



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 14, 2020 – 11:57 am BST

PDB ID : 2KWN  
Title : Solution structure of the double PHD (plant homeodomain) fingers of human transcriptional protein DPF3b bound to a histone H4 peptide containing acetylation at Lysine 16  
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Deposited on : 2010-04-13

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

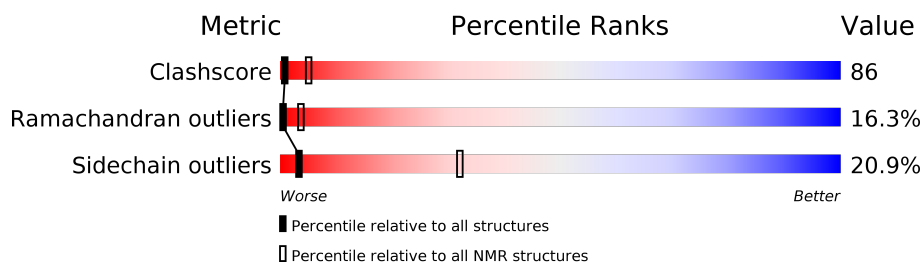
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	B	15	
2	A	114	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	B:17-B:20, A:260-A:368 (113)	0.36	11

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1949 atoms, of which 947 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Histone peptide.

Mol	Chain	Residues	Atoms					Trace
1	B	15	Total	C	H	N	O	0
			255	72	137	29	17	

- Molecule 2 is a protein called Zinc finger protein DPF3.

Mol	Chain	Residues	Atoms					Trace
2	A	114	Total	C	H	N	O	S
			1690	542	810	147	174	17
								0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	259	GLY	-	EXPRESSION TAG	UNP Q92784
A	260	SER	-	EXPRESSION TAG	UNP Q92784

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
3	A	4	Total	Zn
			4	4

## 4 Residue-property plots

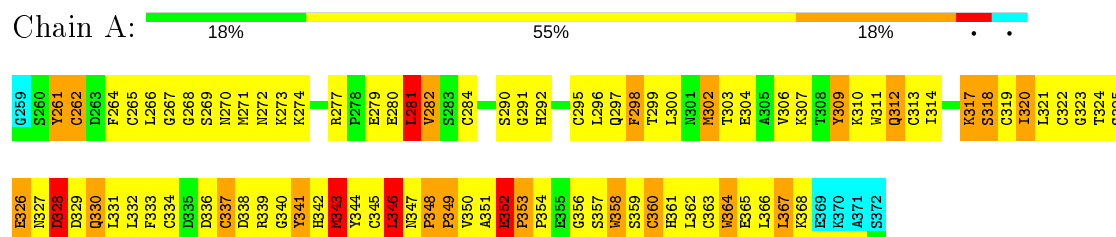
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Histone peptide



- Molecule 2: Zinc finger protein DPF3



### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

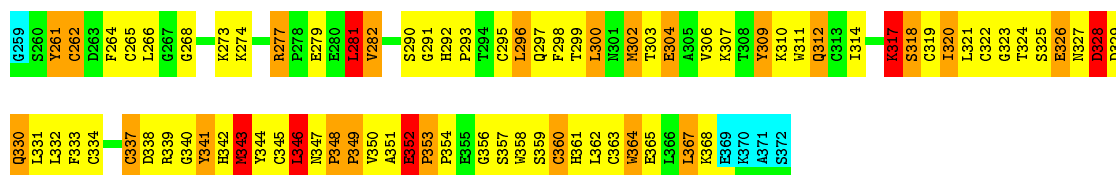
#### 4.2.1 Score per residue for model 1

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3



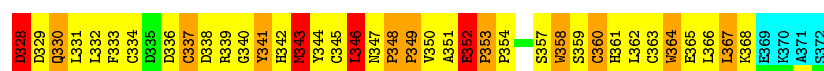
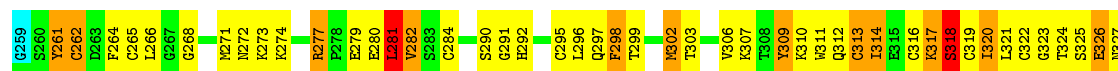


#### 4.2.2 Score per residue for model 2

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3

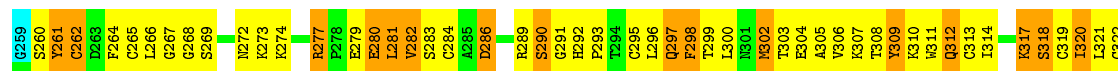
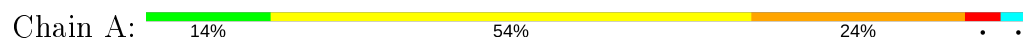


#### 4.2.3 Score per residue for model 3

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3

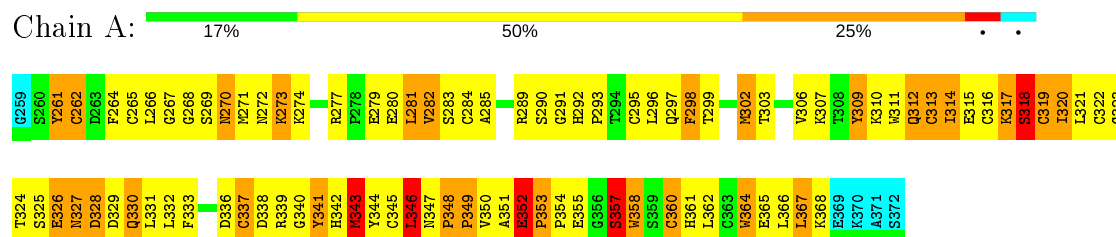


#### 4.2.4 Score per residue for model 4

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3

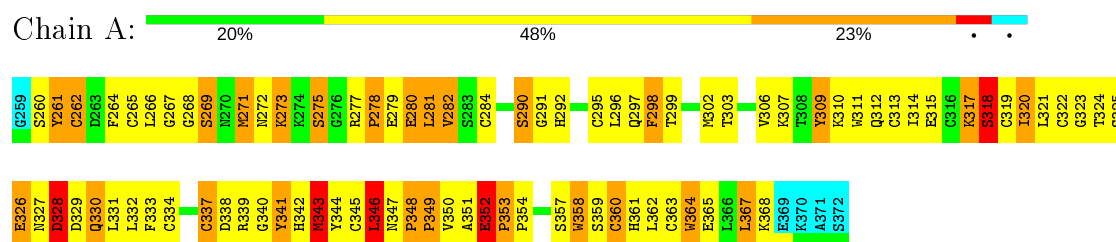


#### 4.2.5 Score per residue for model 5

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3

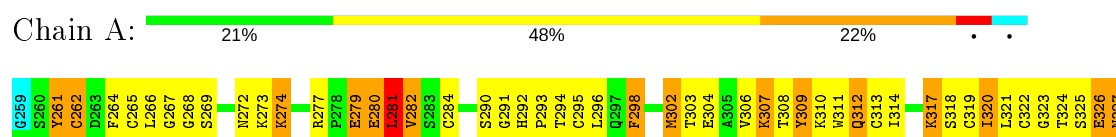


#### 4.2.6 Score per residue for model 6

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3



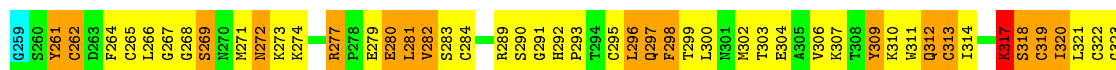
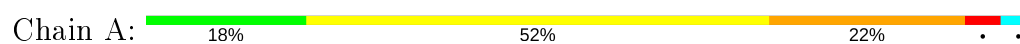


#### 4.2.7 Score per residue for model 7

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3

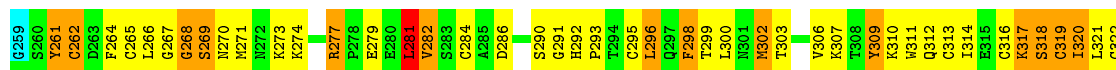
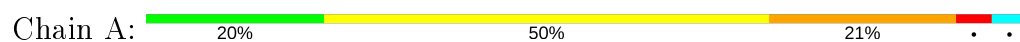


#### 4.2.8 Score per residue for model 8

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3



#### 4.2.9 Score per residue for model 9

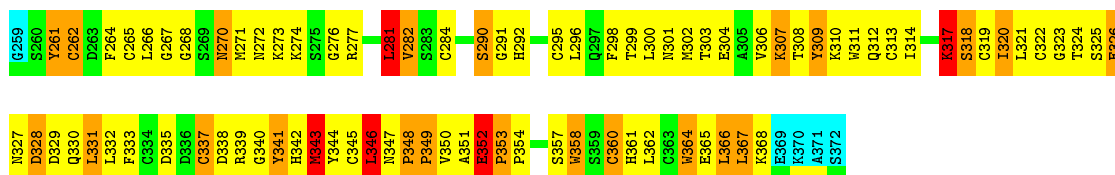
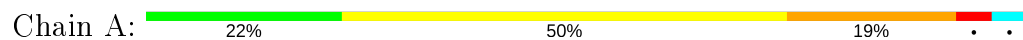
- Molecule 1: Histone peptide







- Molecule 2: Zinc finger protein DPF3

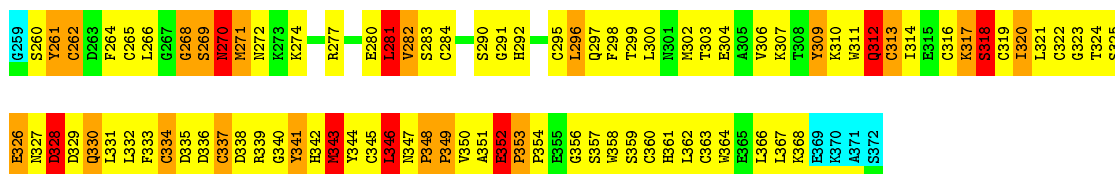
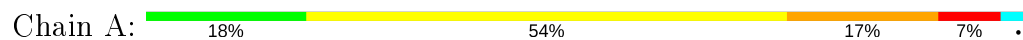


#### 4.2.10 Score per residue for model 10

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3

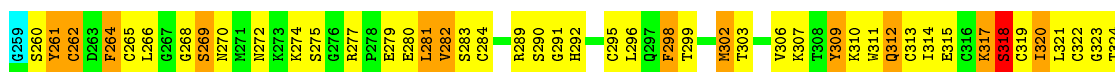


#### 4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3





#### 4.2.12 Score per residue for model 12

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3

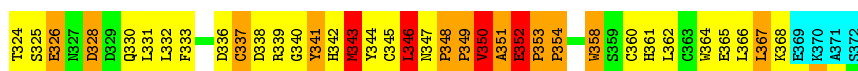
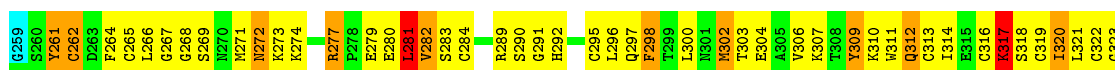


#### 4.2.13 Score per residue for model 13

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3



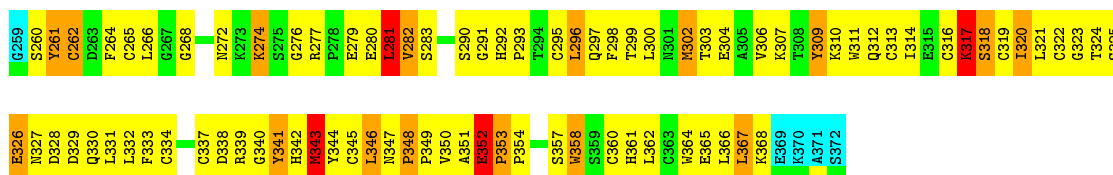
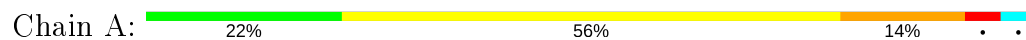
#### 4.2.14 Score per residue for model 14

- Molecule 1: Histone peptide





- Molecule 2: Zinc finger protein DPF3

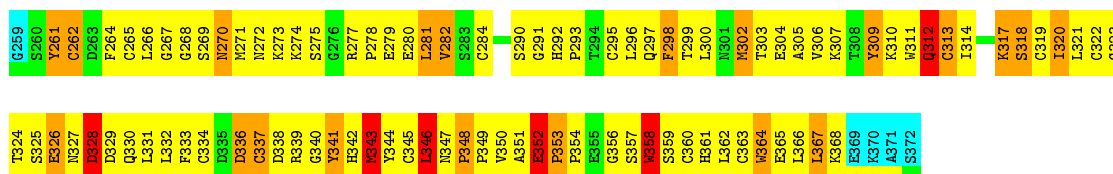
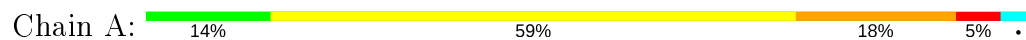


#### 4.2.15 Score per residue for model 15

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3

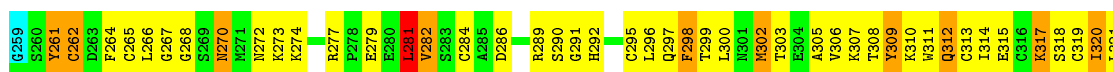
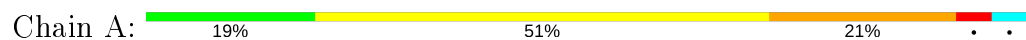


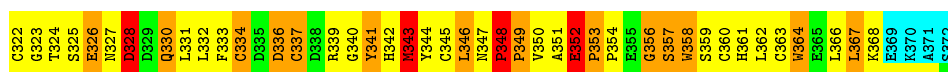
#### 4.2.16 Score per residue for model 16

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3



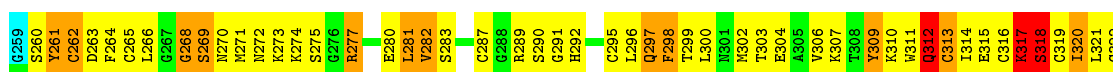
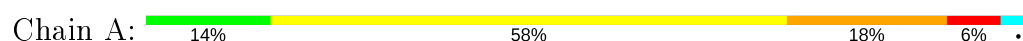


#### 4.2.17 Score per residue for model 17

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3

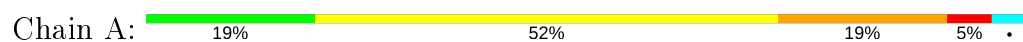


#### 4.2.18 Score per residue for model 18

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3



#### 4.2.19 Score per residue for model 19

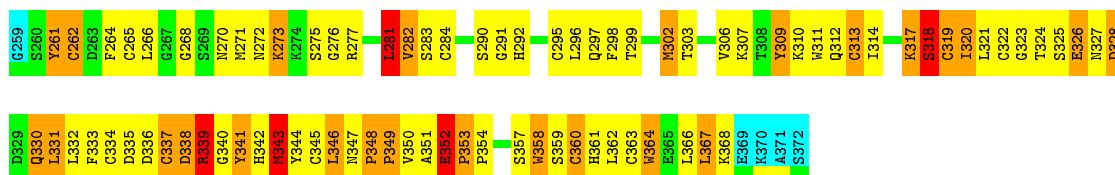
- Molecule 1: Histone peptide





- Molecule 2: Zinc finger protein DPF3

Chain A: 23% 46% 22%



#### 4.2.20 Score per residue for model 20

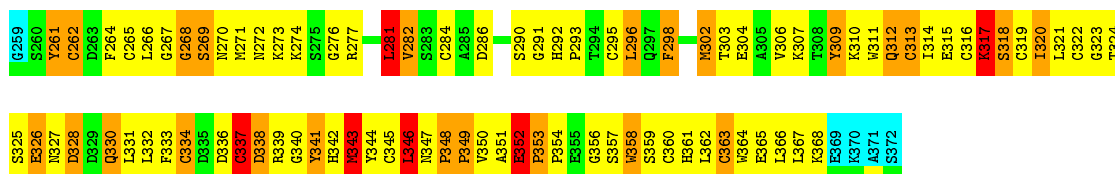
- Molecule 1: Histone peptide

Chain B: 13% 7% 7% 73%



- Molecule 2: Zinc finger protein DPF3

Chain A: 18% 51% 21% 5%



## 5 Refinement protocol and experimental data overview ⓘ

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	refinement	2.2
CNS	structure solution	1.2

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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

There are no covalent bond-length or bond-angle outliers.

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
2	A	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
2	A	339	ARG	Sidechain	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	B	41	47	46	8±2
2	A	846	776	775	145±9
All	All	17820	16460	16420	2936

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 86.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:332:LEU:HD22	2:A:354:PRO:HB2	0.98	1.34	7	19
2:A:350:VAL:HG22	2:A:351:ALA:H	0.86	1.30	13	3
2:A:343:MET:HB3	2:A:350:VAL:HG13	0.85	1.45	19	4
2:A:292:HIS:O	2:A:296:LEU:HD12	0.84	1.73	4	19
2:A:281:LEU:HB3	2:A:290:SER:HG	0.83	1.33	12	1
1:B:18:HIS:HB2	2:A:314:ILE:HB	0.81	1.51	10	3
2:A:269:SER:N	2:A:281:LEU:HD22	0.81	1.89	11	1
2:A:302:MET:SD	2:A:306:VAL:HG11	0.80	2.16	2	13
2:A:325:SER:HA	2:A:331:LEU:HD11	0.80	1.53	2	19
2:A:321:LEU:HD12	2:A:345:CYS:HB3	0.80	1.54	5	20
2:A:339:ARG:HH11	2:A:339:ARG:HG3	0.79	1.37	19	1
2:A:262:CYS:N	2:A:281:LEU:HD22	0.78	1.92	20	19
2:A:350:VAL:HG22	2:A:351:ALA:N	0.77	1.94	13	20
2:A:302:MET:O	2:A:306:VAL:HG13	0.77	1.79	3	13
2:A:314:ILE:HD12	2:A:317:LYS:CD	0.76	2.10	2	3
2:A:314:ILE:HD12	2:A:317:LYS:HG2	0.76	1.55	4	3
2:A:282:VAL:O	2:A:290:SER:HA	0.75	1.81	9	20
2:A:346:LEU:HD11	2:A:350:VAL:HG12	0.75	1.58	9	19
2:A:321:LEU:HD12	2:A:345:CYS:CB	0.75	2.12	14	20
2:A:354:PRO:HB3	2:A:358:TRP:HB2	0.75	1.58	14	19
2:A:353:PRO:HB2	2:A:354:PRO:HD3	0.75	1.59	12	20
2:A:314:ILE:HA	2:A:317:LYS:HD2	0.74	1.59	20	5
2:A:332:LEU:HD22	2:A:354:PRO:HG2	0.74	1.59	8	1
2:A:319:CYS:SG	2:A:321:LEU:HB2	0.74	2.23	20	20
2:A:343:MET:SD	2:A:343:MET:N	0.74	2.60	19	1
2:A:332:LEU:HD21	2:A:343:MET:HG3	0.73	1.61	7	19
2:A:262:CYS:SG	2:A:264:PHE:HB2	0.72	2.24	17	20
2:A:319:CYS:O	2:A:323:GLY:N	0.71	2.23	20	20
2:A:317:LYS:HD3	2:A:318:SER:N	0.71	2.01	3	5
2:A:277:ARG:HD3	2:A:277:ARG:C	0.71	2.05	3	4
1:B:20:LYS:HB3	2:A:314:ILE:HG13	0.71	1.62	1	5
2:A:342:HIS:O	2:A:345:CYS:N	0.70	2.24	13	20
2:A:303:THR:O	2:A:307:LYS:HG3	0.69	1.86	18	19
2:A:277:ARG:C	2:A:277:ARG:HD3	0.69	2.06	12	4
2:A:352:GLU:N	2:A:353:PRO:HD2	0.69	2.02	20	20
2:A:303:THR:HG22	2:A:307:LYS:HE3	0.69	1.65	13	16
2:A:314:ILE:HD12	2:A:317:LYS:HD2	0.69	1.64	1	2
2:A:291:GLY:HA3	2:A:296:LEU:HD21	0.68	1.64	17	1
2:A:293:PRO:HG2	2:A:303:THR:HG23	0.68	1.64	15	2
2:A:277:ARG:HD2	2:A:277:ARG:C	0.68	2.08	18	1
2:A:320:ILE:HG21	2:A:339:ARG:HD2	0.68	1.66	19	1
2:A:362:LEU:O	2:A:366:LEU:HB2	0.68	1.89	10	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:314:ILE:O	2:A:317:LYS:HD2	0.67	1.89	18	9
2:A:364:TRP:O	2:A:368:LYS:HG3	0.67	1.90	10	19
2:A:261:TYR:HA	2:A:281:LEU:HD21	0.67	1.67	11	1
2:A:317:LYS:HD3	2:A:318:SER:H	0.66	1.49	10	3
1:B:20:LYS:HD3	2:A:317:LYS:HE3	0.66	1.67	6	7
2:A:347:ASN:C	2:A:349:PRO:HD3	0.66	2.11	17	5
2:A:360:CYS:N	2:A:363:CYS:SG	0.66	2.68	20	1
2:A:320:ILE:HD12	2:A:339:ARG:HD2	0.66	1.66	5	18
2:A:327:ASN:O	2:A:329:ASP:N	0.66	2.29	14	16
1:B:18:HIS:HB3	2:A:314:ILE:HD13	0.66	1.67	1	15
2:A:350:VAL:HG11	2:A:354:PRO:HG2	0.65	1.68	19	13
2:A:313:CYS:O	2:A:316:CYS:SG	0.65	2.54	20	4
2:A:343:MET:HA	2:A:346:LEU:HD21	0.65	1.67	19	7
2:A:321:LEU:HD11	2:A:341:TYR:CD2	0.65	2.26	14	20
2:A:336:ASP:HB3	2:A:363:CYS:SG	0.65	2.32	16	5
2:A:332:LEU:O	2:A:340:GLY:HA2	0.65	1.92	9	20
2:A:314:ILE:HD12	2:A:317:LYS:CG	0.65	2.22	8	1
2:A:332:LEU:HD22	2:A:354:PRO:CB	0.65	2.17	7	5
2:A:306:VAL:HG12	2:A:337:CYS:O	0.65	1.92	3	3
2:A:342:HIS:HB2	2:A:345:CYS:SG	0.64	2.32	5	19
2:A:359:SER:O	2:A:360:CYS:SG	0.64	2.54	10	6
2:A:331:LEU:HA	2:A:342:HIS:HA	0.64	1.67	9	5
2:A:364:TRP:O	2:A:367:LEU:HB2	0.64	1.91	20	13
2:A:334:CYS:HB2	2:A:360:CYS:HB3	0.64	1.67	15	10
1:B:17:ARG:HG3	1:B:18:HIS:N	0.64	2.07	1	14
2:A:268:GLY:HA2	2:A:281:LEU:HD11	0.64	1.69	15	19
1:B:20:LYS:HE3	2:A:317:LYS:NZ	0.64	2.08	9	2
2:A:320:ILE:HG12	2:A:321:LEU:HD23	0.64	1.70	10	20
2:A:292:HIS:HB2	2:A:295:CYS:SG	0.63	2.34	17	20
2:A:302:MET:HE1	2:A:337:CYS:C	0.63	2.13	8	2
2:A:332:LEU:HD22	2:A:354:PRO:CG	0.63	2.22	8	1
2:A:303:THR:O	2:A:307:LYS:CG	0.63	2.46	6	11
2:A:320:ILE:HD12	2:A:339:ARG:HD3	0.63	1.71	14	1
2:A:272:ASN:N	2:A:277:ARG:O	0.63	2.30	4	7
2:A:347:ASN:O	2:A:348:PRO:C	0.63	2.36	16	1
2:A:350:VAL:HG21	2:A:354:PRO:HD3	0.63	1.71	12	20
2:A:342:HIS:O	2:A:344:TYR:N	0.63	2.31	19	20
2:A:269:SER:HB3	2:A:281:LEU:HB2	0.63	1.71	11	1
2:A:332:LEU:HD11	2:A:350:VAL:CG1	0.63	2.23	8	20
2:A:284:CYS:HB2	2:A:313:CYS:HB3	0.63	1.71	12	16
2:A:347:ASN:O	2:A:349:PRO:N	0.63	2.32	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:334:CYS:HB3	2:A:339:ARG:NH1	0.63	2.09	19	1
2:A:265:CYS:SG	2:A:274:LYS:HG2	0.62	2.34	18	3
2:A:359:SER:O	2:A:363:CYS:HB2	0.62	1.94	3	11
2:A:339:ARG:NE	2:A:362:LEU:HD12	0.62	2.09	14	1
2:A:314:ILE:HA	2:A:317:LYS:CD	0.62	2.24	14	4
2:A:281:LEU:HG	2:A:290:SER:HB3	0.62	1.71	11	1
2:A:302:MET:SD	2:A:306:VAL:CG1	0.62	2.87	2	11
2:A:346:LEU:CD1	2:A:350:VAL:HG12	0.62	2.25	16	16
2:A:330:GLN:HA	2:A:343:MET:SD	0.62	2.35	9	18
2:A:314:ILE:HA	2:A:317:LYS:HD3	0.62	1.72	8	5
2:A:280:GLU:HG2	2:A:307:LYS:HE3	0.61	1.71	6	1
2:A:261:TYR:C	2:A:290:SER:HG	0.61	1.99	3	1
2:A:319:CYS:HA	2:A:340:GLY:O	0.61	1.95	19	20
1:B:20:LYS:HE3	2:A:317:LYS:HZ2	0.61	1.53	9	1
2:A:317:LYS:HZ2	2:A:331:LEU:HB3	0.61	1.55	4	1
1:B:18:HIS:HB3	2:A:314:ILE:HB	0.61	1.71	17	1
2:A:302:MET:HE1	2:A:338:ASP:N	0.61	2.10	8	2
1:B:20:LYS:CE	2:A:317:LYS:HZ2	0.61	2.09	9	1
2:A:332:LEU:HD11	2:A:343:MET:HB3	0.61	1.72	19	1
2:A:281:LEU:HB3	2:A:290:SER:OG	0.61	1.95	5	3
2:A:272:ASN:O	2:A:274:LYS:N	0.61	2.33	4	1
1:B:20:LYS:HG3	2:A:315:GLU:HA	0.61	1.72	11	2
2:A:343:MET:HB3	2:A:350:VAL:CG1	0.60	2.25	19	3
2:A:330:GLN:O	2:A:343:MET:SD	0.60	2.59	6	19
2:A:317:LYS:HA	2:A:317:LYS:NZ	0.60	2.11	17	1
2:A:270:ASN:HD22	2:A:270:ASN:N	0.60	1.95	10	2
2:A:280:GLU:HB3	2:A:307:LYS:NZ	0.60	2.11	18	2
1:B:18:HIS:NE2	2:A:333:PHE:HB3	0.60	2.11	10	4
2:A:346:LEU:N	2:A:346:LEU:HD23	0.60	2.12	14	8
2:A:324:THR:OG1	2:A:326:GLU:HG2	0.60	1.96	12	20
2:A:314:ILE:O	2:A:317:LYS:HB2	0.60	1.97	20	6
2:A:339:ARG:NH2	2:A:360:CYS:HB3	0.60	2.12	19	1
2:A:336:ASP:CB	2:A:363:CYS:SG	0.60	2.90	16	1
2:A:322:CYS:SG	2:A:324:THR:HG22	0.60	2.37	12	1
2:A:350:VAL:CG2	2:A:351:ALA:N	0.59	2.65	13	19
2:A:317:LYS:HE2	2:A:333:PHE:HE2	0.59	1.57	16	7
2:A:314:ILE:CD1	2:A:317:LYS:HD2	0.59	2.27	1	1
2:A:265:CYS:SG	2:A:274:LYS:HG3	0.59	2.37	4	15
2:A:364:TRP:HA	2:A:367:LEU:HB2	0.59	1.74	15	20
2:A:328:ASP:HA	2:A:331:LEU:CG	0.59	2.28	10	18
2:A:332:LEU:CD2	2:A:343:MET:HG3	0.59	2.27	7	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:302:MET:HG3	2:A:303:THR:N	0.59	2.12	20	11
2:A:277:ARG:O	2:A:279:GLU:N	0.59	2.36	5	1
2:A:269:SER:CB	2:A:281:LEU:H	0.59	2.09	11	1
2:A:332:LEU:CG	2:A:343:MET:HG3	0.59	2.27	12	19
2:A:328:ASP:HA	2:A:331:LEU:HG	0.59	1.74	10	13
2:A:346:LEU:HD23	2:A:346:LEU:N	0.59	2.13	19	11
2:A:262:CYS:O	2:A:266:LEU:HD23	0.58	1.98	13	20
1:B:20:LYS:HE3	2:A:317:LYS:HZ1	0.58	1.58	19	1
2:A:302:MET:SD	2:A:337:CYS:N	0.58	2.76	9	2
2:A:279:GLU:CD	2:A:280:GLU:H	0.58	2.02	4	2
2:A:316:CYS:O	2:A:317:LYS:O	0.58	2.22	13	3
2:A:332:LEU:HG	2:A:343:MET:HG3	0.58	1.76	19	9
2:A:332:LEU:CD2	2:A:354:PRO:HG2	0.58	2.26	8	1
1:B:20:LYS:HE2	2:A:317:LYS:NZ	0.58	2.14	6	2
2:A:365:GLU:HA	2:A:368:LYS:HE3	0.58	1.75	8	2
2:A:285:ALA:HB1	2:A:310:LYS:HD3	0.58	1.75	12	2
1:B:18:HIS:HB2	2:A:314:ILE:HD13	0.57	1.76	17	1
2:A:346:LEU:CD1	2:A:346:LEU:N	0.57	2.65	11	1
2:A:324:THR:HG23	2:A:326:GLU:H	0.57	1.59	9	19
2:A:270:ASN:H	2:A:270:ASN:HD22	0.57	1.41	10	1
2:A:317:LYS:HG2	2:A:318:SER:N	0.57	2.13	2	1
2:A:332:LEU:HD21	2:A:343:MET:CG	0.57	2.29	7	18
2:A:327:ASN:C	2:A:329:ASP:H	0.57	2.03	11	3
2:A:330:GLN:HB3	2:A:343:MET:SD	0.57	2.39	19	1
2:A:302:MET:HE1	2:A:334:CYS:O	0.57	1.99	12	1
2:A:328:ASP:HA	2:A:331:LEU:HB3	0.57	1.75	9	1
2:A:357:SER:O	2:A:358:TRP:HB2	0.57	1.99	4	1
2:A:296:LEU:HG	2:A:298:PHE:CE2	0.57	2.34	17	1
2:A:346:LEU:HD13	2:A:346:LEU:H	0.57	1.59	11	1
2:A:360:CYS:O	2:A:364:TRP:CD1	0.57	2.58	18	3
2:A:327:ASN:HB2	2:A:342:HIS:CD2	0.57	2.35	14	7
2:A:317:LYS:NZ	2:A:317:LYS:HA	0.57	2.13	20	1
2:A:317:LYS:HE3	2:A:333:PHE:CD2	0.57	2.35	4	1
2:A:334:CYS:HB3	2:A:339:ARG:CZ	0.57	2.30	19	1
2:A:311:TRP:O	2:A:312:GLN:O	0.56	2.23	17	12
2:A:298:PHE:CD1	2:A:302:MET:SD	0.56	2.98	17	6
2:A:342:HIS:HB3	2:A:344:TYR:CE1	0.56	2.36	19	20
2:A:282:VAL:HG23	2:A:291:GLY:O	0.56	2.01	5	20
2:A:320:ILE:CG2	2:A:339:ARG:HB2	0.56	2.30	19	1
2:A:281:LEU:HD22	2:A:290:SER:HG	0.56	1.61	5	1
2:A:346:LEU:CD2	2:A:350:VAL:HG12	0.56	2.29	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:341:TYR:CZ	2:A:360:CYS:HB2	0.56	2.35	9	17
2:A:262:CYS:HA	2:A:291:GLY:HA2	0.56	1.76	7	16
2:A:272:ASN:HB3	2:A:277:ARG:N	0.56	2.15	5	1
2:A:302:MET:O	2:A:306:VAL:HG22	0.56	1.99	2	17
2:A:306:VAL:HG23	2:A:307:LYS:HD3	0.56	1.76	9	1
2:A:341:TYR:OH	2:A:361:HIS:CD2	0.56	2.59	14	19
2:A:317:LYS:CD	2:A:318:SER:N	0.55	2.69	11	4
2:A:354:PRO:CB	2:A:358:TRP:HB2	0.55	2.31	8	1
2:A:319:CYS:HB2	2:A:331:LEU:HD21	0.55	1.78	12	18
2:A:321:LEU:HD23	2:A:321:LEU:N	0.55	2.15	9	14
1:B:18:HIS:CB	2:A:314:ILE:HB	0.55	2.31	5	5
2:A:299:THR:HG23	2:A:302:MET:H	0.55	1.61	9	14
2:A:309:TYR:CG	2:A:310:LYS:N	0.55	2.75	5	20
2:A:317:LYS:NZ	2:A:331:LEU:CD2	0.55	2.69	9	1
2:A:334:CYS:O	2:A:338:ASP:N	0.55	2.40	3	5
1:B:19:ARG:H	2:A:314:ILE:HD13	0.55	1.61	4	3
2:A:317:LYS:NZ	2:A:331:LEU:HB3	0.55	2.15	4	1
2:A:269:SER:HB2	2:A:281:LEU:H	0.55	1.61	11	2
2:A:320:ILE:HD12	2:A:339:ARG:HH11	0.55	1.62	4	1
2:A:337:CYS:O	2:A:338:ASP:HB3	0.55	2.02	17	9
2:A:339:ARG:O	2:A:339:ARG:NH1	0.55	2.39	19	1
2:A:321:LEU:N	2:A:321:LEU:HD23	0.55	2.16	2	6
2:A:343:MET:CG	2:A:350:VAL:HG13	0.54	2.31	13	2
2:A:332:LEU:CD1	2:A:346:LEU:HD21	0.54	2.31	11	1
2:A:346:LEU:H	2:A:346:LEU:HD23	0.54	1.61	16	9
2:A:339:ARG:NE	2:A:341:TYR:HE1	0.54	2.01	19	1
2:A:272:ASN:ND2	2:A:277:ARG:HA	0.54	2.16	5	1
1:B:19:ARG:O	1:B:20:LYS:HG2	0.54	2.01	5	5
2:A:354:PRO:HB3	2:A:358:TRP:CB	0.54	2.31	16	19
2:A:272:ASN:HD22	2:A:275:SER:H	0.54	1.46	11	3
2:A:272:ASN:HB2	2:A:277:ARG:O	0.54	2.02	11	6
2:A:346:LEU:CD1	2:A:346:LEU:H	0.54	2.15	11	1
2:A:279:GLU:OE1	2:A:293:PRO:HD2	0.54	2.02	4	2
2:A:265:CYS:SG	2:A:274:LYS:CG	0.54	2.96	6	5
2:A:334:CYS:HB3	2:A:339:ARG:NH2	0.54	2.17	19	1
2:A:320:ILE:HD12	2:A:339:ARG:CD	0.54	2.32	14	16
2:A:333:PHE:CD1	2:A:333:PHE:N	0.54	2.76	18	8
2:A:317:LYS:HD2	2:A:317:LYS:N	0.54	2.18	19	3
1:B:20:LYS:H	2:A:314:ILE:HG12	0.54	1.63	19	6
2:A:317:LYS:HZ1	2:A:338:ASP:CG	0.54	2.05	13	1
1:B:20:LYS:CD	2:A:317:LYS:HE3	0.54	2.33	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:262:CYS:SG	2:A:264:PHE:N	0.54	2.79	4	20
2:A:347:ASN:C	2:A:349:PRO:CD	0.53	2.77	16	14
1:B:19:ARG:N	2:A:314:ILE:HD13	0.53	2.18	2	5
2:A:333:PHE:N	2:A:333:PHE:CD1	0.53	2.77	19	7
2:A:360:CYS:SG	2:A:362:LEU:HB2	0.53	2.44	20	11
2:A:298:PHE:CG	2:A:302:MET:SD	0.53	3.02	18	5
1:B:19:ARG:HA	2:A:333:PHE:CZ	0.53	2.39	18	9
2:A:327:ASN:C	2:A:329:ASP:N	0.53	2.62	14	10
2:A:339:ARG:CG	2:A:339:ARG:NH1	0.53	2.72	19	1
2:A:320:ILE:HG21	2:A:339:ARG:HB3	0.53	1.79	3	11
2:A:339:ARG:NE	2:A:341:TYR:CE1	0.53	2.77	19	1
1:B:20:LYS:H	2:A:314:ILE:HD11	0.53	1.63	9	2
2:A:339:ARG:HD2	2:A:362:LEU:HD11	0.52	1.81	3	12
2:A:269:SER:N	2:A:281:LEU:CD2	0.52	2.68	11	1
2:A:281:LEU:HA	2:A:291:GLY:O	0.52	2.02	17	18
2:A:272:ASN:HA	2:A:292:HIS:CE1	0.52	2.39	4	1
1:B:17:ARG:O	1:B:18:HIS:HB3	0.52	2.04	10	3
2:A:296:LEU:HD13	2:A:298:PHE:CE2	0.52	2.40	10	18
1:B:20:LYS:NZ	2:A:325:SER:HB2	0.52	2.19	11	3
1:B:20:LYS:HB3	2:A:314:ILE:CG1	0.52	2.34	4	1
2:A:291:GLY:CA	2:A:296:LEU:HD21	0.52	2.34	17	1
2:A:347:ASN:N	2:A:348:PRO:CD	0.52	2.73	10	19
2:A:332:LEU:HB3	2:A:358:TRP:CE3	0.52	2.40	20	18
2:A:317:LYS:C	2:A:317:LYS:HD3	0.52	2.25	9	1
2:A:269:SER:HB2	2:A:280:GLU:HA	0.52	1.80	7	3
2:A:302:MET:HB2	2:A:336:ASP:CA	0.52	2.34	18	2
2:A:303:THR:HG23	2:A:307:LYS:HE2	0.52	1.82	9	1
2:A:281:LEU:CB	2:A:290:SER:HB3	0.52	2.35	13	12
2:A:292:HIS:C	2:A:296:LEU:HD12	0.52	2.25	4	4
2:A:282:VAL:H	2:A:291:GLY:H	0.51	1.48	7	12
2:A:317:LYS:N	2:A:317:LYS:HD2	0.51	2.20	5	2
1:B:20:LYS:N	2:A:314:ILE:HD11	0.51	2.19	13	5
2:A:334:CYS:SG	2:A:359:SER:HA	0.51	2.45	19	8
2:A:365:GLU:HA	2:A:368:LYS:NZ	0.51	2.21	13	4
2:A:334:CYS:C	2:A:336:ASP:H	0.51	2.09	3	5
2:A:262:CYS:SG	2:A:264:PHE:CB	0.51	2.99	9	20
2:A:364:TRP:O	2:A:368:LYS:HG2	0.51	2.06	3	1
2:A:310:LYS:O	2:A:311:TRP:HB3	0.51	2.06	13	10
2:A:330:GLN:CB	2:A:343:MET:SD	0.51	2.98	19	1
2:A:361:HIS:O	2:A:365:GLU:HG2	0.51	2.05	6	9
2:A:299:THR:HG22	2:A:335:ASP:O	0.51	2.06	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:353:PRO:CB	2:A:354:PRO:HD3	0.51	2.35	19	10
2:A:341:TYR:CG	2:A:358:TRP:HH2	0.51	2.24	12	19
2:A:296:LEU:O	2:A:297:GLN:HB2	0.51	2.04	15	9
2:A:281:LEU:HB2	2:A:290:SER:HB3	0.51	1.82	6	7
2:A:317:LYS:C	2:A:317:LYS:CD	0.51	2.77	16	2
2:A:352:GLU:H	2:A:353:PRO:HD2	0.51	1.66	8	19
2:A:272:ASN:O	2:A:276:GLY:N	0.51	2.43	19	1
2:A:305:ALA:HB3	2:A:337:CYS:HA	0.51	1.82	3	4
2:A:317:LYS:HE3	2:A:333:PHE:CE2	0.51	2.41	4	1
2:A:269:SER:H	2:A:281:LEU:HD21	0.51	1.65	10	4
2:A:272:ASN:ND2	2:A:274:LYS:H	0.51	2.04	11	5
2:A:339:ARG:NH1	2:A:339:ARG:HG3	0.51	2.10	19	1
2:A:317:LYS:CD	2:A:317:LYS:C	0.50	2.79	6	1
2:A:314:ILE:HG23	2:A:315:GLU:N	0.50	2.20	16	5
2:A:261:TYR:HB2	2:A:266:LEU:C	0.50	2.27	14	19
1:B:19:ARG:H	2:A:314:ILE:HG12	0.50	1.66	12	1
2:A:352:GLU:N	2:A:353:PRO:CD	0.50	2.74	9	20
2:A:339:ARG:HD3	2:A:362:LEU:HD12	0.50	1.82	19	1
2:A:351:ALA:C	2:A:352:GLU:HG3	0.50	2.27	5	3
1:B:20:LYS:NZ	2:A:328:ASP:HB3	0.50	2.21	12	2
2:A:317:LYS:NZ	2:A:340:GLY:HA3	0.50	2.20	4	1
2:A:300:LEU:O	2:A:304:GLU:HG3	0.50	2.07	9	7
2:A:328:ASP:HB3	2:A:331:LEU:HD12	0.50	1.82	12	9
2:A:354:PRO:HB2	2:A:358:TRP:HB2	0.50	1.82	8	1
2:A:354:PRO:HB3	2:A:358:TRP:CG	0.50	2.42	20	10
2:A:298:PHE:CG	2:A:302:MET:HG2	0.50	2.41	16	9
2:A:272:ASN:CB	2:A:277:ARG:N	0.50	2.75	5	1
2:A:361:HIS:CD2	2:A:362:LEU:HD22	0.50	2.41	6	2
2:A:306:VAL:HB	2:A:311:TRP:HB2	0.50	1.83	2	16
2:A:311:TRP:O	2:A:312:GLN:C	0.50	2.49	10	2
2:A:274:LYS:NZ	2:A:295:CYS:SG	0.50	2.84	6	1
2:A:334:CYS:SG	2:A:337:CYS:N	0.50	2.84	20	2
1:B:17:ARG:HG3	1:B:18:HIS:H	0.50	1.66	12	2
2:A:296:LEU:HB3	2:A:298:PHE:CE1	0.50	2.41	17	1
2:A:303:THR:O	2:A:306:VAL:HG22	0.50	2.07	18	6
2:A:317:LYS:NZ	2:A:325:SER:HB2	0.50	2.21	9	1
2:A:282:VAL:HG13	2:A:307:LYS:NZ	0.50	2.21	9	1
2:A:269:SER:CB	2:A:280:GLU:HA	0.49	2.37	7	3
2:A:265:CYS:HB3	2:A:273:LYS:HB2	0.49	1.84	5	4
2:A:319:CYS:HB3	2:A:322:CYS:HB2	0.49	1.85	7	19
2:A:317:LYS:O	2:A:318:SER:O	0.49	2.29	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:331:LEU:HB2	2:A:342:HIS:CD2	0.49	2.43	9	1
2:A:302:MET:SD	2:A:335:ASP:C	0.49	2.91	17	2
2:A:334:CYS:SG	2:A:336:ASP:HB3	0.49	2.47	10	4
2:A:269:SER:O	2:A:270:ASN:HB3	0.49	2.07	15	1
2:A:339:ARG:NH1	2:A:362:LEU:HG	0.49	2.23	15	1
2:A:317:LYS:H	2:A:317:LYS:HD2	0.49	1.67	5	1
2:A:360:CYS:O	2:A:363:CYS:SG	0.49	2.71	20	1
2:A:364:TRP:HA	2:A:367:LEU:HD22	0.49	1.83	10	4
2:A:343:MET:O	2:A:346:LEU:HG	0.49	2.08	15	15
2:A:337:CYS:SG	2:A:339:ARG:HG3	0.49	2.48	19	4
2:A:334:CYS:O	2:A:334:CYS:SG	0.49	2.71	20	2
2:A:317:LYS:HZ2	2:A:325:SER:HB2	0.49	1.68	9	1
2:A:269:SER:N	2:A:281:LEU:HD11	0.48	2.23	7	5
2:A:270:ASN:HA	2:A:279:GLU:H	0.48	1.68	11	2
2:A:332:LEU:HD13	2:A:358:TRP:CE2	0.48	2.42	19	8
2:A:267:GLY:CA	2:A:273:LYS:HG3	0.48	2.38	5	11
2:A:281:LEU:HG	2:A:290:SER:CB	0.48	2.38	11	1
2:A:339:ARG:HD3	2:A:362:LEU:CD1	0.48	2.37	19	1
2:A:347:ASN:C	2:A:349:PRO:HD2	0.48	2.29	4	14
2:A:302:MET:HA	2:A:336:ASP:C	0.48	2.29	15	8
1:B:18:HIS:HB2	2:A:314:ILE:CB	0.48	2.33	10	3
2:A:313:CYS:SG	2:A:314:ILE:N	0.48	2.87	7	1
2:A:319:CYS:C	2:A:321:LEU:N	0.48	2.65	16	19
2:A:334:CYS:CB	2:A:360:CYS:HB3	0.48	2.36	10	3
1:B:19:ARG:HA	2:A:333:PHE:CE2	0.48	2.43	20	1
2:A:326:GLU:O	2:A:328:ASP:OD1	0.48	2.32	9	1
2:A:347:ASN:O	2:A:349:PRO:HD2	0.48	2.09	4	14
1:B:17:ARG:CG	1:B:18:HIS:N	0.48	2.77	5	3
2:A:337:CYS:O	2:A:338:ASP:CB	0.47	2.62	3	14
2:A:272:ASN:HD21	2:A:274:LYS:NZ	0.47	2.07	14	1
2:A:320:ILE:HD13	2:A:341:TYR:CE1	0.47	2.44	14	4
2:A:343:MET:HB2	2:A:350:VAL:O	0.47	2.09	19	1
2:A:339:ARG:CD	2:A:362:LEU:HD11	0.47	2.39	10	5
2:A:331:LEU:HD12	2:A:332:LEU:N	0.47	2.24	9	1
2:A:298:PHE:HB3	2:A:302:MET:HG2	0.47	1.86	4	6
2:A:260:SER:HB2	2:A:290:SER:HB3	0.47	1.86	12	1
2:A:327:ASN:O	2:A:330:GLN:N	0.47	2.47	4	1
2:A:339:ARG:HG3	2:A:362:LEU:HD12	0.47	1.84	20	4
2:A:332:LEU:HD11	2:A:350:VAL:HG11	0.47	1.86	5	1
2:A:265:CYS:CB	2:A:273:LYS:HB2	0.47	2.39	1	9
2:A:346:LEU:HD23	2:A:346:LEU:H	0.47	1.69	7	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:20:LYS:CG	2:A:315:GLU:HA	0.47	2.38	16	1
2:A:269:SER:C	2:A:271:MET:H	0.47	2.13	20	4
2:A:281:LEU:HD22	2:A:290:SER:OG	0.47	2.10	12	3
2:A:318:SER:HA	2:A:325:SER:HB2	0.47	1.87	3	2
2:A:272:ASN:HD22	2:A:273:LYS:N	0.47	2.06	7	3
2:A:320:ILE:HB	2:A:339:ARG:HH11	0.47	1.70	7	4
2:A:272:ASN:HB3	2:A:277:ARG:H	0.47	1.68	20	2
2:A:364:TRP:O	2:A:367:LEU:CB	0.47	2.63	13	11
2:A:346:LEU:H	2:A:346:LEU:CD2	0.47	2.23	14	11
2:A:353:PRO:HB2	2:A:354:PRO:CD	0.47	2.39	13	10
2:A:339:ARG:NH2	2:A:358:TRP:CZ3	0.47	2.83	19	1
1:B:19:ARG:N	2:A:314:ILE:CD1	0.47	2.77	2	6
2:A:334:CYS:SG	2:A:336:ASP:N	0.47	2.87	10	2
2:A:303:THR:CG2	2:A:307:LYS:HE3	0.47	2.39	11	14
2:A:275:SER:O	2:A:277:ARG:HG2	0.47	2.10	5	1
2:A:360:CYS:O	2:A:364:TRP:NE1	0.47	2.47	12	3
2:A:352:GLU:C	2:A:354:PRO:HD2	0.47	2.30	8	1
2:A:314:ILE:HD12	2:A:317:LYS:HB2	0.47	1.87	7	2
1:B:20:LYS:HE2	2:A:328:ASP:OD2	0.47	2.10	15	1
2:A:280:GLU:HG2	2:A:307:LYS:HD3	0.46	1.86	13	2
2:A:273:LYS:C	2:A:275:SER:H	0.46	2.13	19	1
2:A:332:LEU:HD11	2:A:343:MET:CB	0.46	2.40	19	1
2:A:359:SER:HB3	2:A:363:CYS:SG	0.46	2.49	20	1
2:A:339:ARG:NH1	2:A:339:ARG:N	0.46	2.63	19	1
2:A:283:SER:HA	2:A:289:ARG:O	0.46	2.11	4	6
1:B:17:ARG:NH1	2:A:335:ASP:HB2	0.46	2.25	9	2
1:B:18:HIS:HA	2:A:314:ILE:HB	0.46	1.87	20	3
2:A:341:TYR:HH	2:A:361:HIS:CD2	0.46	2.28	7	4
2:A:334:CYS:CB	2:A:339:ARG:NH2	0.46	2.78	19	1
2:A:314:ILE:CD1	2:A:317:LYS:HG2	0.46	2.40	13	1
2:A:277:ARG:HB3	2:A:278:PRO:HD2	0.46	1.85	5	1
1:B:20:LYS:HE2	2:A:317:LYS:HZ1	0.46	1.70	6	1
2:A:281:LEU:HB3	2:A:290:SER:CB	0.46	2.41	12	2
2:A:270:ASN:N	2:A:270:ASN:HD22	0.46	2.09	9	1
2:A:342:HIS:C	2:A:344:TYR:N	0.46	2.69	19	19
2:A:359:SER:CA	2:A:363:CYS:SG	0.46	3.04	20	1
2:A:359:SER:C	2:A:363:CYS:SG	0.46	2.94	20	1
2:A:361:HIS:CD2	2:A:362:LEU:N	0.46	2.84	14	4
1:B:17:ARG:HG3	1:B:18:HIS:ND1	0.46	2.26	7	2
2:A:319:CYS:HB3	2:A:323:GLY:H	0.46	1.70	20	11
2:A:364:TRP:CA	2:A:367:LEU:HB2	0.46	2.40	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:317:LYS:O	2:A:318:SER:C	0.46	2.54	4	2
2:A:364:TRP:CE3	2:A:368:LYS:HE3	0.46	2.46	10	9
2:A:316:CYS:O	2:A:317:LYS:C	0.46	2.54	8	2
2:A:264:PHE:N	2:A:264:PHE:CD1	0.46	2.84	11	6
2:A:343:MET:HG3	2:A:351:ALA:N	0.46	2.25	13	1
2:A:360:CYS:O	2:A:363:CYS:HB2	0.46	2.11	16	1
2:A:293:PRO:CG	2:A:303:THR:HG23	0.46	2.39	6	2
2:A:328:ASP:HB2	2:A:331:LEU:HD12	0.46	1.86	7	1
2:A:284:CYS:SG	2:A:286:ASP:HB2	0.46	2.51	3	1
2:A:341:TYR:HB2	2:A:346:LEU:CD2	0.46	2.40	2	11
2:A:280:GLU:HB3	2:A:307:LYS:HE2	0.46	1.88	11	2
2:A:317:LYS:HD3	2:A:317:LYS:C	0.46	2.31	6	2
2:A:269:SER:CA	2:A:281:LEU:HG	0.45	2.41	5	5
2:A:342:HIS:O	2:A:343:MET:C	0.45	2.55	11	17
2:A:312:GLN:O	2:A:317:LYS:NZ	0.45	2.48	13	1
2:A:272:ASN:HD21	2:A:279:GLU:HB2	0.45	1.72	3	3
1:B:20:LYS:N	2:A:314:ILE:CG1	0.45	2.79	20	1
2:A:331:LEU:HG	2:A:342:HIS:CD2	0.45	2.47	2	13
2:A:302:MET:HB2	2:A:336:ASP:HA	0.45	1.89	10	1
2:A:292:HIS:O	2:A:295:CYS:N	0.45	2.50	4	8
2:A:319:CYS:O	2:A:320:ILE:C	0.45	2.54	20	14
2:A:361:HIS:HD2	2:A:362:LEU:N	0.45	2.09	14	1
2:A:321:LEU:CD1	2:A:345:CYS:HB3	0.45	2.37	3	3
2:A:318:SER:HA	2:A:325:SER:HB3	0.45	1.87	10	8
2:A:346:LEU:CD2	2:A:346:LEU:H	0.45	2.24	6	3
2:A:269:SER:O	2:A:270:ASN:CB	0.45	2.65	15	1
2:A:268:GLY:CA	2:A:281:LEU:HD11	0.45	2.42	6	16
2:A:314:ILE:O	2:A:317:LYS:HG3	0.45	2.11	4	1
2:A:282:VAL:HG21	2:A:298:PHE:CE2	0.45	2.47	17	5
2:A:343:MET:HB3	2:A:350:VAL:O	0.45	2.12	4	8
2:A:350:VAL:CG2	2:A:351:ALA:H	0.45	2.24	5	2
2:A:302:MET:SD	2:A:337:CYS:CA	0.45	3.04	9	2
2:A:333:PHE:N	2:A:333:PHE:CD2	0.45	2.84	14	1
1:B:17:ARG:NH1	2:A:298:PHE:HA	0.45	2.26	9	3
2:A:293:PRO:HG3	2:A:303:THR:HG23	0.45	1.89	7	1
2:A:313:CYS:SG	2:A:315:GLU:HB2	0.45	2.52	4	1
2:A:261:TYR:HB2	2:A:267:GLY:N	0.45	2.27	16	7
2:A:272:ASN:CB	2:A:277:ARG:H	0.45	2.24	5	1
2:A:314:ILE:CD1	2:A:317:LYS:CD	0.45	2.95	1	1
2:A:359:SER:O	2:A:360:CYS:O	0.45	2.35	18	4
2:A:366:LEU:O	2:A:366:LEU:HD13	0.45	2.12	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:17:ARG:NH1	2:A:335:ASP:HB3	0.45	2.27	7	1
2:A:336:ASP:O	2:A:337:CYS:SG	0.45	2.75	3	2
1:B:17:ARG:HH21	2:A:297:GLN:HB3	0.45	1.71	3	1
2:A:320:ILE:HG21	2:A:341:TYR:CE1	0.44	2.47	12	15
1:B:20:LYS:HE3	2:A:328:ASP:CB	0.44	2.42	13	1
2:A:292:HIS:O	2:A:296:LEU:HD23	0.44	2.12	17	1
2:A:260:SER:HB3	2:A:290:SER:HB3	0.44	1.87	3	2
2:A:317:LYS:NZ	2:A:331:LEU:HD13	0.44	2.28	2	1
2:A:312:GLN:O	2:A:313:CYS:O	0.44	2.36	20	2
1:B:17:ARG:NH2	2:A:297:GLN:HB3	0.44	2.26	7	1
2:A:269:SER:HB3	2:A:281:LEU:HD22	0.44	1.87	11	1
2:A:296:LEU:O	2:A:297:GLN:CB	0.44	2.65	17	1
2:A:352:GLU:H	2:A:353:PRO:CD	0.44	2.25	8	11
2:A:327:ASN:O	2:A:330:GLN:HG3	0.44	2.12	10	9
2:A:314:ILE:HD12	2:A:317:LYS:HD3	0.44	1.88	14	2
2:A:261:TYR:O	2:A:290:SER:HB2	0.44	2.12	10	2
2:A:364:TRP:HE3	2:A:368:LYS:HE3	0.44	1.73	10	1
1:B:19:ARG:O	1:B:20:LYS:HB2	0.44	2.11	20	1
2:A:334:CYS:SG	2:A:336:ASP:CB	0.44	3.06	3	2
2:A:343:MET:SD	2:A:351:ALA:HA	0.44	2.52	13	1
2:A:347:ASN:HB3	2:A:348:PRO:HD3	0.44	1.89	6	8
2:A:356:GLY:O	2:A:357:SER:HB2	0.44	2.11	16	2
2:A:366:LEU:HD13	2:A:366:LEU:O	0.44	2.12	10	2
2:A:314:ILE:O	2:A:317:LYS:CG	0.44	2.66	4	1
2:A:261:TYR:CE1	2:A:266:LEU:HD22	0.44	2.48	19	16
2:A:341:TYR:CB	2:A:346:LEU:CD2	0.44	2.95	19	8
2:A:297:GLN:O	2:A:298:PHE:C	0.44	2.56	18	2
2:A:261:TYR:C	2:A:290:SER:OG	0.44	2.55	3	3
1:B:18:HIS:NE2	2:A:338:ASP:OD1	0.44	2.50	14	1
2:A:314:ILE:C	2:A:316:CYS:N	0.44	2.72	2	2
2:A:280:GLU:HB3	2:A:307:LYS:HZ2	0.44	1.72	18	1
2:A:330:GLN:NE2	2:A:344:TYR:CE1	0.44	2.86	9	1
2:A:331:LEU:CA	2:A:342:HIS:HA	0.44	2.41	9	1
2:A:296:LEU:HB3	2:A:298:PHE:CD1	0.44	2.48	17	1
2:A:293:PRO:HA	2:A:296:LEU:HD12	0.44	1.89	20	7
2:A:269:SER:H	2:A:281:LEU:CD2	0.43	2.26	8	3
2:A:260:SER:HB3	2:A:290:SER:OG	0.43	2.13	14	4
2:A:269:SER:OG	2:A:280:GLU:HA	0.43	2.12	10	3
2:A:312:GLN:O	2:A:313:CYS:C	0.43	2.53	7	2
2:A:314:ILE:O	2:A:315:GLU:C	0.43	2.56	20	1
2:A:347:ASN:CB	2:A:348:PRO:HD2	0.43	2.44	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:346:LEU:N	2:A:346:LEU:CD2	0.43	2.82	5	3
2:A:314:ILE:CD1	2:A:317:LYS:HD3	0.43	2.43	12	2
2:A:357:SER:O	2:A:358:TRP:CB	0.43	2.66	7	1
2:A:272:ASN:HB3	2:A:276:GLY:N	0.43	2.28	14	3
2:A:314:ILE:HG23	2:A:315:GLU:H	0.43	1.73	5	2
2:A:354:PRO:HA	2:A:357:SER:O	0.43	2.14	4	1
2:A:261:TYR:HB2	2:A:266:LEU:HA	0.43	1.91	20	4
2:A:356:GLY:O	2:A:357:SER:OG	0.43	2.36	6	1
2:A:268:GLY:C	2:A:281:LEU:HD21	0.43	2.34	7	1
2:A:346:LEU:HD21	2:A:350:VAL:HG12	0.43	1.91	11	1
2:A:312:GLN:HB3	2:A:316:CYS:O	0.43	2.14	4	1
1:B:18:HIS:O	1:B:19:ARG:HB3	0.43	2.13	20	2
2:A:317:LYS:HA	2:A:317:LYS:HZ2	0.43	1.72	17	1
2:A:320:ILE:HG21	2:A:339:ARG:HB2	0.43	1.90	19	1
2:A:331:LEU:HD23	2:A:342:HIS:N	0.43	2.29	13	2
2:A:304:GLU:HA	2:A:307:LYS:HD2	0.43	1.90	6	1
2:A:307:LYS:N	2:A:307:LYS:HD3	0.43	2.28	9	1
2:A:331:LEU:CB	2:A:342:HIS:CD2	0.43	3.02	9	1
2:A:300:LEU:O	2:A:304:GLU:HB3	0.43	2.13	1	1
1:B:19:ARG:H	2:A:314:ILE:CD1	0.43	2.27	1	1
2:A:272:ASN:CB	2:A:277:ARG:O	0.43	2.67	19	3
1:B:20:LYS:N	2:A:314:ILE:HG12	0.43	2.28	20	2
2:A:261:TYR:CA	2:A:281:LEU:HD21	0.43	2.43	11	1
2:A:299:THR:HG21	2:A:336:ASP:OD1	0.43	2.13	3	2
2:A:319:CYS:O	2:A:321:LEU:N	0.42	2.52	6	4
2:A:314:ILE:O	2:A:317:LYS:HD3	0.42	2.14	2	1
2:A:317:LYS:HG3	2:A:318:SER:H	0.42	1.73	15	1
2:A:302:MET:HA	2:A:336:ASP:O	0.42	2.14	10	1
2:A:346:LEU:HD12	2:A:349:PRO:HA	0.42	1.91	13	1
2:A:299:THR:HG22	2:A:302:MET:HB3	0.42	1.90	18	1
2:A:328:ASP:HA	2:A:331:LEU:HB2	0.42	1.91	20	1
2:A:272:ASN:CG	2:A:277:ARG:O	0.42	2.58	16	1
2:A:341:TYR:HB2	2:A:346:LEU:HD22	0.42	1.91	2	4
2:A:313:CYS:O	2:A:317:LYS:N	0.42	2.52	5	2
2:A:359:SER:O	2:A:364:TRP:CD1	0.42	2.72	8	1
2:A:314:ILE:C	2:A:316:CYS:H	0.42	2.17	2	2
2:A:272:ASN:ND2	2:A:279:GLU:HB2	0.42	2.29	3	1
2:A:293:PRO:HB3	2:A:303:THR:OG1	0.42	2.15	3	1
2:A:275:SER:C	2:A:277:ARG:N	0.42	2.72	5	1
2:A:346:LEU:HD22	2:A:349:PRO:HA	0.42	1.92	11	1
2:A:296:LEU:HD22	2:A:298:PHE:CZ	0.42	2.50	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:341:TYR:CE1	2:A:360:CYS:HB2	0.42	2.49	20	1
2:A:269:SER:OG	2:A:280:GLU:HG3	0.42	2.14	6	1
2:A:350:VAL:HG21	2:A:354:PRO:CD	0.42	2.44	12	2
2:A:269:SER:HA	2:A:280:GLU:HA	0.42	1.92	18	1
2:A:289:ARG:NH2	2:A:315:GLU:HG3	0.42	2.29	18	1
2:A:317:LYS:CD	2:A:318:SER:H	0.42	2.27	5	1
2:A:284:CYS:SG	2:A:312:GLN:HA	0.42	2.55	20	1
2:A:262:CYS:O	2:A:266:LEU:N	0.42	2.51	17	2
2:A:335:ASP:CG	2:A:335:ASP:O	0.42	2.59	19	1
2:A:363:CYS:O	2:A:366:LEU:HB3	0.42	2.15	10	2
2:A:269:SER:O	2:A:279:GLU:N	0.42	2.53	5	1
2:A:314:ILE:O	2:A:316:CYS:N	0.42	2.53	20	1
2:A:314:ILE:HA	2:A:317:LYS:HB3	0.41	1.92	4	3
2:A:290:SER:OG	2:A:291:GLY:N	0.41	2.53	5	1
2:A:269:SER:HA	2:A:281:LEU:HD13	0.41	1.92	11	1
2:A:268:GLY:C	2:A:270:ASN:H	0.41	2.18	4	1
1:B:17:ARG:HG2	1:B:18:HIS:CG	0.41	2.50	18	1
2:A:272:ASN:ND2	2:A:275:SER:N	0.41	2.68	17	1
1:B:18:HIS:CA	2:A:314:ILE:HB	0.41	2.45	17	1
2:A:339:ARG:CD	2:A:362:LEU:HD12	0.41	2.45	14	1
2:A:346:LEU:CD2	2:A:346:LEU:N	0.41	2.80	19	1
1:B:17:ARG:NH2	2:A:297:GLN:NE2	0.41	2.68	18	1
2:A:318:SER:O	2:A:319:CYS:C	0.41	2.57	4	1
2:A:330:GLN:O	2:A:331:LEU:C	0.41	2.59	19	1
2:A:311:TRP:O	2:A:313:CYS:N	0.41	2.54	7	1
2:A:269:SER:N	2:A:281:LEU:HG	0.41	2.31	17	1
2:A:270:ASN:ND2	2:A:270:ASN:N	0.41	2.66	10	1
2:A:346:LEU:HG	2:A:358:TRP:HZ2	0.41	1.76	11	1
1:B:20:LYS:HZ3	2:A:325:SER:HB2	0.41	1.75	11	1
2:A:351:ALA:C	2:A:352:GLU:HG2	0.41	2.36	14	1
2:A:332:LEU:N	2:A:341:TYR:O	0.41	2.53	7	4
2:A:272:ASN:HD22	2:A:275:SER:N	0.41	2.10	11	1
1:B:20:LYS:HB3	2:A:314:ILE:HG12	0.41	1.92	4	1
2:A:270:ASN:C	2:A:278:PRO:HA	0.41	2.36	15	1
2:A:337:CYS:SG	2:A:339:ARG:NH1	0.41	2.94	19	1
2:A:268:GLY:N	2:A:271:MET:O	0.41	2.54	5	1
2:A:334:CYS:C	2:A:336:ASP:N	0.41	2.74	3	1
2:A:336:ASP:O	2:A:337:CYS:HB3	0.41	2.16	13	1
2:A:321:LEU:CD2	2:A:321:LEU:N	0.41	2.84	20	2
2:A:280:GLU:O	2:A:307:LYS:NZ	0.41	2.53	18	1
1:B:17:ARG:HH12	2:A:298:PHE:HA	0.41	1.76	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:284:CYS:HB2	2:A:313:CYS:H	0.41	1.75	20	1
2:A:363:CYS:O	2:A:367:LEU:N	0.41	2.54	15	1
1:B:20:LYS:HE3	2:A:314:ILE:HD11	0.41	1.92	5	1
2:A:285:ALA:HB1	2:A:310:LYS:CD	0.41	2.46	12	1
2:A:331:LEU:HA	2:A:342:HIS:CA	0.41	2.42	9	1
2:A:336:ASP:OD2	2:A:363:CYS:SG	0.41	2.79	15	1
2:A:300:LEU:O	2:A:304:GLU:HB2	0.41	2.15	3	1
2:A:281:LEU:HG	2:A:281:LEU:H	0.40	1.49	10	2
1:B:17:ARG:HH21	2:A:297:GLN:NE2	0.40	2.15	3	1
2:A:282:VAL:N	2:A:291:GLY:O	0.40	2.54	17	1
2:A:348:PRO:N	2:A:349:PRO:CD	0.40	2.84	19	1
2:A:267:GLY:CA	2:A:273:LYS:HG2	0.40	2.46	8	1
2:A:306:VAL:CG1	2:A:311:TRP:CD1	0.40	3.05	9	1
1:B:20:LYS:HB2	2:A:314:ILE:CD1	0.40	2.46	11	1
2:A:352:GLU:HG3	2:A:353:PRO:HD2	0.40	1.93	20	1
2:A:361:HIS:O	2:A:365:GLU:HB3	0.40	2.16	20	1
2:A:296:LEU:HG	2:A:298:PHE:CZ	0.40	2.52	17	1
2:A:361:HIS:CD2	2:A:362:LEU:HG	0.40	2.50	14	1
2:A:328:ASP:CB	2:A:331:LEU:HD23	0.40	2.47	9	1
1:B:18:HIS:C	2:A:314:ILE:HG12	0.40	2.37	1	1
2:A:319:CYS:O	2:A:322:CYS:N	0.40	2.55	13	1
2:A:320:ILE:CD1	2:A:362:LEU:HD21	0.40	2.46	6	1
2:A:317:LYS:HZ1	2:A:331:LEU:CD2	0.40	2.28	9	1
2:A:320:ILE:CG2	2:A:341:TYR:CE1	0.40	3.05	9	2
2:A:343:MET:HA	2:A:346:LEU:HD11	0.40	1.92	19	1
2:A:321:LEU:HD21	2:A:341:TYR:CD2	0.40	2.51	12	1
2:A:333:PHE:CD2	2:A:333:PHE:N	0.40	2.87	20	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	B	4/15 (27%)	0±0 (6±11%)	2±1 (55±20%)	2±1 (39±18%)	0	0
2	A	109/114 (96%)	69±2 (64±2%)	23±3 (21±2%)	17±2 (16±2%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2260/2580 (88%)	1392 (62%)	499 (22%)	369 (16%)	0 4

All 37 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	A	353	PRO	20
2	A	348	PRO	20
2	A	337	CYS	20
2	A	343	MET	20
2	A	352	GLU	20
2	A	312	GLN	20
2	A	326	GLU	19
2	A	357	SER	18
2	A	346	LEU	17
2	A	328	ASP	17
2	A	298	PHE	15
2	A	349	PRO	15
2	A	281	LEU	14
2	A	360	CYS	12
1	B	20	LYS	12
2	A	358	TRP	11
2	A	317	LYS	11
2	A	318	SER	10
1	B	17	ARG	9
2	A	279	GLU	8
2	A	356	GLY	8
2	A	313	CYS	8
2	A	270	ASN	6
1	B	19	ARG	5
2	A	269	SER	5
2	A	268	GLY	5
1	B	18	HIS	5
2	A	280	GLU	4
2	A	319	CYS	4
2	A	338	ASP	3
2	A	273	LYS	2
2	A	351	ALA	1
2	A	339	ARG	1
2	A	354	PRO	1
2	A	350	VAL	1
2	A	331	LEU	1

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Mol	Chain	Res	Type	Models (Total)
2	A	278	PRO	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	B	4/9 (44%)	3±1 (86±18%)	1±1 (14±18%)	7	47
2	A	98/101 (97%)	77±2 (79±2%)	21±2 (21±2%)	3	31
All	All	2040/2200 (93%)	1613 (79%)	427 (21%)	3	32

All 62 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	A	346	LEU	20
2	A	262	CYS	20
2	A	343	MET	20
2	A	309	TYR	20
2	A	352	GLU	20
2	A	282	VAL	20
2	A	320	ILE	20
2	A	261	TYR	20
2	A	341	TYR	20
2	A	318	SER	18
2	A	281	LEU	17
2	A	317	LYS	17
2	A	328	ASP	17
2	A	330	GLN	16
2	A	367	LEU	15
2	A	302	MET	14
2	A	364	TRP	11
2	A	271	MET	10
2	A	277	ARG	9
2	A	358	TRP	7
1	B	20	LYS	7
2	A	296	LEU	7
2	A	297	GLN	6

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Mol	Chain	Res	Type	Models (Total)
2	A	308	THR	4
2	A	283	SER	4
2	A	290	SER	4
2	A	270	ASN	4
2	A	286	ASP	4
2	A	312	GLN	4
2	A	272	ASN	3
2	A	327	ASN	3
2	A	334	CYS	3
2	A	300	LEU	3
1	B	19	ARG	3
2	A	336	ASP	3
2	A	304	GLU	2
2	A	359	SER	2
2	A	274	LYS	2
2	A	269	SER	2
2	A	314	ILE	2
2	A	289	ARG	2
2	A	307	LYS	2
2	A	264	PHE	1
2	A	348	PRO	1
2	A	287	CYS	1
2	A	339	ARG	1
2	A	363	CYS	1
2	A	366	LEU	1
2	A	263	ASP	1
2	A	280	GLU	1
2	A	350	VAL	1
2	A	294	THR	1
2	A	337	CYS	1
2	A	284	CYS	1
2	A	355	GLU	1
2	A	273	LYS	1
2	A	275	SER	1
2	A	331	LEU	1
2	A	335	ASP	1
1	B	18	HIS	1
2	A	357	SER	1
2	A	313	CYS	1



### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	ALY	B	16	1	10,11,12	0.58±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	ALY	B	16	1	7,12,14	0.97±0.05	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ALY	B	16	1	-	0±0,9,10,12	-

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

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

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided