9	7
1:A:155:LEU:N	1:A:155:LEU:CD2	0.58	2.67	5	1
1:A:161:THR:O	1:A:163:ARG:N	0.57	2.37	8	10
1:A:166:GLN:OE1	1:A:189:LEU:HD11	0.57	1.98	1	1
2:B:36:ASN:H	2:B:36:ASN:HD22	0.57	1.39	1	2
1:A:77:HIS:CG	2:B:39:THR:O	0.57	2.57	7	1
2:B:20:ASN:ND2	2:B:21:GLU:H	0.57	1.97	9	1
1:A:182:THR:O	1:A:184:ALA:N	0.57	2.37	2	8
2:B:7:SER:O	2:B:9:MET:N	0.57	2.37	8	8
1:A:77:HIS:N	1:A:77:HIS:ND1	0.57	2.51	8	1
2:B:8:ASP:O	2:B:10:ASP:N	0.57	2.36	10	8
2:B:56:GLU:O	2:B:57:GLU:C	0.57	2.48	3	4
2:B:12:ALA:O	2:B:16:ALA:N	0.57	2.37	6	2
2:B:29:LEU:N	2:B:29:LEU:HD13	0.57	2.14	3	1
1:A:53:LYS:O	1:A:55:SER:N	0.57	2.37	9	3
1:A:166:GLN:NE2	1:A:186:GLY:N	0.57	2.52	10	1
1:A:93:THR:C	1:A:95:ALA:N	0.57	2.63	6	10
1:A:115:LEU:O	1:A:119:ALA:HB3	0.57	2.00	1	4
2:B:38:ILE:C	2:B:38:ILE:HD12	0.57	2.25	9	3
1:A:174:GLU:H	1:A:174:GLU:CD	0.57	2.08	2	8
2:B:56:GLU:CD	2:B:57:GLU:N	0.57	2.63	9	1
1:A:118:HIS:C	1:A:120:THR:H	0.57	2.06	6	3
1:A:126:GLY:C	1:A:128:LYS:H	0.56	2.08	1	10
2:B:58:LEU:HD23	2:B:58:LEU:C	0.56	2.25	6	1
1:A:122:ARG:NE	1:A:122:ARG:H	0.56	1.97	8	1
1:A:21:GLY:O	1:A:22:ILE:O	0.56	2.23	3	10
2:B:20:ASN:O	2:B:22:GLY:N	0.56	2.39	1	6
2:B:36:ASN:C	2:B:37:ILE:HD13	0.56	2.25	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:THR:OG1	1:A:5:TYR:N	0.56	2.37	10	5
1:A:24:GLN:NE2	1:A:24:GLN:C	0.56	2.64	4	1
2:B:27:ASP:O	2:B:28:ASP:C	0.56	2.48	8	1
1:A:164:HIS:ND1	1:A:164:HIS:N	0.56	2.52	9	1
1:A:129:ALA:O	1:A:132:TYR:N	0.56	2.39	10	5
2:B:15:ASP:OD1	2:B:16:ALA:N	0.56	2.39	1	2
2:B:23:GLU:O	2:B:26:GLU:N	0.56	2.39	1	1
2:B:52:LYS:O	2:B:55:ALA:N	0.56	2.38	1	1
2:B:29:LEU:H	2:B:29:LEU:CD1	0.56	2.06	3	1
1:A:176:ASP:O	1:A:180:ARG:N	0.56	2.39	9	1
1:A:32:SER:O	1:A:36:ASP:N	0.56	2.39	8	9
1:A:93:THR:C	1:A:95:ALA:H	0.56	2.08	1	10
2:B:25:GLU:H	2:B:25:GLU:CD	0.56	2.09	6	1
1:A:16:THR:O	1:A:17:HIS:CG	0.56	2.59	4	10
2:B:20:ASN:ND2	2:B:22:GLY:H	0.56	1.98	3	1
1:A:9:ILE:O	1:A:13:LEU:N	0.56	2.38	1	9
1:A:139:TYR:CD1	1:A:139:TYR:C	0.56	2.83	6	6
1:A:89:TYR:CD1	1:A:101:ARG:NH1	0.56	2.74	5	1
2:B:60:LYS:C	2:B:62:GLU:N	0.56	2.64	6	6
1:A:96:GLN:H	1:A:101:ARG:NE	0.56	1.98	5	1
1:A:164:HIS:N	1:A:164:HIS:CD2	0.56	2.69	10	1
1:A:92:SER:O	1:A:94:GLN:N	0.55	2.38	5	1
1:A:94:GLN:O	1:A:95:ALA:HB3	0.55	2.01	8	1
1:A:111:ILE:O	1:A:114:TYR:N	0.55	2.39	3	10
2:B:23:GLU:O	2:B:25:GLU:N	0.55	2.40	8	2
1:A:128:LYS:CD	1:A:128:LYS:H	0.55	2.15	6	1
1:A:77:HIS:CE1	2:B:40:SER:N	0.55	2.73	1	1
1:A:152:ALA:HB2	1:A:164:HIS:CD2	0.55	2.36	3	2
1:A:94:GLN:O	1:A:95:ALA:HB2	0.55	2.00	9	2
1:A:166:GLN:HE22	1:A:188:VAL:H	0.55	1.43	10	1
1:A:33:PHE:O	1:A:36:ASP:N	0.55	2.39	2	9
2:B:35:SER:C	2:B:37:ILE:N	0.55	2.64	2	4
2:B:18:MET:O	2:B:20:ASN:N	0.55	2.39	5	2
1:A:15:GLN:N	1:A:15:GLN:CD	0.55	2.64	6	9
1:A:65:ALA:O	1:A:69:ILE:N	0.55	2.37	4	6
1:A:126:GLY:C	1:A:128:LYS:N	0.55	2.61	1	10
1:A:148:ALA:O	1:A:152:ALA:N	0.55	2.40	5	2
2:B:58:LEU:O	2:B:60:LYS:N	0.55	2.40	1	1
1:A:97:SER:O	1:A:101:ARG:N	0.55	2.35	5	9
2:B:28:ASP:O	2:B:30:ALA:N	0.55	2.40	3	2
2:B:35:SER:C	2:B:36:ASN:ND2	0.55	2.64	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:GLN:H	1:A:24:GLN:CD	0.55	2.09	1	5
1:A:93:THR:O	1:A:95:ALA:N	0.55	2.40	1	10
2:B:28:ASP:CG	2:B:29:LEU:N	0.55	2.63	9	1
1:A:24:GLN:N	1:A:24:GLN:CD	0.55	2.65	10	4
1:A:152:ALA:O	1:A:156:LYS:N	0.55	2.39	7	3
2:B:58:LEU:C	2:B:60:LYS:H	0.55	2.10	1	1
2:B:57:GLU:O	2:B:62:GLU:N	0.55	2.39	3	1
2:B:56:GLU:C	2:B:58:LEU:N	0.55	2.62	1	2
2:B:14:LEU:H	2:B:14:LEU:CD2	0.55	2.11	5	2
1:A:166:GLN:NE2	1:A:166:GLN:C	0.55	2.65	9	2
1:A:175:LEU:O	1:A:178:LEU:N	0.54	2.38	8	9
1:A:157:VAL:C	1:A:159:ARG:N	0.54	2.64	4	8
2:B:54:THR:CG2	2:B:55:ALA:N	0.54	2.70	6	3
1:A:90:SER:O	1:A:94:GLN:NE2	0.54	2.39	3	1
1:A:52:ASN:O	1:A:52:ASN:ND2	0.54	2.40	6	2
1:A:156:LYS:NZ	1:A:164:HIS:CD2	0.54	2.75	6	1
1:A:164:HIS:CD2	1:A:164:HIS:H	0.54	2.21	1	2
1:A:156:LYS:NZ	1:A:164:HIS:NE2	0.54	2.54	2	2
1:A:165:LEU:O	1:A:169:ILE:N	0.54	2.38	6	5
2:B:54:THR:HG23	2:B:55:ALA:H	0.54	1.61	6	1
1:A:163:ARG:O	1:A:166:GLN:N	0.54	2.39	1	2
2:B:58:LEU:C	2:B:58:LEU:HD23	0.54	2.26	1	2
1:A:92:SER:O	1:A:94:GLN:NE2	0.54	2.40	3	4
1:A:94:GLN:N	1:A:94:GLN:CD	0.54	2.64	3	1
2:B:20:ASN:CG	2:B:21:GLU:N	0.54	2.65	9	2
1:A:94:GLN:O	1:A:95:ALA:CB	0.54	2.55	8	3
2:B:22:GLY:O	2:B:24:GLU:N	0.54	2.39	5	2
1:A:25:LYS:O	1:A:28:SER:N	0.54	2.40	5	10
1:A:145:LEU:O	1:A:149:GLY:N	0.54	2.40	4	2
1:A:156:LYS:C	1:A:157:VAL:HG22	0.54	2.27	3	3
2:B:21:GLU:CD	2:B:21:GLU:H	0.54	2.10	2	1
1:A:75:ALA:O	1:A:78:ALA:N	0.54	2.41	3	8
1:A:161:THR:H	1:A:164:HIS:HD1	0.54	1.45	2	1
1:A:82:GLY:O	1:A:86:VAL:HG23	0.54	2.03	8	3
1:A:44:GLU:N	1:A:44:GLU:OE1	0.54	2.41	4	2
1:A:7:SER:O	1:A:10:TYR:N	0.54	2.41	4	5
1:A:90:SER:O	1:A:92:SER:N	0.54	2.41	9	6
2:B:31:GLU:O	2:B:33:ASP:N	0.54	2.40	3	2
2:B:42:ARG:O	2:B:44:THR:N	0.54	2.41	4	1
1:A:44:GLU:OE1	1:A:44:GLU:N	0.54	2.41	8	2
1:A:17:HIS:NE2	1:A:150:ASN:OD1	0.54	2.41	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:TYR:O	1:A:6:SER:C	0.54	2.51	3	6
1:A:16:THR:O	1:A:17:HIS:CD2	0.54	2.61	10	3
2:B:35:SER:C	2:B:36:ASN:HD22	0.54	2.11	6	3
1:A:92:SER:C	1:A:94:GLN:N	0.54	2.65	5	1
1:A:8:TYR:OH	2:B:7:SER:N	0.54	2.41	7	1
2:B:14:LEU:HD22	2:B:14:LEU:H	0.54	1.62	9	1
1:A:126:GLY:O	1:A:128:LYS:N	0.53	2.41	1	8
1:A:119:ALA:HB1	1:A:123:THR:OG1	0.53	2.02	3	2
2:B:46:GLY:O	2:B:47:LYS:O	0.53	2.26	9	4
1:A:112:LYS:NZ	2:B:15:ASP:N	0.53	2.56	5	1
1:A:161:THR:OG1	1:A:164:HIS:CE1	0.53	2.61	6	1
1:A:180:ARG:N	1:A:180:ARG:NE	0.53	2.56	6	1
1:A:61:GLU:N	1:A:61:GLU:OE1	0.53	2.41	1	5
2:B:22:GLY:C	2:B:24:GLU:N	0.53	2.67	5	3
1:A:121:GLY:C	1:A:123:THR:N	0.53	2.65	6	3
1:A:185:SER:C	1:A:187:GLY:N	0.53	2.65	2	2
2:B:43:ARG:O	2:B:43:ARG:NE	0.53	2.42	2	1
1:A:94:GLN:N	1:A:94:GLN:OE1	0.53	2.41	3	1
1:A:122:ARG:NE	1:A:122:ARG:N	0.53	2.56	8	1
2:B:26:GLU:O	2:B:28:ASP:N	0.53	2.41	8	1
1:A:119:ALA:O	1:A:121:GLY:N	0.53	2.42	1	2
1:A:177:SER:O	1:A:180:ARG:NE	0.53	2.41	8	2
2:B:34:THR:O	2:B:37:ILE:N	0.53	2.40	2	2
1:A:77:HIS:CD2	2:B:38:ILE:HD11	0.53	2.38	4	1
1:A:40:ARG:NH1	1:A:178:LEU:O	0.53	2.42	7	1
1:A:33:PHE:O	1:A:37:ILE:N	0.53	2.39	8	9
1:A:5:TYR:O	1:A:7:SER:N	0.53	2.41	2	1
2:B:61:LYS:CD	2:B:62:GLU:N	0.53	2.71	9	1
2:B:28:ASP:O	2:B:29:LEU:C	0.53	2.52	10	3
1:A:128:LYS:NZ	2:B:27:ASP:CG	0.53	2.67	2	1
1:A:89:TYR:O	1:A:101:ARG:NE	0.53	2.42	9	2
1:A:60:ARG:NH1	2:B:27:ASP:O	0.53	2.42	10	1
2:B:35:SER:O	2:B:37:ILE:N	0.53	2.42	7	4
2:B:13:LYS:O	2:B:16:ALA:N	0.53	2.42	5	1
2:B:54:THR:O	2:B:58:LEU:N	0.53	2.36	9	2
1:A:3:GLU:OE2	1:A:4:THR:N	0.53	2.42	9	1
1:A:87:THR:HG23	1:A:88:LYS:N	0.53	2.19	9	1
1:A:43:THR:O	1:A:47:LYS:N	0.53	2.42	4	3
2:B:16:ALA:C	2:B:18:MET:H	0.53	2.10	4	1
1:A:17:HIS:CE1	1:A:150:ASN:OD1	0.53	2.62	9	3
2:B:36:ASN:H	2:B:36:ASN:ND2	0.53	2.00	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:THR:HG22	1:A:93:THR:O	0.53	2.04	4	1
1:A:77:HIS:CE1	2:B:40:SER:O	0.53	2.62	6	1
1:A:63:GLN:NE2	1:A:63:GLN:C	0.53	2.67	10	1
1:A:24:GLN:NE2	1:A:24:GLN:N	0.53	2.56	1	4
1:A:85:ALA:HB1	1:A:131:ILE:HD11	0.53	1.81	5	7
1:A:180:ARG:N	1:A:180:ARG:CD	0.53	2.72	7	5
1:A:63:GLN:NE2	2:B:28:ASP:OD2	0.53	2.42	4	1
2:B:30:ALA:C	2:B:32:ILE:N	0.53	2.66	10	6
1:A:77:HIS:CD2	2:B:38:ILE:HD13	0.53	2.39	3	1
1:A:77:HIS:ND1	2:B:36:ASN:O	0.53	2.42	7	1
1:A:73:GLU:O	1:A:77:HIS:ND1	0.53	2.42	8	3
1:A:16:THR:O	1:A:17:HIS:ND1	0.52	2.42	6	4
1:A:39:GLU:OE1	1:A:118:HIS:NE2	0.52	2.42	10	1
1:A:101:ARG:C	1:A:103:GLY:N	0.52	2.67	8	7
1:A:90:SER:C	1:A:92:SER:N	0.52	2.67	5	6
1:A:143:GLU:C	1:A:145:LEU:N	0.52	2.65	3	1
2:B:29:LEU:N	2:B:29:LEU:CD2	0.52	2.63	3	1
2:B:45:ARG:C	2:B:45:ARG:NE	0.52	2.67	4	1
1:A:150:ASN:O	1:A:150:ASN:ND2	0.52	2.42	5	1
2:B:43:ARG:C	2:B:43:ARG:NE	0.52	2.68	9	1
1:A:92:SER:O	1:A:93:THR:CB	0.52	2.57	1	1
1:A:179:ILE:O	1:A:180:ARG:C	0.52	2.51	4	5
2:B:8:ASP:N	2:B:8:ASP:OD1	0.52	2.42	1	1
1:A:125:VAL:O	2:B:20:ASN:ND2	0.52	2.42	4	1
1:A:63:GLN:HE21	1:A:63:GLN:C	0.52	2.13	9	2
1:A:179:ILE:C	1:A:181:ALA:N	0.52	2.68	9	9
2:B:30:ALA:O	2:B:32:ILE:N	0.52	2.42	10	3
1:A:75:ALA:O	1:A:79:VAL:N	0.52	2.41	8	8
2:B:9:MET:O	2:B:13:LYS:NZ	0.52	2.42	1	1
1:A:166:GLN:N	1:A:166:GLN:OE1	0.52	2.42	2	1
1:A:105:GLN:N	1:A:105:GLN:CD	0.52	2.68	4	1
1:A:4:THR:OG1	1:A:31:ASN:ND2	0.52	2.43	5	2
1:A:119:ALA:O	1:A:120:THR:CB	0.52	2.58	7	2
1:A:173:ASP:OD2	2:B:61:LYS:NZ	0.52	2.42	7	1
2:B:36:ASN:O	2:B:36:ASN:ND2	0.52	2.42	7	1
1:A:117:ARG:HE	1:A:117:ARG:C	0.52	2.13	10	1
2:B:26:GLU:O	2:B:27:ASP:C	0.52	2.51	8	7
2:B:33:ASP:N	2:B:33:ASP:OD1	0.52	2.42	1	1
1:A:179:ILE:O	1:A:179:ILE:CG2	0.52	2.57	6	5
2:B:29:LEU:HD22	2:B:29:LEU:H	0.52	1.62	3	1
1:A:120:THR:OG1	1:A:122:ARG:NH2	0.52	2.42	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:51:TYR:O	2:B:52:LYS:C	0.52	2.53	8	1
1:A:166:GLN:NE2	1:A:185:SER:H	0.52	2.03	10	1
1:A:54:LYS:C	1:A:56:THR:N	0.52	2.66	8	4
2:B:19:GLY:O	2:B:20:ASN:ND2	0.52	2.43	1	1
2:B:31:GLU:N	2:B:31:GLU:CD	0.52	2.67	5	4
2:B:56:GLU:O	2:B:58:LEU:N	0.52	2.42	3	2
1:A:118:HIS:C	1:A:120:THR:N	0.52	2.67	4	4
1:A:137:LEU:O	1:A:141:THR:N	0.52	2.39	10	7
2:B:60:LYS:O	2:B:62:GLU:N	0.52	2.42	2	6
1:A:77:HIS:NE2	2:B:40:SER:O	0.52	2.42	6	1
1:A:110:ARG:NE	1:A:114:TYR:OH	0.52	2.42	8	1
1:A:61:GLU:N	1:A:61:GLU:CD	0.52	2.67	9	5
1:A:65:ALA:O	1:A:68:LEU:N	0.52	2.43	6	7
1:A:188:VAL:O	1:A:188:VAL:HG22	0.52	2.05	9	4
1:A:112:LYS:NZ	2:B:15:ASP:C	0.52	2.67	4	1
1:A:122:ARG:O	1:A:123:THR:C	0.52	2.53	5	1
2:B:17:LEU:HD23	2:B:17:LEU:O	0.52	2.05	9	1
1:A:161:THR:C	1:A:163:ARG:N	0.52	2.68	3	10
2:B:52:LYS:NZ	2:B:56:GLU:CD	0.52	2.68	2	1
1:A:124:ARG:NH2	2:B:20:ASN:O	0.52	2.42	5	1
1:A:112:LYS:NZ	2:B:15:ASP:O	0.51	2.41	1	1
2:B:22:GLY:C	2:B:24:GLU:H	0.51	2.13	5	5
1:A:31:ASN:C	1:A:31:ASN:ND2	0.51	2.67	3	1
1:A:63:GLN:NE2	2:B:28:ASP:OD1	0.51	2.42	3	1
1:A:89:TYR:CE2	2:B:24:GLU:OE2	0.51	2.63	4	1
2:B:13:LYS:O	2:B:17:LEU:N	0.51	2.42	7	3
1:A:58:SER:N	1:A:61:GLU:OE1	0.51	2.43	6	1
1:A:39:GLU:OE2	1:A:118:HIS:CE1	0.51	2.63	10	1
1:A:24:GLN:N	1:A:24:GLN:OE1	0.51	2.42	2	2
2:B:51:TYR:O	2:B:52:LYS:CB	0.51	2.58	5	3
1:A:63:GLN:NE2	2:B:28:ASP:CG	0.51	2.67	3	1
2:B:57:GLU:O	2:B:61:LYS:N	0.51	2.42	5	1
2:B:37:ILE:HG22	2:B:37:ILE:O	0.51	2.04	7	1
2:B:20:ASN:C	2:B:22:GLY:H	0.51	2.13	8	5
1:A:166:GLN:NE2	1:A:166:GLN:O	0.51	2.43	9	2
1:A:63:GLN:OE1	1:A:67:ARG:NH1	0.51	2.44	10	1
1:A:154:ASP:OD1	1:A:154:ASP:N	0.51	2.42	10	1
2:B:17:LEU:C	2:B:19:GLY:N	0.51	2.66	1	2
1:A:160:ILE:CG2	1:A:161:THR:N	0.51	2.74	3	5
1:A:61:GLU:OE1	1:A:61:GLU:N	0.51	2.43	6	1
1:A:92:SER:O	1:A:93:THR:OG1	0.51	2.27	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:20:ASN:C	2:B:22:GLY:N	0.51	2.69	7	7
2:B:8:ASP:C	2:B:10:ASP:N	0.51	2.68	2	5
2:B:23:GLU:C	2:B:25:GLU:H	0.51	2.14	8	2
2:B:27:ASP:N	2:B:27:ASP:OD1	0.51	2.42	5	1
1:A:28:SER:O	1:A:32:SER:N	0.51	2.41	7	6
1:A:63:GLN:C	1:A:63:GLN:NE2	0.51	2.68	9	1
1:A:171:GLY:O	1:A:173:ASP:N	0.51	2.43	8	3
2:B:34:THR:C	2:B:36:ASN:N	0.51	2.68	8	2
1:A:60:ARG:NH2	2:B:26:GLU:O	0.51	2.42	10	1
1:A:156:LYS:O	1:A:157:VAL:CG1	0.51	2.57	3	4
1:A:94:GLN:C	1:A:101:ARG:NH1	0.51	2.68	9	3
1:A:176:ASP:O	1:A:180:ARG:CD	0.51	2.59	7	1
1:A:106:PHE:CD1	1:A:138:GLU:OE1	0.51	2.63	1	1
1:A:58:SER:C	1:A:60:ARG:N	0.51	2.68	9	2
1:A:38:PHE:CD1	1:A:38:PHE:C	0.51	2.86	4	2
1:A:152:ALA:O	1:A:157:VAL:N	0.51	2.44	4	1
2:B:36:ASN:HD22	2:B:36:ASN:N	0.51	1.97	4	1
1:A:92:SER:C	1:A:94:GLN:H	0.51	2.14	5	1
2:B:43:ARG:C	2:B:43:ARG:HE	0.51	2.14	9	1
2:B:61:LYS:O	2:B:62:GLU:O	0.51	2.28	9	1
1:A:187:GLY:O	1:A:188:VAL:C	0.50	2.52	2	2
2:B:31:GLU:CD	2:B:31:GLU:H	0.50	2.12	5	2
2:B:54:THR:CG2	2:B:55:ALA:H	0.50	2.19	6	1
2:B:33:ASP:OD1	2:B:36:ASN:ND2	0.50	2.44	8	1
1:A:34:VAL:CG2	1:A:141:THR:OG1	0.50	2.60	9	2
2:B:16:ALA:C	2:B:18:MET:N	0.50	2.66	4	4
2:B:52:LYS:NZ	2:B:56:GLU:OE2	0.50	2.45	1	1
2:B:23:GLU:C	2:B:25:GLU:N	0.50	2.69	8	2
1:A:111:ILE:C	1:A:113:ARG:N	0.50	2.68	4	10
1:A:3:GLU:C	1:A:4:THR:HG23	0.50	2.29	2	2
2:B:8:ASP:C	2:B:10:ASP:H	0.50	2.15	3	5
2:B:20:ASN:ND2	2:B:20:ASN:C	0.50	2.67	3	1
2:B:16:ALA:O	2:B:17:LEU:CB	0.50	2.60	7	2
2:B:20:ASN:OD1	2:B:22:GLY:N	0.50	2.45	1	1
1:A:146:GLU:OE1	2:B:45:ARG:N	0.50	2.41	3	1
1:A:180:ARG:N	1:A:180:ARG:HE	0.50	2.05	6	1
1:A:163:ARG:NH2	2:B:52:LYS:CE	0.50	2.74	7	1
1:A:128:LYS:HZ2	1:A:128:LYS:HB3	0.50	1.67	8	1
1:A:48:LEU:C	1:A:48:LEU:CD1	0.50	2.84	8	10
2:B:58:LEU:C	2:B:60:LYS:N	0.50	2.70	1	1
2:B:29:LEU:H	2:B:29:LEU:CD2	0.50	2.19	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ILE:O	1:A:22:ILE:HG23	0.50	2.06	4	3
2:B:29:LEU:O	2:B:30:ALA:HB2	0.50	2.06	9	2
2:B:32:ILE:C	2:B:34:THR:H	0.50	2.15	5	2
1:A:187:GLY:C	1:A:189:LEU:H	0.50	2.14	8	1
1:A:11:LYS:C	1:A:15:GLN:NE2	0.50	2.70	9	1
1:A:31:ASN:HD22	1:A:31:ASN:N	0.50	2.04	9	1
1:A:166:GLN:NE2	1:A:188:VAL:H	0.50	2.04	10	1
1:A:47:LYS:C	1:A:49:ALA:N	0.50	2.68	3	5
1:A:38:PHE:CD1	1:A:38:PHE:O	0.50	2.64	10	2
2:B:13:LYS:NZ	2:B:13:LYS:CB	0.50	2.75	9	3
1:A:17:HIS:NE2	1:A:150:ASN:CG	0.50	2.70	10	1
1:A:101:ARG:O	1:A:103:GLY:N	0.50	2.45	8	4
1:A:128:LYS:NZ	2:B:27:ASP:OD1	0.50	2.42	2	1
2:B:54:THR:C	2:B:56:GLU:N	0.50	2.70	7	4
2:B:13:LYS:O	2:B:15:ASP:N	0.50	2.45	5	1
2:B:31:GLU:O	2:B:32:ILE:O	0.50	2.30	10	3
1:A:33:PHE:C	1:A:37:ILE:HG22	0.50	2.31	6	2
1:A:185:SER:C	1:A:187:GLY:H	0.50	2.14	8	1
1:A:129:ALA:O	1:A:130:ALA:C	0.50	2.55	6	9
1:A:149:GLY:C	1:A:151:ALA:N	0.50	2.70	5	3
1:A:176:ASP:C	1:A:178:LEU:N	0.50	2.67	2	8
2:B:11:ASP:O	2:B:12:ALA:C	0.50	2.54	9	4
1:A:54:LYS:C	1:A:56:THR:H	0.50	2.13	5	2
1:A:147:LEU:O	1:A:151:ALA:HB3	0.49	2.07	5	1
1:A:182:THR:O	1:A:183:ILE:C	0.49	2.55	8	2
1:A:59:ALA:HB2	1:A:128:LYS:O	0.49	2.06	8	1
1:A:17:HIS:CE1	1:A:150:ASN:CG	0.49	2.90	10	1
1:A:39:GLU:CD	1:A:118:HIS:CE1	0.49	2.90	10	1
1:A:9:ILE:C	1:A:11:LYS:N	0.49	2.69	9	9
2:B:61:LYS:O	2:B:62:GLU:C	0.49	2.55	9	3
1:A:167:LEU:HD12	1:A:168:ALA:N	0.49	2.22	9	1
1:A:52:ASN:N	1:A:52:ASN:HD22	0.49	2.05	3	3
2:B:60:LYS:C	2:B:62:GLU:H	0.49	2.15	7	4
1:A:5:TYR:CZ	1:A:34:VAL:CG1	0.49	2.95	4	1
2:B:18:MET:SD	2:B:18:MET:O	0.49	2.70	9	1
2:B:56:GLU:OE1	2:B:57:GLU:N	0.49	2.45	9	1
1:A:133:LEU:HD13	1:A:133:LEU:O	0.49	2.08	10	1
1:A:89:TYR:O	1:A:101:ARG:NH1	0.49	2.41	5	1
1:A:3:GLU:CG	1:A:4:THR:N	0.49	2.75	2	1
1:A:118:HIS:O	1:A:120:THR:N	0.49	2.45	4	2
1:A:77:HIS:NE2	2:B:40:SER:C	0.49	2.70	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:51:TYR:CD1	2:B:51:TYR:N	0.49	2.80	10	1
1:A:161:THR:C	1:A:163:ARG:H	0.49	2.14	5	9
1:A:94:GLN:OE1	1:A:94:GLN:CA	0.49	2.60	3	1
1:A:12:VAL:O	1:A:16:THR:HG22	0.49	2.07	4	1
2:B:54:THR:O	2:B:56:GLU:N	0.49	2.45	7	3
1:A:120:THR:HG23	1:A:121:GLY:N	0.49	2.21	9	1
1:A:149:GLY:C	1:A:151:ALA:H	0.49	2.15	2	5
1:A:145:LEU:HD23	1:A:145:LEU:O	0.49	2.08	7	1
1:A:39:GLU:O	1:A:43:THR:OG1	0.49	2.31	5	10
1:A:96:GLN:O	1:A:97:SER:O	0.49	2.30	4	5
2:B:54:THR:O	2:B:55:ALA:C	0.49	2.56	9	5
1:A:178:LEU:C	1:A:178:LEU:CD1	0.49	2.85	7	3
2:B:13:LYS:O	2:B:14:LEU:C	0.49	2.56	5	2
2:B:38:ILE:O	2:B:39:THR:OG1	0.49	2.29	7	2
2:B:62:GLU:O	2:B:62:GLU:CG	0.49	2.60	9	1
2:B:13:LYS:CG	2:B:14:LEU:H	0.48	2.21	6	1
1:A:86:VAL:CG1	2:B:27:ASP:OD1	0.48	2.61	8	1
1:A:99:SER:OG	2:B:9:MET:SD	0.48	2.70	8	1
2:B:28:ASP:CG	2:B:29:LEU:H	0.48	2.15	9	1
1:A:105:GLN:CD	1:A:105:GLN:N	0.48	2.70	1	1
2:B:29:LEU:N	2:B:29:LEU:CD1	0.48	2.76	1	2
2:B:20:ASN:ND2	2:B:21:GLU:N	0.48	2.60	9	2
2:B:12:ALA:O	2:B:13:LYS:C	0.48	2.54	6	1
1:A:5:TYR:CD1	1:A:5:TYR:N	0.48	2.79	5	4
2:B:25:GLU:CG	2:B:26:GLU:N	0.48	2.76	10	1
1:A:114:TYR:N	1:A:114:TYR:CD1	0.48	2.78	4	7
1:A:119:ALA:C	1:A:121:GLY:N	0.48	2.70	1	2
2:B:24:GLU:O	2:B:27:ASP:OD2	0.48	2.32	4	2
2:B:52:LYS:O	2:B:53:LYS:C	0.48	2.56	7	6
2:B:34:THR:C	2:B:36:ASN:H	0.48	2.16	8	2
2:B:40:SER:C	2:B:42:ARG:H	0.48	2.16	7	4
1:A:54:LYS:O	1:A:55:SER:C	0.48	2.57	10	4
2:B:40:SER:OG	2:B:41:GLY:N	0.48	2.44	4	1
1:A:167:LEU:C	1:A:167:LEU:CD1	0.48	2.85	9	3
1:A:180:ARG:HD3	1:A:180:ARG:H	0.48	1.69	6	1
2:B:13:LYS:CG	2:B:14:LEU:N	0.48	2.75	10	2
1:A:13:LEU:HD12	1:A:20:THR:HG21	0.48	1.84	3	1
1:A:177:SER:O	1:A:180:ARG:CZ	0.48	2.62	7	1
2:B:51:TYR:O	2:B:54:THR:N	0.48	2.35	8	1
1:A:39:GLU:O	1:A:43:THR:CB	0.48	2.62	3	9
1:A:106:PHE:O	1:A:108:VAL:N	0.48	2.46	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:TYR:CD1	1:A:114:TYR:N	0.48	2.79	2	3
1:A:31:ASN:O	1:A:35:ASN:N	0.48	2.45	3	1
2:B:17:LEU:C	2:B:19:GLY:H	0.48	2.17	4	2
2:B:52:LYS:N	2:B:52:LYS:CD	0.48	2.76	7	2
2:B:27:ASP:OD1	2:B:28:ASP:N	0.48	2.47	10	1
1:A:185:SER:O	1:A:187:GLY:N	0.48	2.47	2	2
1:A:16:THR:C	1:A:17:HIS:CG	0.48	2.91	3	1
1:A:41:ILE:HG22	1:A:42:ALA:N	0.48	2.24	4	2
1:A:119:ALA:O	1:A:120:THR:C	0.48	2.57	10	2
1:A:121:GLY:C	1:A:123:THR:H	0.48	2.16	2	5
1:A:149:GLY:O	1:A:151:ALA:N	0.48	2.46	2	2
1:A:176:ASP:C	1:A:178:LEU:H	0.48	2.17	7	1
1:A:5:TYR:CE2	1:A:110:ARG:NH2	0.48	2.82	8	1
1:A:83:THR:O	1:A:84:ARG:C	0.48	2.56	10	10
1:A:96:GLN:O	1:A:100:ALA:HB3	0.48	2.08	2	1
2:B:22:GLY:O	2:B:23:GLU:C	0.48	2.56	2	1
1:A:10:TYR:CD1	1:A:10:TYR:C	0.48	2.91	3	1
1:A:11:LYS:C	1:A:15:GLN:HE21	0.48	2.17	9	1
1:A:149:GLY:O	1:A:153:LYS:CG	0.48	2.62	10	1
1:A:162:PRO:HA	1:A:165:LEU:HD12	0.47	1.86	3	3
2:B:9:MET:O	2:B:11:ASP:N	0.47	2.40	4	1
1:A:174:GLU:CD	1:A:174:GLU:N	0.47	2.72	8	1
1:A:98:SER:C	1:A:100:ALA:H	0.47	2.18	8	2
1:A:121:GLY:O	1:A:123:THR:N	0.47	2.47	6	2
2:B:30:ALA:C	2:B:32:ILE:H	0.47	2.17	10	4
2:B:27:ASP:OD1	2:B:29:LEU:CD1	0.47	2.62	4	1
2:B:32:ILE:C	2:B:34:THR:N	0.47	2.69	10	2
1:A:3:GLU:O	1:A:4:THR:O	0.47	2.32	10	2
1:A:11:LYS:O	1:A:15:GLN:OE1	0.47	2.31	3	4
1:A:59:ALA:CA	1:A:128:LYS:O	0.47	2.62	6	2
1:A:60:ARG:NE	1:A:61:GLU:OE1	0.47	2.47	8	1
1:A:113:ARG:CZ	2:B:11:ASP:OD2	0.47	2.63	8	1
1:A:52:ASN:C	1:A:54:LYS:N	0.47	2.73	3	4
1:A:83:THR:OG1	1:A:84:ARG:N	0.47	2.46	8	2
2:B:7:SER:C	2:B:9:MET:N	0.47	2.69	4	2
1:A:117:ARG:C	1:A:117:ARG:NE	0.47	2.73	10	1
2:B:23:GLU:O	2:B:24:GLU:C	0.47	2.57	1	3
2:B:9:MET:CG	2:B:9:MET:O	0.47	2.62	2	1
2:B:25:GLU:C	2:B:27:ASP:N	0.47	2.72	2	2
2:B:32:ILE:O	2:B:32:ILE:CG2	0.47	2.62	4	1
1:A:13:LEU:O	1:A:17:HIS:O	0.47	2.33	4	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:166:GLN:NE2	1:A:167:LEU:CD2	0.47	2.78	1	1
2:B:25:GLU:CD	2:B:25:GLU:N	0.47	2.72	1	2
2:B:44:THR:HG22	2:B:45:ARG:H	0.47	1.66	1	1
1:A:128:LYS:NZ	2:B:21:GLU:OE1	0.47	2.46	4	1
2:B:61:LYS:CD	2:B:61:LYS:C	0.47	2.87	9	1
1:A:75:ALA:O	1:A:76:LYS:C	0.47	2.57	2	10
1:A:52:ASN:OD1	1:A:52:ASN:O	0.47	2.32	4	2
2:B:32:ILE:CD1	2:B:35:SER:OG	0.47	2.63	4	1
1:A:128:LYS:CD	1:A:128:LYS:N	0.47	2.76	6	1
2:B:34:THR:OG1	2:B:38:ILE:O	0.47	2.32	6	1
2:B:28:ASP:O	2:B:29:LEU:O	0.47	2.33	7	1
1:A:58:SER:C	1:A:60:ARG:H	0.47	2.17	9	1
1:A:182:THR:C	1:A:184:ALA:N	0.47	2.72	7	3
2:B:52:LYS:HZ2	2:B:56:GLU:CD	0.47	2.17	2	1
1:A:105:GLN:N	1:A:105:GLN:NE2	0.47	2.63	4	1
1:A:118:HIS:O	1:A:118:HIS:ND1	0.47	2.48	7	1
1:A:75:ALA:C	1:A:79:VAL:HG23	0.47	2.35	8	1
1:A:89:TYR:O	1:A:89:TYR:CG	0.47	2.67	9	1
1:A:186:GLY:C	1:A:188:VAL:H	0.47	2.16	4	2
2:B:40:SER:C	2:B:42:ARG:N	0.47	2.71	3	4
1:A:27:MET:O	1:A:31:ASN:CG	0.47	2.57	8	4
1:A:58:SER:O	1:A:60:ARG:N	0.47	2.48	9	1
1:A:77:HIS:ND1	1:A:77:HIS:N	0.47	2.62	10	2
1:A:85:ALA:O	1:A:89:TYR:N	0.47	2.38	9	1
1:A:89:TYR:O	1:A:89:TYR:CD1	0.47	2.68	9	1
1:A:94:GLN:O	1:A:101:ARG:NH1	0.47	2.48	2	1
1:A:48:LEU:CD1	1:A:61:GLU:OE2	0.47	2.63	7	2
2:B:25:GLU:N	2:B:25:GLU:CD	0.47	2.73	4	1
1:A:94:GLN:C	1:A:101:ARG:HH11	0.46	2.19	10	4
1:A:87:THR:HA	2:B:29:LEU:HD12	0.46	1.86	3	1
2:B:7:SER:C	2:B:9:MET:H	0.46	2.19	4	3
1:A:96:GLN:H	1:A:101:ARG:HE	0.46	1.49	5	1
1:A:164:HIS:CD2	1:A:164:HIS:N	0.46	2.84	7	1
1:A:122:ARG:N	1:A:122:ARG:CD	0.46	2.77	8	1
2:B:46:GLY:O	2:B:47:LYS:C	0.46	2.58	9	1
1:A:52:ASN:C	1:A:54:LYS:H	0.46	2.18	1	6
1:A:96:GLN:O	1:A:97:SER:CB	0.46	2.63	1	1
1:A:101:ARG:C	1:A:103:GLY:H	0.46	2.18	5	3
1:A:24:GLN:CD	1:A:25:LYS:H	0.46	2.18	5	3
1:A:167:LEU:HD12	1:A:167:LEU:N	0.46	2.26	2	1
1:A:176:ASP:O	1:A:178:LEU:N	0.46	2.49	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:60:LYS:O	2:B:61:LYS:C	0.46	2.58	4	5
2:B:24:GLU:O	2:B:24:GLU:CG	0.46	2.62	4	1
1:A:180:ARG:CD	1:A:180:ARG:H	0.46	2.22	6	1
1:A:13:LEU:HD12	1:A:145:LEU:HD21	0.46	1.86	1	1
1:A:88:LYS:C	1:A:90:SER:N	0.46	2.73	2	1
1:A:188:VAL:O	1:A:189:LEU:C	0.46	2.59	2	3
1:A:114:TYR:O	1:A:118:HIS:CB	0.46	2.64	9	3
1:A:90:SER:C	1:A:92:SER:H	0.46	2.18	5	1
1:A:8:TYR:O	1:A:9:ILE:C	0.46	2.58	8	1
2:B:33:ASP:OD1	2:B:33:ASP:N	0.46	2.48	2	1
1:A:89:TYR:O	1:A:101:ARG:CD	0.46	2.63	4	1
1:A:128:LYS:CE	2:B:21:GLU:OE1	0.46	2.63	4	1
2:B:29:LEU:O	2:B:30:ALA:CB	0.46	2.62	7	1
2:B:32:ILE:O	2:B:34:THR:N	0.46	2.48	10	1
1:A:123:THR:O	1:A:124:ARG:O	0.46	2.32	10	4
1:A:126:GLY:CA	2:B:20:ASN:OD1	0.46	2.63	3	1
1:A:145:LEU:HD23	1:A:145:LEU:C	0.46	2.35	7	1
1:A:173:ASP:CB	2:B:61:LYS:NZ	0.46	2.79	7	1
2:B:43:ARG:O	2:B:44:THR:C	0.46	2.58	8	1
2:B:38:ILE:C	2:B:38:ILE:CD1	0.46	2.89	9	1
2:B:19:GLY:O	2:B:21:GLU:N	0.46	2.47	10	1
1:A:48:LEU:O	1:A:52:ASN:CG	0.46	2.59	2	4
1:A:177:SER:C	1:A:180:ARG:NE	0.46	2.74	1	1
1:A:55:SER:O	1:A:57:ILE:N	0.46	2.48	4	3
1:A:87:THR:O	1:A:88:LYS:C	0.46	2.59	4	8
2:B:9:MET:C	2:B:11:ASP:H	0.46	2.17	5	2
1:A:112:LYS:NZ	2:B:12:ALA:O	0.46	2.41	7	1
1:A:3:GLU:CD	1:A:4:THR:N	0.46	2.73	9	1
1:A:55:SER:O	1:A:56:THR:O	0.46	2.34	9	1
1:A:83:THR:HG21	2:B:31:GLU:HB2	0.46	1.87	7	1
1:A:53:LYS:C	1:A:55:SER:H	0.46	2.18	10	1
1:A:39:GLU:O	1:A:40:ARG:C	0.46	2.59	4	9
1:A:118:HIS:O	1:A:119:ALA:C	0.46	2.59	5	5
1:A:24:GLN:CD	1:A:24:GLN:H	0.46	2.19	10	1
1:A:148:ALA:O	1:A:152:ALA:CB	0.46	2.64	5	2
2:B:20:ASN:O	2:B:21:GLU:C	0.46	2.58	1	4
2:B:11:ASP:O	2:B:13:LYS:N	0.46	2.48	3	1
2:B:54:THR:O	2:B:58:LEU:CB	0.46	2.64	7	4
1:A:80:SER:OG	2:B:35:SER:CB	0.46	2.64	9	1
2:B:34:THR:O	2:B:35:SER:C	0.46	2.58	6	2
1:A:21:GLY:N	1:A:158:LYS:O	0.46	2.43	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:THR:C	1:A:125:VAL:H	0.46	2.20	5	1
2:B:39:THR:OG1	2:B:42:ARG:NH2	0.46	2.49	5	1
2:B:56:GLU:CG	2:B:57:GLU:N	0.46	2.79	9	1
2:B:25:GLU:CD	2:B:25:GLU:H	0.45	2.18	1	1
2:B:11:ASP:C	2:B:13:LYS:N	0.45	2.72	3	1
1:A:120:THR:HG23	1:A:121:GLY:H	0.45	1.71	9	1
1:A:128:LYS:HZ1	1:A:128:LYS:HA	0.45	1.71	9	1
2:B:17:LEU:O	2:B:19:GLY:N	0.45	2.50	1	1
1:A:48:LEU:O	1:A:52:ASN:CB	0.45	2.64	4	1
1:A:137:LEU:O	1:A:141:THR:OG1	0.45	2.34	9	5
1:A:186:GLY:O	1:A:188:VAL:HG22	0.45	2.12	1	2
2:B:23:GLU:CD	2:B:23:GLU:N	0.45	2.74	3	1
1:A:137:LEU:O	1:A:138:GLU:C	0.45	2.60	6	1
1:A:57:ILE:O	1:A:129:ALA:CB	0.45	2.64	10	1
1:A:59:ALA:HB1	1:A:63:GLN:HE21	0.45	1.71	4	1
1:A:177:SER:C	1:A:180:ARG:CZ	0.45	2.89	7	1
1:A:12:VAL:O	1:A:16:THR:HG23	0.45	2.11	1	1
1:A:112:LYS:HZ1	1:A:116:LYS:HG3	0.45	1.72	1	1
2:B:44:THR:CG2	2:B:45:ARG:N	0.45	2.78	1	1
1:A:47:LYS:C	1:A:49:ALA:H	0.45	2.19	10	2
1:A:178:LEU:O	1:A:180:ARG:NE	0.45	2.49	6	1
1:A:3:GLU:O	1:A:4:THR:C	0.45	2.57	7	2
1:A:156:LYS:NZ	1:A:163:ARG:HH22	0.45	2.01	2	1
1:A:138:GLU:O	1:A:142:ALA:CB	0.45	2.65	3	1
1:A:152:ALA:HB2	1:A:164:HIS:CG	0.45	2.47	3	2
2:B:20:ASN:HD22	2:B:22:GLY:H	0.45	1.53	3	1
1:A:117:ARG:CG	1:A:118:HIS:N	0.45	2.78	7	2
1:A:163:ARG:C	1:A:165:LEU:N	0.45	2.73	3	3
1:A:170:ARG:NH1	1:A:176:ASP:OD2	0.45	2.42	2	1
2:B:44:THR:O	2:B:45:ARG:O	0.45	2.34	3	1
1:A:137:LEU:O	1:A:141:THR:CB	0.45	2.65	9	4
2:B:33:ASP:C	2:B:35:SER:N	0.45	2.72	8	1
2:B:8:ASP:O	2:B:9:MET:CB	0.45	2.65	9	1
1:A:33:PHE:O	1:A:34:VAL:C	0.45	2.58	2	10
1:A:64:THR:O	1:A:65:ALA:C	0.45	2.60	3	7
1:A:23:SER:OG	1:A:160:ILE:O	0.45	2.35	7	2
1:A:166:GLN:NE2	1:A:189:LEU:CD1	0.45	2.80	6	1
1:A:7:SER:O	1:A:8:TYR:C	0.45	2.60	1	6
1:A:90:SER:O	1:A:91:SER:C	0.45	2.59	1	5
1:A:91:SER:O	1:A:92:SER:O	0.45	2.35	9	4
1:A:188:VAL:O	1:A:188:VAL:CG2	0.45	2.61	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:GLN:O	1:A:67:ARG:N	0.45	2.42	6	3
1:A:72:GLY:O	1:A:76:LYS:N	0.45	2.42	7	1
2:B:36:ASN:ND2	2:B:36:ASN:C	0.45	2.75	7	1
1:A:83:THR:HG22	2:B:28:ASP:OD2	0.45	2.12	3	1
1:A:77:HIS:NE2	2:B:38:ILE:CD1	0.45	2.80	4	1
1:A:87:THR:OG1	2:B:29:LEU:HD22	0.45	2.12	5	1
1:A:166:GLN:OE1	1:A:166:GLN:C	0.45	2.60	5	1
1:A:56:THR:O	1:A:56:THR:CG2	0.45	2.64	10	1
2:B:51:TYR:C	2:B:53:LYS:H	0.44	2.19	1	1
1:A:28:SER:O	1:A:32:SER:CB	0.44	2.65	7	4
1:A:173:ASP:CB	2:B:61:LYS:HZ1	0.44	2.26	7	1
2:B:11:ASP:CG	2:B:12:ALA:N	0.44	2.75	9	1
1:A:3:GLU:C	1:A:4:THR:CG2	0.44	2.90	10	1
1:A:53:LYS:O	1:A:54:LYS:C	0.44	2.61	3	5
1:A:56:THR:O	1:A:61:GLU:OE2	0.44	2.34	10	2
1:A:169:ILE:HG21	1:A:183:ILE:HD11	0.44	1.89	1	1
1:A:166:GLN:OE1	1:A:188:VAL:HG12	0.44	2.11	3	1
2:B:20:ASN:C	2:B:20:ASN:HD22	0.44	2.19	3	1
1:A:58:SER:O	1:A:61:GLU:OE1	0.44	2.36	6	1
2:B:20:ASN:C	2:B:21:GLU:CD	0.44	2.85	6	1
2:B:25:GLU:C	2:B:27:ASP:H	0.44	2.17	2	1
1:A:6:SER:O	1:A:7:SER:C	0.44	2.58	3	2
1:A:49:ALA:O	1:A:53:LYS:N	0.44	2.51	4	1
1:A:122:ARG:O	1:A:123:THR:O	0.44	2.35	6	1
2:B:23:GLU:N	2:B:23:GLU:CD	0.44	2.75	7	1
1:A:127:SER:O	1:A:131:ILE:CG2	0.44	2.65	1	1
1:A:13:LEU:CD2	1:A:20:THR:O	0.44	2.65	2	5
1:A:40:ARG:O	1:A:44:GLU:OE2	0.44	2.36	7	4
1:A:124:ARG:O	1:A:125:VAL:C	0.44	2.61	5	2
2:B:19:GLY:O	2:B:21:GLU:OE2	0.44	2.35	6	1
2:B:58:LEU:C	2:B:58:LEU:CD2	0.44	2.90	6	2
2:B:29:LEU:HD12	2:B:30:ALA:N	0.44	2.27	8	1
2:B:52:LYS:C	2:B:54:THR:N	0.44	2.69	10	1
1:A:12:VAL:O	1:A:16:THR:OG1	0.44	2.32	1	1
1:A:65:ALA:O	1:A:66:VAL:C	0.44	2.59	6	10
1:A:54:LYS:O	1:A:55:SER:OG	0.44	2.36	2	2
1:A:33:PHE:CZ	1:A:37:ILE:HG21	0.44	2.48	3	3
1:A:22:ILE:O	1:A:22:ILE:CG2	0.44	2.66	4	2
1:A:77:HIS:CD2	2:B:38:ILE:CG1	0.44	3.00	4	1
2:B:15:ASP:O	2:B:17:LEU:CD1	0.44	2.66	4	1
1:A:151:ALA:O	1:A:155:LEU:N	0.44	2.51	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:GLY:O	1:A:187:GLY:O	0.44	2.35	8	1
2:B:7:SER:O	2:B:8:ASP:C	0.44	2.60	10	1
1:A:48:LEU:HD12	1:A:49:ALA:N	0.44	2.26	2	3
1:A:81:GLU:OE1	2:B:42:ARG:NH2	0.44	2.49	2	1
2:B:17:LEU:N	2:B:17:LEU:CD1	0.44	2.80	4	1
2:B:58:LEU:HD23	2:B:58:LEU:O	0.44	2.13	6	1
1:A:166:GLN:CD	1:A:166:GLN:C	0.44	2.86	7	1
1:A:93:THR:C	1:A:94:GLN:CD	0.44	2.86	9	6
1:A:119:ALA:O	1:A:120:THR:OG1	0.44	2.36	2	3
1:A:123:THR:C	1:A:125:VAL:N	0.44	2.75	5	1
2:B:42:ARG:C	2:B:44:THR:H	0.44	2.21	6	1
1:A:112:LYS:NZ	2:B:16:ALA:CB	0.44	2.80	7	1
2:B:21:GLU:O	2:B:22:GLY:O	0.44	2.36	10	2
1:A:109:GLY:O	1:A:110:ARG:C	0.44	2.61	10	1
1:A:83:THR:C	1:A:85:ALA:N	0.44	2.74	5	2
1:A:111:ILE:O	1:A:112:LYS:C	0.44	2.60	7	7
2:B:30:ALA:O	2:B:31:GLU:C	0.44	2.61	2	2
1:A:143:GLU:C	1:A:145:LEU:H	0.44	2.20	3	1
1:A:146:GLU:CD	2:B:45:ARG:N	0.44	2.76	3	1
2:B:25:GLU:O	2:B:27:ASP:OD1	0.44	2.36	3	1
1:A:178:LEU:C	1:A:180:ARG:HE	0.44	2.21	5	1
1:A:3:GLU:O	1:A:4:THR:OG1	0.44	2.33	9	2
1:A:72:GLY:O	1:A:73:GLU:C	0.44	2.60	6	9
1:A:186:GLY:C	1:A:188:VAL:N	0.44	2.74	4	3
2:B:19:GLY:O	2:B:20:ASN:CG	0.44	2.61	1	1
2:B:21:GLU:O	2:B:22:GLY:C	0.44	2.61	7	3
1:A:10:TYR:CZ	1:A:11:LYS:CE	0.44	3.01	3	1
1:A:90:SER:O	1:A:94:GLN:CD	0.44	2.61	3	1
1:A:12:VAL:O	1:A:16:THR:CG2	0.44	2.66	4	1
1:A:5:TYR:CD1	1:A:31:ASN:ND2	0.43	2.86	1	1
1:A:59:ALA:CB	2:B:28:ASP:OD2	0.43	2.66	2	1
1:A:119:ALA:C	1:A:120:THR:CG2	0.43	2.91	2	1
1:A:146:GLU:CD	2:B:43:ARG:O	0.43	2.61	4	1
2:B:20:ASN:O	2:B:21:GLU:CD	0.43	2.61	6	2
1:A:112:LYS:C	1:A:112:LYS:CD	0.43	2.91	7	1
1:A:8:TYR:O	1:A:11:LYS:CG	0.43	2.66	8	1
2:B:32:ILE:O	2:B:32:ILE:HG23	0.43	2.12	8	1
1:A:87:THR:CG2	1:A:88:LYS:N	0.43	2.81	9	1
1:A:60:ARG:O	1:A:61:GLU:C	0.43	2.59	10	1
1:A:77:HIS:N	1:A:77:HIS:HD1	0.43	2.11	10	1
1:A:151:ALA:O	1:A:154:ASP:OD1	0.43	2.36	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:ILE:C	1:A:43:THR:N	0.43	2.76	1	1
1:A:85:ALA:CB	1:A:131:ILE:HD11	0.43	2.43	1	3
1:A:89:TYR:CE1	1:A:94:GLN:NE2	0.43	2.87	1	1
2:B:33:ASP:OD1	2:B:34:THR:N	0.43	2.51	2	1
2:B:33:ASP:C	2:B:35:SER:H	0.43	2.20	2	1
1:A:155:LEU:N	1:A:155:LEU:HD22	0.43	2.28	5	1
1:A:146:GLU:OE2	2:B:44:THR:O	0.43	2.36	1	1
2:B:11:ASP:O	2:B:15:ASP:OD1	0.43	2.36	1	2
2:B:10:ASP:O	2:B:11:ASP:CG	0.43	2.62	6	1
1:A:8:TYR:OH	2:B:8:ASP:CG	0.43	2.62	8	1
1:A:105:GLN:CD	1:A:105:GLN:H	0.43	2.21	1	1
1:A:175:LEU:O	1:A:176:ASP:C	0.43	2.61	10	7
2:B:59:ASP:OD1	2:B:59:ASP:O	0.43	2.37	2	2
1:A:66:VAL:HG21	1:A:136:VAL:HG11	0.43	1.91	3	1
1:A:143:GLU:O	1:A:145:LEU:N	0.43	2.51	3	1
2:B:27:ASP:O	2:B:28:ASP:CG	0.43	2.61	7	1
1:A:125:VAL:O	2:B:19:GLY:O	0.43	2.36	10	1
2:B:11:ASP:O	2:B:15:ASP:CG	0.43	2.61	1	3
2:B:31:GLU:O	2:B:32:ILE:C	0.43	2.61	1	1
1:A:31:ASN:O	1:A:35:ASN:CB	0.43	2.67	3	2
1:A:52:ASN:OD1	1:A:54:LYS:NZ	0.43	2.51	6	1
1:A:172:ASP:O	1:A:173:ASP:C	0.43	2.61	9	4
1:A:24:GLN:C	1:A:24:GLN:CD	0.43	2.87	4	1
1:A:70:LEU:HD23	1:A:178:LEU:HD22	0.43	1.90	4	1
1:A:127:SER:OG	2:B:24:GLU:CD	0.43	2.61	4	1
1:A:156:LYS:C	1:A:157:VAL:CG2	0.43	2.92	4	1
2:B:10:ASP:C	2:B:11:ASP:OD1	0.43	2.61	4	2
2:B:23:GLU:O	2:B:23:GLU:OE1	0.43	2.36	5	1
1:A:60:ARG:O	1:A:63:GLN:N	0.43	2.52	10	1
1:A:146:GLU:OE2	2:B:44:THR:N	0.43	2.52	1	1
1:A:59:ALA:O	1:A:63:GLN:CG	0.43	2.67	3	1
1:A:124:ARG:O	2:B:20:ASN:OD1	0.43	2.36	4	1
2:B:59:ASP:O	2:B:59:ASP:OD1	0.43	2.36	5	1
1:A:121:GLY:O	1:A:122:ARG:C	0.43	2.62	6	2
2:B:37:ILE:O	2:B:38:ILE:C	0.43	2.61	7	1
1:A:147:LEU:O	1:A:148:ALA:C	0.43	2.61	10	4
1:A:115:LEU:O	1:A:119:ALA:CB	0.43	2.67	4	1
1:A:138:GLU:CD	1:A:138:GLU:O	0.43	2.61	4	3
2:B:40:SER:O	2:B:42:ARG:NH1	0.43	2.52	5	1
1:A:166:GLN:O	1:A:170:ARG:CG	0.43	2.66	10	1
1:A:160:ILE:C	1:A:160:ILE:HD13	0.43	2.39	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:174:GLU:O	1:A:175:LEU:C	0.43	2.60	6	2
2:B:27:ASP:C	2:B:28:ASP:OD1	0.43	2.62	4	1
1:A:96:GLN:O	1:A:96:GLN:CD	0.43	2.62	7	1
1:A:44:GLU:N	1:A:44:GLU:CD	0.43	2.77	8	1
2:B:34:THR:O	2:B:36:ASN:N	0.43	2.52	8	1
1:A:4:THR:C	1:A:6:SER:H	0.43	2.22	1	1
1:A:32:SER:O	1:A:36:ASP:CG	0.43	2.62	3	4
1:A:166:GLN:OE1	1:A:166:GLN:O	0.43	2.36	1	1
1:A:176:ASP:O	1:A:177:SER:C	0.43	2.62	2	2
1:A:138:GLU:C	1:A:138:GLU:CD	0.43	2.87	6	2
1:A:174:GLU:O	1:A:177:SER:N	0.43	2.52	4	1
2:B:24:GLU:O	2:B:27:ASP:CG	0.43	2.62	6	1
2:B:27:ASP:O	2:B:28:ASP:OD1	0.43	2.37	7	1
1:A:28:SER:O	1:A:32:SER:OG	0.43	2.37	8	1
2:B:10:ASP:OD1	2:B:10:ASP:C	0.43	2.61	10	1
1:A:70:LEU:O	1:A:72:GLY:N	0.42	2.52	6	5
1:A:185:SER:O	1:A:186:GLY:C	0.42	2.60	2	1
1:A:32:SER:O	1:A:36:ASP:OD2	0.42	2.37	7	2
1:A:146:GLU:CD	1:A:146:GLU:C	0.42	2.86	7	1
1:A:86:VAL:HG11	2:B:27:ASP:O	0.42	2.13	8	1
1:A:159:ARG:O	1:A:160:ILE:C	0.42	2.60	1	1
1:A:88:LYS:O	1:A:90:SER:N	0.42	2.52	2	1
1:A:131:ILE:O	1:A:135:ALA:N	0.42	2.50	3	1
1:A:147:LEU:O	1:A:151:ALA:HB2	0.42	2.14	3	2
1:A:154:ASP:OD1	1:A:154:ASP:C	0.42	2.62	3	1
1:A:88:LYS:O	1:A:89:TYR:C	0.42	2.62	4	2
1:A:148:ALA:O	1:A:152:ALA:HB2	0.42	2.13	5	1
1:A:167:LEU:CD2	2:B:52:LYS:H	0.42	2.26	6	1
1:A:145:LEU:O	1:A:146:GLU:C	0.42	2.60	7	1
1:A:25:LYS:C	1:A:28:SER:H	0.42	2.22	6	3
1:A:127:SER:HG	2:B:27:ASP:CG	0.42	2.22	1	1
2:B:12:ALA:C	2:B:15:ASP:OD1	0.42	2.61	1	1
1:A:59:ALA:O	1:A:63:GLN:CD	0.42	2.62	3	1
1:A:165:LEU:O	1:A:166:GLN:C	0.42	2.60	3	1
2:B:19:GLY:C	2:B:21:GLU:OE2	0.42	2.62	6	1
1:A:25:LYS:O	1:A:29:ILE:N	0.42	2.42	9	1
2:B:24:GLU:OE1	2:B:27:ASP:OD2	0.42	2.37	9	1
1:A:123:THR:O	1:A:124:ARG:C	0.42	2.63	10	1
2:B:24:GLU:CD	2:B:24:GLU:O	0.42	2.62	10	1
1:A:162:PRO:CB	1:A:185:SER:OG	0.42	2.67	5	1
2:B:43:ARG:O	2:B:45:ARG:N	0.42	2.53	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:SER:O	1:A:94:GLN:OE1	0.42	2.37	7	1
1:A:87:THR:O	1:A:91:SER:OG	0.42	2.36	9	1
1:A:101:ARG:O	1:A:102:ALA:C	0.42	2.63	2	1
2:B:23:GLU:N	2:B:23:GLU:OE1	0.42	2.52	2	1
2:B:7:SER:O	2:B:11:ASP:OD1	0.42	2.36	4	1
2:B:29:LEU:C	2:B:29:LEU:CD1	0.42	2.93	8	2
1:A:172:ASP:O	1:A:174:GLU:N	0.42	2.53	8	1
1:A:64:THR:O	1:A:67:ARG:N	0.42	2.52	2	1
1:A:137:LEU:O	1:A:139:TYR:N	0.42	2.52	6	1
1:A:143:GLU:O	1:A:144:VAL:C	0.42	2.62	7	1
1:A:173:ASP:OD2	2:B:59:ASP:O	0.42	2.37	7	1
1:A:172:ASP:C	1:A:174:GLU:N	0.42	2.77	8	1
1:A:30:LEU:O	1:A:34:VAL:N	0.42	2.49	10	1
1:A:70:LEU:O	1:A:71:PRO:C	0.42	2.63	3	6
1:A:148:ALA:O	1:A:149:GLY:C	0.42	2.61	4	1
1:A:166:GLN:C	1:A:166:GLN:CD	0.42	2.87	9	3
2:B:13:LYS:C	2:B:15:ASP:N	0.42	2.76	5	1
2:B:30:ALA:O	2:B:31:GLU:OE2	0.42	2.37	6	1
1:A:40:ARG:O	1:A:44:GLU:CD	0.42	2.63	7	1
2:B:38:ILE:C	2:B:39:THR:OG1	0.42	2.62	10	1
1:A:178:LEU:O	1:A:178:LEU:CD1	0.42	2.67	2	2
1:A:81:GLU:OE2	1:A:81:GLU:O	0.42	2.37	3	1
2:B:41:GLY:C	2:B:43:ARG:N	0.42	2.76	4	1
1:A:166:GLN:C	1:A:166:GLN:OE1	0.42	2.62	7	1
1:A:97:SER:O	1:A:100:ALA:N	0.42	2.53	8	1
1:A:187:GLY:C	1:A:189:LEU:N	0.42	2.78	8	1
2:B:24:GLU:OE2	2:B:27:ASP:OD1	0.42	2.37	9	1
1:A:81:GLU:CD	2:B:40:SER:O	0.42	2.63	10	1
1:A:32:SER:O	1:A:36:ASP:OD1	0.42	2.38	10	2
1:A:63:GLN:O	1:A:64:THR:C	0.42	2.63	4	1
1:A:137:LEU:C	1:A:139:TYR:N	0.42	2.77	6	1
2:B:29:LEU:C	2:B:29:LEU:HD12	0.42	2.39	6	1
1:A:52:ASN:O	1:A:52:ASN:CG	0.42	2.62	8	2
2:B:20:ASN:O	2:B:21:GLU:OE2	0.42	2.38	9	1
1:A:180:ARG:O	1:A:181:ALA:C	0.42	2.62	10	1
1:A:52:ASN:OD1	1:A:54:LYS:CE	0.42	2.67	6	1
1:A:123:THR:C	1:A:124:ARG:O	0.42	2.62	10	2
1:A:180:ARG:HD2	1:A:180:ARG:N	0.41	2.30	2	1
1:A:41:ILE:O	1:A:43:THR:N	0.41	2.53	3	1
1:A:138:GLU:CD	1:A:138:GLU:C	0.41	2.88	4	1
1:A:170:ARG:O	1:A:171:GLY:C	0.41	2.62	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:LEU:O	1:A:75:ALA:C	0.41	2.63	5	3
1:A:110:ARG:O	1:A:114:TYR:CE1	0.41	2.73	4	1
2:B:11:ASP:O	2:B:15:ASP:OD2	0.41	2.38	4	1
1:A:96:GLN:C	1:A:97:SER:OG	0.41	2.61	1	1
1:A:5:TYR:CD2	1:A:31:ASN:OD1	0.41	2.74	3	1
1:A:24:GLN:O	1:A:27:MET:N	0.41	2.54	4	1
2:B:45:ARG:C	2:B:45:ARG:CD	0.41	2.94	4	1
1:A:126:GLY:O	1:A:127:SER:C	0.41	2.63	5	1
1:A:83:THR:OG1	2:B:32:ILE:CG2	0.41	2.68	9	1
1:A:62:ILE:HD12	1:A:132:TYR:HB3	0.41	1.90	10	1
1:A:102:ALA:O	1:A:104:LEU:CD2	0.41	2.69	10	1
1:A:180:ARG:C	1:A:180:ARG:CD	0.41	2.93	2	1
1:A:3:GLU:O	1:A:6:SER:OG	0.41	2.37	3	2
1:A:31:ASN:C	1:A:31:ASN:HD22	0.41	2.23	3	1
1:A:87:THR:O	1:A:90:SER:N	0.41	2.49	3	1
1:A:160:ILE:O	1:A:161:THR:HG23	0.41	2.15	6	1
1:A:145:LEU:C	1:A:145:LEU:CD2	0.41	2.94	7	1
1:A:87:THR:OG1	1:A:91:SER:OG	0.41	2.38	9	1
2:B:24:GLU:OE1	2:B:27:ASP:CG	0.41	2.63	9	1
1:A:8:TYR:OH	2:B:8:ASP:OD2	0.41	2.37	1	1
1:A:9:ILE:O	1:A:10:TYR:C	0.41	2.64	1	4
1:A:58:SER:O	1:A:59:ALA:C	0.41	2.63	2	2
1:A:101:ARG:CA	1:A:101:ARG:HE	0.41	2.28	3	1
1:A:170:ARG:NH2	1:A:176:ASP:OD2	0.41	2.45	3	1
1:A:5:TYR:CE1	1:A:34:VAL:CG1	0.41	3.03	4	1
1:A:181:ALA:O	1:A:182:THR:OG1	0.41	2.36	5	1
1:A:59:ALA:HB3	2:B:28:ASP:CG	0.41	2.41	8	1
1:A:53:LYS:N	1:A:53:LYS:CD	0.41	2.83	9	1
1:A:89:TYR:OH	1:A:94:GLN:OE1	0.41	2.39	1	1
1:A:45:ALA:O	1:A:49:ALA:CB	0.41	2.68	7	1
2:B:42:ARG:O	2:B:43:ARG:C	0.41	2.64	7	1
1:A:127:SER:OG	2:B:27:ASP:OD2	0.41	2.37	1	1
1:A:138:GLU:O	1:A:138:GLU:OE2	0.41	2.39	4	2
1:A:83:THR:O	1:A:85:ALA:N	0.41	2.54	1	1
1:A:114:TYR:O	1:A:118:HIS:N	0.41	2.52	4	2
1:A:123:THR:O	1:A:123:THR:CG2	0.41	2.68	5	1
1:A:24:GLN:CD	1:A:24:GLN:N	0.41	2.78	6	1
1:A:48:LEU:CD1	1:A:61:GLU:CD	0.41	2.94	7	1
1:A:86:VAL:O	1:A:87:THR:C	0.41	2.64	9	1
1:A:3:GLU:C	1:A:4:THR:O	0.41	2.64	1	1
1:A:3:GLU:C	1:A:4:THR:OG1	0.41	2.64	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:40:SER:O	2:B:44:THR:OG1	0.41	2.37	2	1
2:B:10:ASP:N	2:B:10:ASP:OD1	0.41	2.53	6	1
1:A:112:LYS:HZ3	2:B:16:ALA:CB	0.41	2.27	7	1
1:A:163:ARG:HH21	2:B:52:LYS:CE	0.41	2.28	7	1
1:A:146:GLU:OE2	2:B:45:ARG:N	0.41	2.42	8	1
1:A:33:PHE:C	1:A:35:ASN:N	0.41	2.77	2	1
2:B:61:LYS:O	2:B:62:GLU:CG	0.41	2.69	3	1
2:B:19:GLY:O	2:B:20:ASN:C	0.41	2.63	7	1
1:A:171:GLY:O	2:B:58:LEU:HD22	0.40	2.16	1	1
1:A:10:TYR:CD1	1:A:10:TYR:O	0.40	2.74	3	1
1:A:154:ASP:OD1	1:A:154:ASP:O	0.40	2.39	3	1
1:A:52:ASN:ND2	1:A:54:LYS:CE	0.40	2.85	4	1
1:A:115:LEU:HD11	1:A:133:LEU:HD22	0.40	1.91	4	1
2:B:38:ILE:O	2:B:38:ILE:HG23	0.40	2.16	6	1
1:A:61:GLU:O	1:A:64:THR:OG1	0.40	2.38	7	1
1:A:81:GLU:O	1:A:85:ALA:CB	0.40	2.70	8	1
1:A:141:THR:O	1:A:145:LEU:HD13	0.40	2.16	3	1
1:A:124:ARG:NH1	2:B:18:MET:CE	0.40	2.85	7	1
1:A:8:TYR:OH	2:B:8:ASP:OD1	0.40	2.39	8	1
1:A:115:LEU:HD11	1:A:133:LEU:HD12	0.40	1.93	8	1
2:B:43:ARG:C	2:B:43:ARG:CD	0.40	2.94	9	1
2:B:46:GLY:O	2:B:47:LYS:CG	0.40	2.69	10	1
1:A:31:ASN:OD1	1:A:31:ASN:C	0.40	2.64	1	1
1:A:90:SER:O	1:A:94:GLN:OE1	0.40	2.40	3	1
1:A:119:ALA:O	1:A:123:THR:OG1	0.40	2.35	3	1
1:A:26:SER:OG	1:A:160:ILE:O	0.40	2.33	5	1
1:A:99:SER:CB	2:B:7:SER:O	0.40	2.69	9	1
2:B:32:ILE:CG1	2:B:33:ASP:H	0.40	2.29	10	1
1:A:94:GLN:CD	1:A:94:GLN:N	0.40	2.80	6	1
1:A:12:VAL:O	1:A:12:VAL:HG12	0.40	2.15	10	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	187/192 (97%)	128±4 (69±2%)	40±4 (22±2%)	18±3 (10±1%)	1	10
2	B	52/62 (84%)	21±2 (41±3%)	20±3 (39±5%)	10±2 (20±4%)	0	2
All	All	2390/2540 (94%)	1496 (63%)	607 (25%)	287 (12%)	1	7

All 83 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	22	ILE	10
1	A	107	PRO	10
1	A	162	PRO	10
1	A	185	SER	10
1	A	180	ARG	9
1	A	183	ILE	9
1	A	97	SER	8
1	A	120	THR	7
2	B	28	ASP	7
2	B	30	ALA	7
1	A	92	SER	7
1	A	94	GLN	6
2	B	32	ILE	6
2	B	47	LYS	6
1	A	7	SER	5
1	A	71	PRO	5
1	A	6	SER	5
2	B	8	ASP	5
1	A	3	GLU	5
1	A	96	GLN	5
1	A	187	GLY	5
1	A	91	SER	5
1	A	4	THR	4
1	A	127	SER	4
1	A	156	LYS	4
2	B	20	ASN	4
2	B	42	ARG	4
1	A	56	THR	4
1	A	124	ARG	4
1	A	129	ALA	4
2	B	29	LEU	4
2	B	44	THR	4
2	B	10	ASP	4
2	B	24	GLU	3
2	B	40	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	A	55	SER	3
1	A	157	VAL	3
1	A	172	ASP	3
1	A	188	VAL	3
2	B	9	MET	3
2	B	23	GLU	3
2	B	52	LYS	3
2	B	22	GLY	3
1	A	158	LYS	3
1	A	95	ALA	3
2	B	19	GLY	3
1	A	93	THR	2
2	B	21	GLU	2
2	B	31	GLU	2
2	B	33	ASP	2
1	A	87	THR	2
1	A	171	GLY	2
2	B	35	SER	2
2	B	43	ARG	2
2	B	61	LYS	2
2	B	12	ALA	2
2	B	45	ARG	2
1	A	181	ALA	2
1	A	123	THR	2
2	B	36	ASN	2
2	B	51	TYR	2
1	A	160	ILE	1
2	B	59	ASP	1
1	A	150	ASN	1
2	B	11	ASP	1
1	A	42	ALA	1
2	B	57	GLU	1
1	A	41	ILE	1
1	A	57	ILE	1
1	A	119	ALA	1
1	A	161	THR	1
2	B	14	LEU	1
2	B	18	MET	1
2	B	55	ALA	1
1	A	69	ILE	1
1	A	102	ALA	1
2	B	27	ASP	1

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Mol	Chain	Res	Type	Models (Total)
2	B	46	GLY	1
1	A	54	LYS	1
2	B	37	ILE	1
2	B	38	ILE	1
2	B	39	THR	1
2	B	7	SER	1

6.3.2 Protein sidechains ⓘ

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	153/158 (97%)	131±2 (86±2%)	22±2 (14±2%)	5	44
2	B	45/54 (83%)	38±2 (85±4%)	7±2 (15±4%)	5	42
All	All	1980/2120 (93%)	1696 (86%)	284 (14%)	5	44

All 88 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	10	TYR	10
1	A	34	VAL	10
1	A	62	ILE	10
2	B	36	ASN	10
1	A	15	GLN	9
1	A	97	SER	9
1	A	178	LEU	9
1	A	66	VAL	8
2	B	13	LYS	8
1	A	127	SER	7
1	A	112	LYS	7
2	B	62	GLU	7
1	A	24	GLN	6
1	A	4	THR	6
1	A	37	ILE	5
1	A	61	GLU	5
1	A	128	LYS	5
1	A	132	TYR	5

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Mol	Chain	Res	Type	Models (Total)
1	A	174	GLU	5
1	A	117	ARG	5
1	A	5	TYR	4
1	A	22	ILE	4
1	A	55	SER	4
1	A	167	LEU	4
1	A	3	GLU	4
1	A	157	VAL	4
1	A	180	ARG	4
2	B	29	LEU	4
1	A	44	GLU	4
1	A	120	THR	4
2	B	31	GLU	4
2	B	52	LYS	3
2	B	60	LYS	3
1	A	139	TYR	3
1	A	183	ILE	3
2	B	39	THR	3
2	B	14	LEU	3
2	B	27	ASP	3
2	B	61	LYS	3
1	A	116	LYS	3
1	A	52	ASN	2
1	A	131	ILE	2
1	A	188	VAL	2
2	B	28	ASP	2
1	A	23	SER	2
1	A	83	THR	2
2	B	23	GLU	2
1	A	31	ASN	2
1	A	94	GLN	2
1	A	101	ARG	2
1	A	106	PHE	2
1	A	123	THR	2
2	B	18	MET	2
1	A	156	LYS	2
1	A	185	SER	2
1	A	14	LYS	2
2	B	54	THR	2
1	A	63	GLN	2
1	A	164	HIS	2
1	A	160	ILE	1

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Mol	Chain	Res	Type	Models (Total)
2	B	8	ASP	1
2	B	20	ASN	1
2	B	24	GLU	1
2	B	37	ILE	1
1	A	88	LYS	1
1	A	166	GLN	1
1	A	13	LEU	1
1	A	38	PHE	1
2	B	45	ARG	1
1	A	35	ASN	1
1	A	92	SER	1
1	A	98	SER	1
1	A	155	LEU	1
2	B	21	GLU	1
1	A	58	SER	1
1	A	60	ARG	1
1	A	86	VAL	1
1	A	96	GLN	1
1	A	146	GLU	1
1	A	175	LEU	1
1	A	77	HIS	1
1	A	189	LEU	1
2	B	32	ILE	1
2	B	40	SER	1
1	A	25	LYS	1
1	A	153	LYS	1
1	A	133	LEU	1
2	B	53	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided