



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2025 – 03:10 PM EDT

PDB ID : 2KWO  
Title : Solution structure of the double PHD (plant homeodomain) fingers of human transcriptional protein DPF3b bound to a histone H4 peptide containing N-terminal acetylation at Serine 1  
Authors : Zeng, L.; Zhang, Q.; Li, S.; Plotnikov, A.N.; Walsh, M.J.; Zhou, M.  
Deposited on : 2010-04-14

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.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.41.4

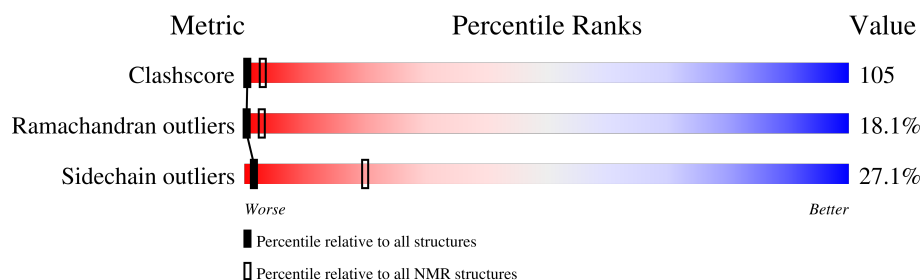
# 1 Overall quality at a glance

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	20	100%
2	A	114	11% 53% 25% 6% 6%

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:261-A:367 (107)	0.63	12

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. No single-model clusters were found.

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

### 3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1997 atoms, of which 970 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Histone peptide.

Mol	Chain	Residues	Atoms					Trace
1	B	20	Total	C	H	N	O	0
			303	84	160	36	23	

- 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).

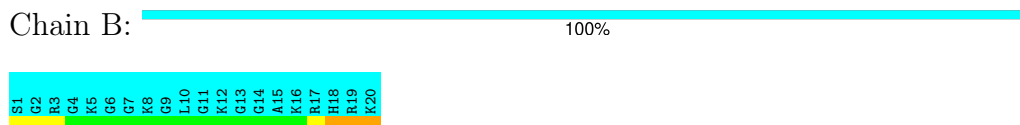
Mol	Chain	Residues	Atoms	
3	A	4	Total	Zn
			4	4

## 4 Residue-property plots

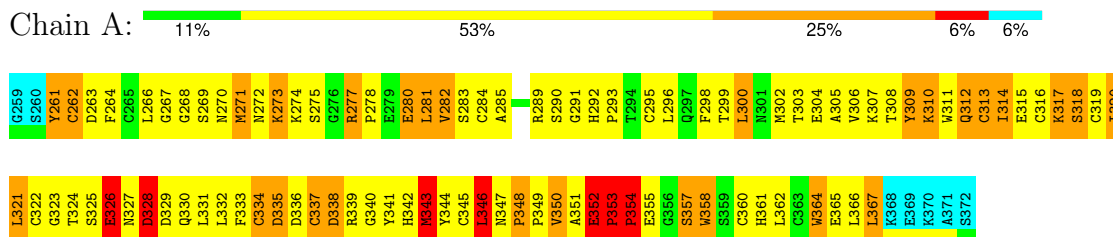
### 4.1 Average score per residue in the NMR ensemble

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



- Molecule 2: Zinc finger protein DPF3

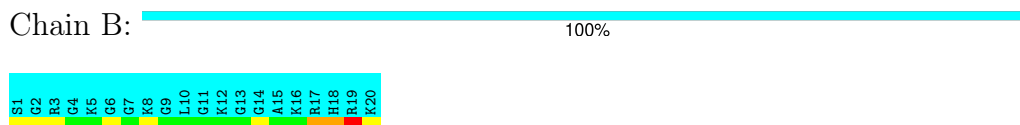


### 4.2 Scores per residue for each member of the ensemble

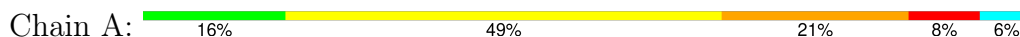
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3

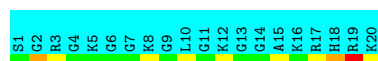




#### 4.2.2 Score per residue for model 2

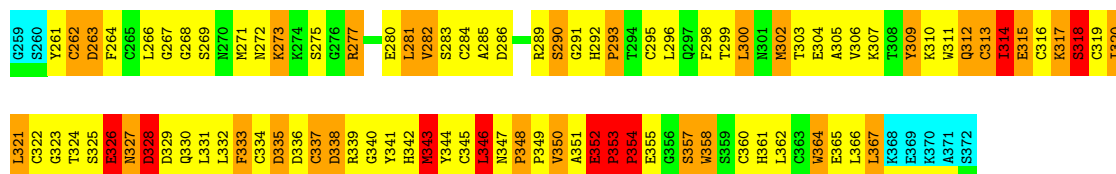
- Molecule 1: Histone peptide

Chain B: 100%



- Molecule 2: Zinc finger protein DPF3

Chain A: 13% 48% 25% 8% 6%



#### 4.2.3 Score per residue for model 3

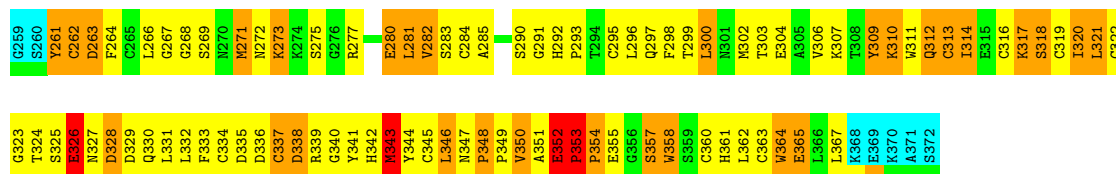
- Molecule 1: Histone peptide

Chain B: 100%



- Molecule 2: Zinc finger protein DPF3

Chain A: 16% 49% 25% 6%



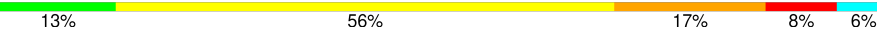
#### 4.2.4 Score per residue for model 4

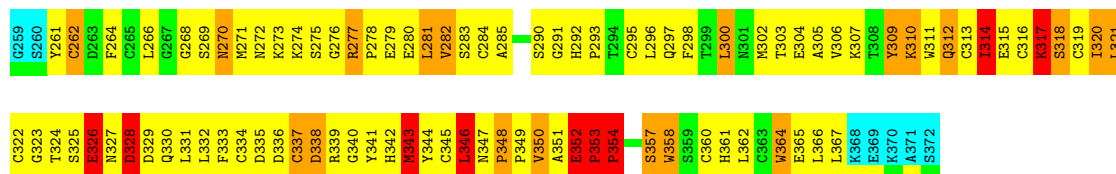
- Molecule 1: Histone peptide

Chain B:  100%



- Molecule 2: Zinc finger protein DPF3

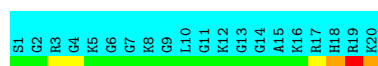
Chain A:  13% 56% 17% 8% 6%




#### 4.2.5 Score per residue for model 5

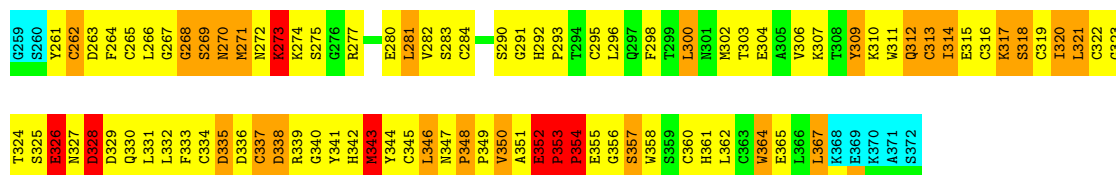
- Molecule 1: Histone peptide

Chain B:  100%



- Molecule 2: Zinc finger protein DPF3

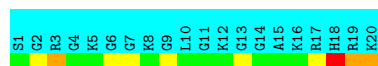
Chain A:  15% 52% 21% 6% 6%




#### 4.2.6 Score per residue for model 6

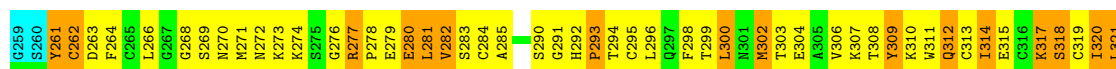
- Molecule 1: Histone peptide

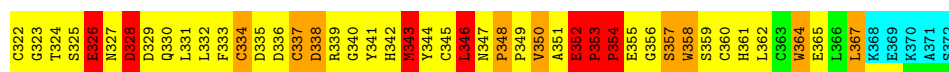
Chain B:  100%



- Molecule 2: Zinc finger protein DPF3

Chain A:  11% 54% 22% 6% 6%

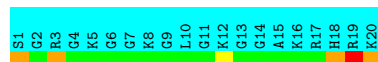




#### 4.2.7 Score per residue for model 7

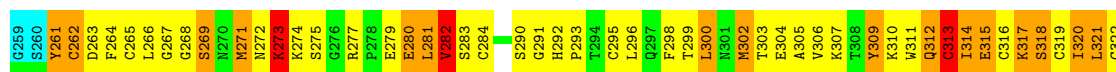
- Molecule 1: Histone peptide

Chain B:  100%



- Molecule 2: Zinc finger protein DPF3

Chain A:  12% 48% 25% 8% 6%




#### 4.2.8 Score per residue for model 8

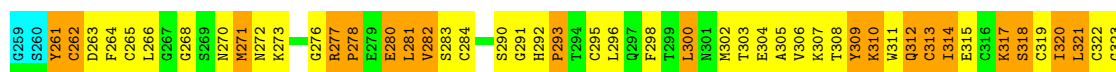
- Molecule 1: Histone peptide

Chain B:  100%



- Molecule 2: Zinc finger protein DPF3

Chain A:  15% 45% 28% 6% 6%

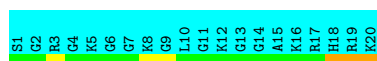


#### 4.2.9 Score per residue for model 9

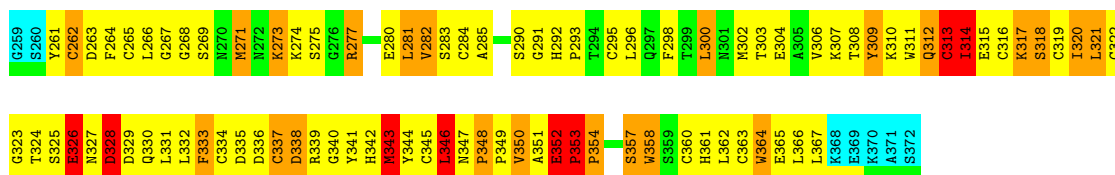
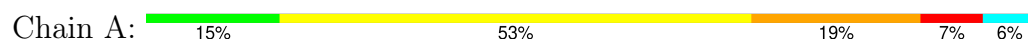
- Molecule 1: Histone peptide

Chain B:  100%





- Molecule 2: Zinc finger protein DPF3

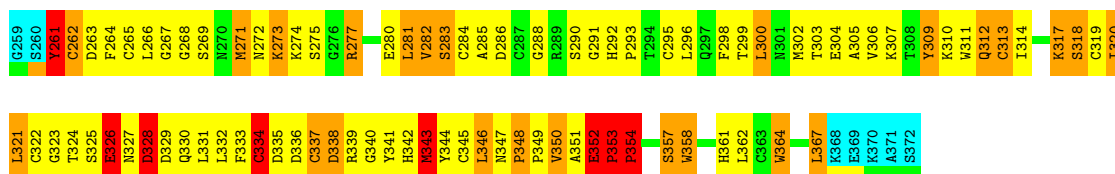
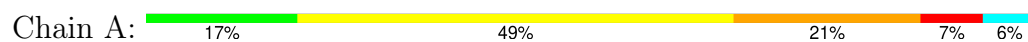


#### 4.2.10 Score per residue for model 10

- Molecule 1: Histone peptide

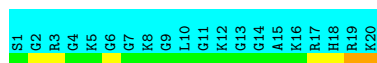


- Molecule 2: Zinc finger protein DPF3

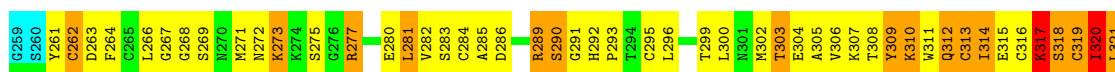
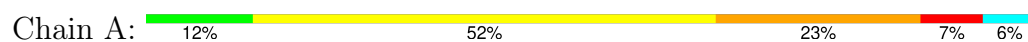


#### 4.2.11 Score per residue for model 11

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3

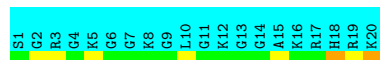




#### 4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Histone peptide

Chain B:  100%



- Molecule 2: Zinc finger protein DPF3

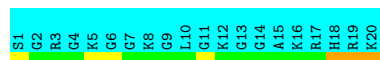
Chain A:  11% 50% 26% 6% 6%




#### 4.2.13 Score per residue for model 13

- Molecule 1: Histone peptide

Chain B:  100%



- Molecule 2: Zinc finger protein DPF3

Chain A:  12% 54% 23% 6%



#### 4.2.14 Score per residue for model 14

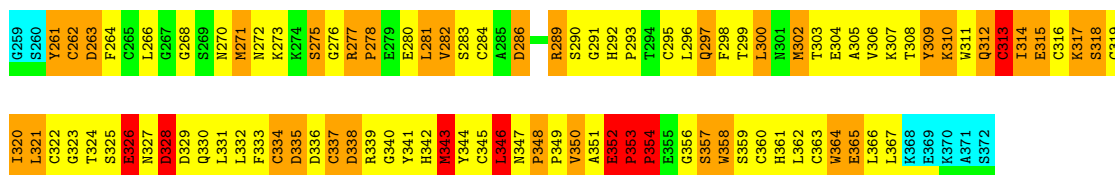
- Molecule 1: Histone peptide

Chain B:  100%



- Molecule 2: Zinc finger protein DPF3

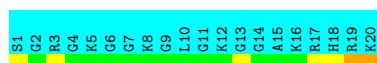
Chain A: 10% 48% 29% 7% 6%



#### 4.2.15 Score per residue for model 15

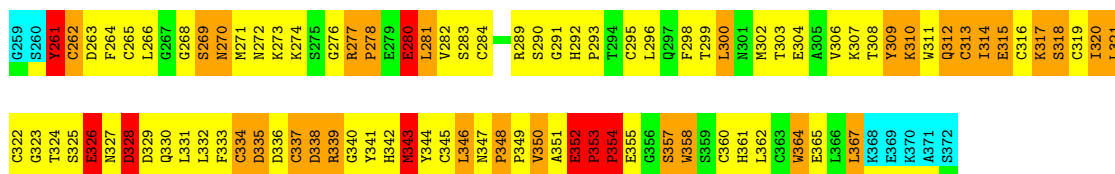
- Molecule 1: Histone peptide

Chain B: 100%



- Molecule 2: Zinc finger protein DPF3

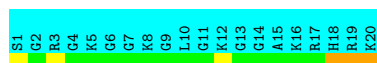
Chain A: 13% 48% 25% 7% 6%



#### 4.2.16 Score per residue for model 16

- Molecule 1: Histone peptide

Chain B: 100%



- Molecule 2: Zinc finger protein DPF3

Chain A: 11% 56% 20% 7% 6%

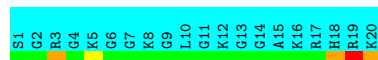




#### 4.2.17 Score per residue for model 17

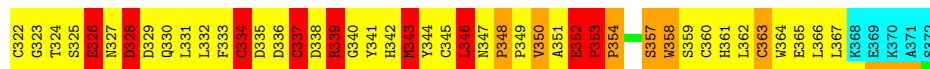
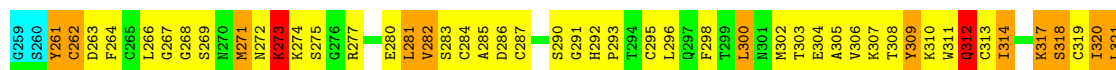
- Molecule 1: Histone peptide

Chain B: 100%



- Molecule 2: Zinc finger protein DPF3

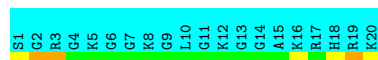
Chain A: 13% 55% 16% 10% 6%



#### 4.2.18 Score per residue for model 18

- Molecule 1: Histone peptide

Chain B: 100%



- Molecule 2: Zinc finger protein DPF3

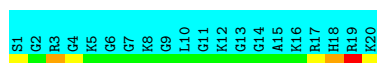
Chain A: 18% 47% 22% 7% 6%



#### 4.2.19 Score per residue for model 19

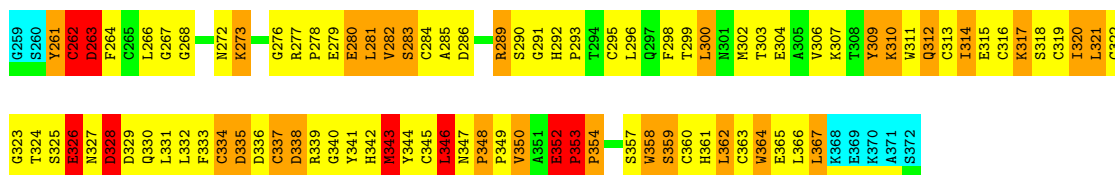
- Molecule 1: Histone peptide

Chain B: 100%



- Molecule 2: Zinc finger protein DPF3

Chain A: 14% 49% 24% 7% 6%



#### 4.2.20 Score per residue for model 20

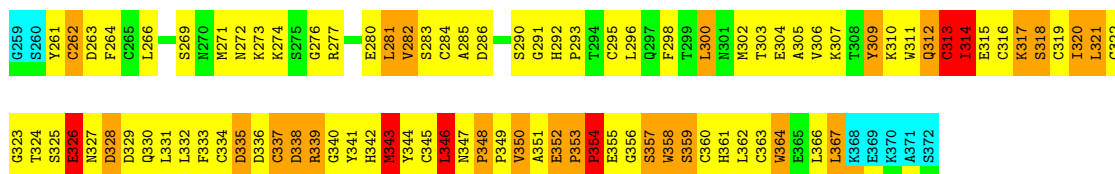
- Molecule 1: Histone peptide

Chain B: 100%



- Molecule 2: Zinc finger protein DPF3

Chain A: 14% 54% 21% 5% 6%



## 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.

## 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, SAC

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
2	A	0.58±0.02	0±0/853 ( 0.0± 0.0%)	0.78±0.02	1±0/1157 ( 0.1± 0.0%)
All	All	0.58	0/17060 ( 0.0%)	0.78	19/23140 ( 0.1%)

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
2	A	353	PRO	N-CA-CB	-6.34	95.62	102.60	13	18
2	A	354	PRO	N-CA-CB	-5.54	96.50	102.60	20	1

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	0	0	0	0±0
2	A	831	758	757	167±11
All	All	16700	15160	15140	3334

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 105.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:282:VAL:HG23	2:A:291:GLY:O	0.99	1.56	10	1
2:A:314:ILE:HD13	2:A:317:LYS:HD3	0.98	1.34	6	2
2:A:282:VAL:HG12	2:A:291:GLY:O	0.91	1.64	15	2
2:A:354:PRO:HB2	2:A:358:TRP:HB2	0.88	1.45	20	20
2:A:314:ILE:HG22	2:A:315:GLU:N	0.86	1.84	14	9
2:A:314:ILE:HD12	2:A:317:LYS:HE3	0.84	1.49	2	5
2:A:293:PRO:HG2	2:A:303:THR:HG23	0.83	1.48	10	14
2:A:352:GLU:H	2:A:353:PRO:HD2	0.82	1.34	20	20
2:A:320:ILE:HD12	2:A:339:ARG:HD3	0.82	1.50	17	8
2:A:282:VAL:HG13	2:A:291:GLY:O	0.82	1.73	11	1
2:A:352:GLU:N	2:A:353:PRO:HD2	0.82	1.89	20	20
2:A:350:VAL:HG21	2:A:354:PRO:HD2	0.82	1.51	12	19
2:A:282:VAL:HG22	2:A:291:GLY:O	0.81	1.76	3	16
2:A:303:THR:HG22	2:A:307:LYS:HE2	0.80	1.52	10	18
2:A:342:HIS:HB2	2:A:345:CYS:SG	0.79	2.18	11	20
2:A:346:LEU:H	2:A:346:LEU:HD13	0.79	1.38	9	2
2:A:364:TRP:HA	2:A:367:LEU:HB2	0.78	1.53	8	20
2:A:314:ILE:HA	2:A:317:LYS:CD	0.77	2.08	6	3
2:A:314:ILE:CG2	2:A:315:GLU:N	0.77	2.47	9	10
2:A:332:LEU:HG	2:A:343:MET:HG3	0.77	1.57	11	19
2:A:332:LEU:HD13	2:A:358:TRP:CE2	0.76	2.16	9	19
2:A:314:ILE:HD12	2:A:317:LYS:CE	0.75	2.10	10	8
2:A:325:SER:HA	2:A:331:LEU:HD11	0.75	1.57	5	20
2:A:314:ILE:O	2:A:317:LYS:HD2	0.74	1.82	20	11
2:A:346:LEU:H	2:A:346:LEU:CD1	0.74	1.96	9	2
2:A:314:ILE:HD13	2:A:317:LYS:CE	0.74	2.12	19	1
2:A:350:VAL:HG23	2:A:352:GLU:H	0.73	1.43	17	2
2:A:321:LEU:N	2:A:321:LEU:HD23	0.73	1.99	18	3
2:A:321:LEU:HD23	2:A:321:LEU:N	0.72	1.99	10	17
2:A:353:PRO:HB2	2:A:354:PRO:HD3	0.72	1.60	5	20
2:A:314:ILE:HD12	2:A:317:LYS:CD	0.72	2.14	10	1
2:A:292:HIS:HB2	2:A:295:CYS:SG	0.72	2.25	14	20
2:A:281:LEU:HD22	2:A:290:SER:HG	0.72	1.45	2	2
2:A:324:THR:HG23	2:A:326:GLU:H	0.72	1.44	20	19
2:A:317:LYS:HD3	2:A:318:SER:N	0.72	1.99	20	6
2:A:317:LYS:HD3	2:A:318:SER:H	0.71	1.45	3	10
2:A:332:LEU:HD12	2:A:346:LEU:HD21	0.71	1.60	9	2
2:A:337:CYS:SG	2:A:339:ARG:HG3	0.71	2.25	10	12
2:A:314:ILE:O	2:A:317:LYS:HB3	0.71	1.86	13	4
2:A:364:TRP:HA	2:A:367:LEU:CB	0.71	2.16	14	3
2:A:317:LYS:HG3	2:A:318:SER:N	0.71	2.00	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:341:TYR:HH	2:A:361:HIS:CG	0.71	2.04	18	2
2:A:272:ASN:N	2:A:277:ARG:O	0.70	2.24	5	10
2:A:314:ILE:HD12	2:A:317:LYS:HD3	0.70	1.62	10	1
2:A:333:PHE:N	2:A:333:PHE:CD1	0.70	2.60	15	3
2:A:314:ILE:O	2:A:316:CYS:N	0.70	2.25	7	10
2:A:317:LYS:CD	2:A:318:SER:N	0.70	2.54	4	9
2:A:334:CYS:HA	2:A:358:TRP:O	0.70	1.86	17	19
2:A:293:PRO:N	2:A:296:LEU:HD12	0.69	2.03	2	16
2:A:303:THR:O	2:A:306:VAL:HG22	0.69	1.87	11	2
2:A:314:ILE:HD13	2:A:317:LYS:CD	0.69	2.15	6	2
2:A:262:CYS:N	2:A:281:LEU:HD22	0.69	2.03	13	17
2:A:350:VAL:HB	2:A:353:PRO:HG2	0.69	1.63	20	1
2:A:317:LYS:HD2	2:A:318:SER:H	0.69	1.47	5	2
2:A:281:LEU:HD22	2:A:290:SER:OG	0.68	1.89	11	2
2:A:332:LEU:HD22	2:A:343:MET:CG	0.68	2.18	5	1
2:A:314:ILE:HA	2:A:317:LYS:HD2	0.68	1.64	19	4
2:A:272:ASN:O	2:A:274:LYS:N	0.68	2.27	1	4
2:A:314:ILE:O	2:A:317:LYS:HE3	0.68	1.89	3	6
2:A:353:PRO:HB2	2:A:354:PRO:CD	0.67	2.20	8	17
2:A:284:CYS:HB3	2:A:312:GLN:HA	0.67	1.64	17	1
2:A:332:LEU:HD13	2:A:358:TRP:CD2	0.67	2.25	7	19
2:A:284:CYS:SG	2:A:287:CYS:N	0.67	2.68	16	1
2:A:328:ASP:HA	2:A:331:LEU:HG	0.66	1.66	11	19
2:A:322:CYS:SG	2:A:324:THR:HG22	0.66	2.30	13	2
2:A:317:LYS:N	2:A:317:LYS:HD2	0.66	2.04	11	1
2:A:262:CYS:SG	2:A:264:PHE:HB2	0.66	2.30	1	20
2:A:317:LYS:HD2	2:A:317:LYS:N	0.66	2.05	9	7
2:A:302:MET:O	2:A:306:VAL:HG22	0.66	1.91	2	15
2:A:350:VAL:CG2	2:A:351:ALA:N	0.66	2.58	17	1
2:A:346:LEU:CD1	2:A:346:LEU:N	0.66	2.58	8	2
2:A:302:MET:SD	2:A:337:CYS:N	0.66	2.69	15	15
2:A:292:HIS:C	2:A:296:LEU:HD12	0.66	2.11	2	2
2:A:332:LEU:HB3	2:A:358:TRP:CZ3	0.66	2.26	8	19
2:A:298:PHE:CD2	2:A:302:MET:SD	0.66	2.89	7	1
2:A:293:PRO:CG	2:A:303:THR:HG23	0.65	2.21	15	18
2:A:333:PHE:CD1	2:A:333:PHE:N	0.65	2.63	2	16
2:A:330:GLN:O	2:A:343:MET:SD	0.65	2.54	5	20
2:A:343:MET:HB3	2:A:350:VAL:HG22	0.65	1.68	12	18
2:A:350:VAL:HG21	2:A:354:PRO:CD	0.65	2.22	5	4
2:A:283:SER:HA	2:A:290:SER:HA	0.65	1.69	16	20
2:A:332:LEU:HB3	2:A:358:TRP:CE3	0.65	2.27	11	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:343:MET:HG2	2:A:350:VAL:HG22	0.65	1.67	14	18
2:A:346:LEU:HD23	2:A:346:LEU:N	0.65	2.06	11	16
2:A:354:PRO:HG3	2:A:358:TRP:CD1	0.65	2.27	12	18
2:A:314:ILE:O	2:A:317:LYS:CD	0.64	2.44	14	13
2:A:350:VAL:HG11	2:A:354:PRO:HD3	0.64	1.68	11	1
2:A:350:VAL:HG11	2:A:353:PRO:HB2	0.64	1.69	11	1
2:A:321:LEU:HD11	2:A:341:TYR:CD2	0.64	2.27	1	19
2:A:332:LEU:HG	2:A:343:MET:CG	0.64	2.23	9	18
2:A:321:LEU:HD12	2:A:345:CYS:C	0.64	2.13	2	20
2:A:337:CYS:O	2:A:338:ASP:HB3	0.64	1.93	15	10
2:A:314:ILE:O	2:A:317:LYS:CE	0.64	2.45	5	11
2:A:354:PRO:CB	2:A:358:TRP:HB2	0.63	2.23	7	18
2:A:319:CYS:SG	2:A:321:LEU:HB2	0.63	2.33	8	20
2:A:332:LEU:O	2:A:340:GLY:HA2	0.63	1.93	1	16
2:A:317:LYS:CD	2:A:318:SER:H	0.63	2.05	7	8
2:A:341:TYR:HB3	2:A:346:LEU:CD2	0.63	2.23	11	7
2:A:269:SER:OG	2:A:281:LEU:N	0.63	2.31	3	3
2:A:320:ILE:HG22	2:A:340:GLY:O	0.63	1.94	1	20
2:A:339:ARG:NE	2:A:362:LEU:HD12	0.63	2.08	15	6
2:A:282:VAL:HG21	2:A:306:VAL:HG23	0.63	1.69	18	2
2:A:302:MET:HB2	2:A:335:ASP:O	0.63	1.93	11	18
2:A:353:PRO:CB	2:A:354:PRO:CD	0.63	2.77	12	15
2:A:298:PHE:CE2	2:A:302:MET:SD	0.63	2.92	7	1
2:A:262:CYS:O	2:A:266:LEU:HD23	0.62	1.95	13	18
2:A:353:PRO:CB	2:A:354:PRO:HD3	0.62	2.24	12	18
2:A:275:SER:HB3	2:A:277:ARG:HE	0.62	1.55	4	2
2:A:262:CYS:HA	2:A:291:GLY:HA2	0.62	1.71	19	20
2:A:321:LEU:HD12	2:A:345:CYS:CB	0.62	2.25	1	18
2:A:314:ILE:HD12	2:A:317:LYS:HE2	0.62	1.72	17	4
2:A:272:ASN:CG	2:A:277:ARG:H	0.62	1.97	13	2
2:A:334:CYS:O	2:A:338:ASP:N	0.62	2.33	17	13
2:A:346:LEU:H	2:A:346:LEU:HD23	0.62	1.55	2	2
2:A:364:TRP:HB3	2:A:367:LEU:HD12	0.61	1.72	9	1
2:A:313:CYS:O	2:A:317:LYS:HB3	0.61	1.94	12	2
2:A:319:CYS:HB3	2:A:323:GLY:H	0.61	1.54	1	17
2:A:282:VAL:CG2	2:A:296:LEU:HD11	0.61	2.25	19	16
2:A:296:LEU:HB3	2:A:298:PHE:CE1	0.61	2.30	3	18
2:A:350:VAL:HG12	2:A:351:ALA:H	0.61	1.55	11	1
2:A:339:ARG:HB2	2:A:341:TYR:OH	0.61	1.94	12	1
2:A:346:LEU:N	2:A:346:LEU:HD23	0.61	2.09	15	2
2:A:272:ASN:CB	2:A:277:ARG:N	0.61	2.63	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:284:CYS:SG	2:A:312:GLN:HA	0.61	2.35	19	11
2:A:314:ILE:O	2:A:317:LYS:N	0.61	2.32	18	10
2:A:263:ASP:HB3	2:A:289:ARG:HE	0.61	1.55	14	1
2:A:282:VAL:O	2:A:290:SER:HA	0.61	1.96	3	19
2:A:272:ASN:HB2	2:A:276:GLY:H	0.61	1.56	19	1
2:A:331:LEU:O	2:A:333:PHE:CE1	0.61	2.53	20	19
2:A:350:VAL:HG23	2:A:351:ALA:N	0.61	2.10	17	2
2:A:346:LEU:HD23	2:A:346:LEU:H	0.61	1.55	14	16
2:A:364:TRP:C	2:A:366:LEU:N	0.60	2.48	9	3
2:A:314:ILE:HG22	2:A:315:GLU:H	0.60	1.56	9	9
2:A:317:LYS:HZ3	2:A:338:ASP:C	0.60	1.99	13	2
2:A:341:TYR:O	2:A:342:HIS:C	0.60	2.38	1	20
2:A:320:ILE:HD12	2:A:339:ARG:HE	0.60	1.57	10	1
2:A:342:HIS:O	2:A:344:TYR:N	0.60	2.35	9	20
2:A:361:HIS:CD2	2:A:362:LEU:N	0.60	2.69	4	19
2:A:317:LYS:O	2:A:318:SER:O	0.60	2.19	4	9
2:A:314:ILE:HA	2:A:317:LYS:NZ	0.60	2.11	19	2
2:A:269:SER:HB2	2:A:280:GLU:HA	0.60	1.72	7	12
2:A:341:TYR:CB	2:A:346:LEU:HD12	0.60	2.27	9	2
2:A:334:CYS:SG	2:A:334:CYS:O	0.59	2.59	18	2
2:A:293:PRO:HA	2:A:296:LEU:HD12	0.59	1.74	18	16
2:A:302:MET:SD	2:A:306:VAL:HG11	0.59	2.38	7	1
2:A:321:LEU:HD12	2:A:345:CYS:HB3	0.59	1.74	1	17
2:A:272:ASN:HB3	2:A:277:ARG:N	0.59	2.12	12	6
2:A:341:TYR:HB3	2:A:346:LEU:HD12	0.59	1.73	9	2
2:A:334:CYS:H	2:A:341:TYR:HE1	0.59	1.41	12	1
2:A:293:PRO:CA	2:A:296:LEU:HD12	0.58	2.28	13	18
2:A:317:LYS:HE2	2:A:333:PHE:CE2	0.58	2.34	12	4
2:A:352:GLU:N	2:A:353:PRO:CD	0.58	2.65	20	20
2:A:284:CYS:HB2	2:A:313:CYS:HB3	0.58	1.75	15	13
2:A:320:ILE:HD12	2:A:339:ARG:NE	0.58	2.14	10	1
2:A:282:VAL:HG11	2:A:306:VAL:CG2	0.58	2.29	3	16
2:A:342:HIS:O	2:A:345:CYS:N	0.58	2.37	2	20
2:A:304:GLU:O	2:A:308:THR:HG23	0.58	1.98	13	11
2:A:346:LEU:HD22	2:A:349:PRO:HA	0.58	1.76	9	2
2:A:320:ILE:HG21	2:A:339:ARG:HB3	0.57	1.75	13	17
2:A:314:ILE:O	2:A:317:LYS:NZ	0.57	2.35	5	2
2:A:318:SER:HB2	2:A:325:SER:N	0.57	2.14	19	3
2:A:319:CYS:HB3	2:A:323:GLY:N	0.57	2.14	2	8
2:A:334:CYS:SG	2:A:359:SER:O	0.57	2.62	19	1
2:A:337:CYS:O	2:A:338:ASP:CB	0.57	2.51	11	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:282:VAL:HG13	2:A:282:VAL:O	0.57	2.00	18	2
2:A:319:CYS:HA	2:A:340:GLY:O	0.57	1.98	14	20
2:A:262:CYS:O	2:A:264:PHE:HD1	0.57	1.81	19	1
2:A:303:THR:O	2:A:307:LYS:HE2	0.57	2.00	11	2
2:A:341:TYR:CD1	2:A:341:TYR:N	0.57	2.70	12	1
2:A:284:CYS:HB3	2:A:288:GLY:CA	0.57	2.30	16	1
2:A:309:TYR:CG	2:A:310:LYS:N	0.56	2.73	16	20
2:A:341:TYR:CZ	2:A:360:CYS:HB2	0.56	2.35	16	17
2:A:331:LEU:O	2:A:333:PHE:CE2	0.56	2.58	8	1
2:A:268:GLY:HA2	2:A:281:LEU:HD11	0.56	1.77	10	19
2:A:332:LEU:HD12	2:A:346:LEU:HD11	0.56	1.75	4	17
2:A:303:THR:O	2:A:307:LYS:HE3	0.56	2.00	8	16
2:A:296:LEU:HD13	2:A:298:PHE:CE2	0.56	2.35	7	16
2:A:332:LEU:HD21	2:A:354:PRO:HG2	0.56	1.76	7	3
2:A:334:CYS:O	2:A:334:CYS:SG	0.56	2.63	17	2
2:A:341:TYR:CE1	2:A:358:TRP:HZ3	0.56	2.18	12	1
2:A:314:ILE:HD13	2:A:317:LYS:HG3	0.56	1.77	4	2
2:A:354:PRO:O	2:A:356:GLY:N	0.56	2.39	6	4
2:A:350:VAL:HG21	2:A:354:PRO:HD3	0.56	1.77	20	2
2:A:262:CYS:HA	2:A:290:SER:O	0.56	2.01	14	7
2:A:298:PHE:CG	2:A:302:MET:SD	0.56	2.99	6	4
2:A:312:GLN:HB3	2:A:316:CYS:SG	0.56	2.41	18	4
2:A:359:SER:O	2:A:360:CYS:SG	0.56	2.64	19	1
2:A:342:HIS:HB3	2:A:344:TYR:CE1	0.55	2.36	6	18
2:A:280:GLU:HG2	2:A:307:LYS:HD2	0.55	1.79	8	13
2:A:318:SER:HB3	2:A:325:SER:N	0.55	2.17	8	3
2:A:318:SER:O	2:A:319:CYS:C	0.55	2.45	11	1
2:A:330:GLN:HA	2:A:343:MET:SD	0.55	2.41	10	14
2:A:314:ILE:C	2:A:317:LYS:HD2	0.55	2.21	3	2
2:A:293:PRO:HG3	2:A:303:THR:HG23	0.55	1.78	15	4
2:A:347:ASN:N	2:A:348:PRO:CD	0.55	2.69	4	20
2:A:302:MET:SD	2:A:335:ASP:HA	0.55	2.42	14	2
2:A:272:ASN:HB3	2:A:276:GLY:C	0.55	2.21	12	4
2:A:343:MET:HE3	2:A:350:VAL:HG22	0.55	1.79	17	1
2:A:332:LEU:HG	2:A:358:TRP:CD2	0.55	2.36	5	1
2:A:343:MET:HA	2:A:346:LEU:HD21	0.55	1.78	5	13
2:A:320:ILE:HD12	2:A:339:ARG:CD	0.55	2.29	17	2
2:A:321:LEU:N	2:A:321:LEU:CD2	0.55	2.70	3	20
2:A:302:MET:HG3	2:A:306:VAL:HG13	0.55	1.78	2	2
2:A:363:CYS:O	2:A:366:LEU:HB3	0.55	2.02	17	2
2:A:285:ALA:HB3	2:A:310:LYS:HG3	0.55	1.79	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:302:MET:SD	2:A:338:ASP:N	0.55	2.80	14	6
2:A:364:TRP:HA	2:A:367:LEU:HG	0.55	1.77	9	1
2:A:282:VAL:H	2:A:291:GLY:H	0.54	1.44	1	7
2:A:315:GLU:HA	2:A:317:LYS:HZ1	0.54	1.61	15	3
2:A:298:PHE:HB3	2:A:302:MET:HG2	0.54	1.80	6	1
2:A:320:ILE:HG21	2:A:341:TYR:CE2	0.54	2.37	12	1
2:A:346:LEU:HD13	2:A:358:TRP:CZ2	0.54	2.37	12	16
2:A:352:GLU:H	2:A:353:PRO:CD	0.54	2.12	20	19
2:A:332:LEU:HD11	2:A:354:PRO:HG2	0.54	1.78	5	1
2:A:346:LEU:HG	2:A:358:TRP:CZ2	0.54	2.37	8	2
2:A:339:ARG:HD2	2:A:362:LEU:HD23	0.54	1.79	16	1
2:A:298:PHE:HZ	2:A:311:TRP:NE1	0.54	2.00	17	10
2:A:262:CYS:HA	2:A:291:GLY:CA	0.54	2.32	19	2
2:A:283:SER:HA	2:A:289:ARG:O	0.54	2.02	16	2
2:A:300:LEU:O	2:A:304:GLU:HG3	0.54	2.03	2	18
2:A:343:MET:CG	2:A:350:VAL:HG22	0.54	2.32	12	18
2:A:328:ASP:H	2:A:342:HIS:HE2	0.54	1.46	2	2
2:A:314:ILE:O	2:A:315:GLU:C	0.54	2.46	14	10
2:A:314:ILE:HD12	2:A:317:LYS:HG2	0.54	1.80	8	2
2:A:289:ARG:HG3	2:A:289:ARG:O	0.54	2.03	19	1
2:A:328:ASP:HA	2:A:331:LEU:CG	0.54	2.33	3	18
2:A:303:THR:HG22	2:A:307:LYS:CE	0.54	2.33	13	2
2:A:343:MET:HB3	2:A:350:VAL:HG13	0.54	1.80	17	1
2:A:313:CYS:O	2:A:316:CYS:SG	0.54	2.66	18	1
2:A:310:LYS:HG2	2:A:312:GLN:HG3	0.53	1.78	18	1
2:A:314:ILE:CA	2:A:317:LYS:HD2	0.53	2.33	19	3
2:A:361:HIS:CD2	2:A:362:LEU:HD22	0.53	2.39	16	2
2:A:302:MET:SD	2:A:337:CYS:C	0.53	2.87	20	6
2:A:272:ASN:O	2:A:276:GLY:N	0.53	2.42	4	2
2:A:275:SER:HB3	2:A:277:ARG:NE	0.53	2.19	11	2
2:A:327:ASN:C	2:A:329:ASP:H	0.53	2.06	16	19
2:A:330:GLN:O	2:A:331:LEU:C	0.53	2.45	5	20
2:A:282:VAL:HG21	2:A:296:LEU:CD1	0.53	2.33	19	10
2:A:272:ASN:HB2	2:A:277:ARG:N	0.53	2.18	6	2
2:A:334:CYS:HB2	2:A:360:CYS:N	0.53	2.19	8	4
2:A:303:THR:HG22	2:A:307:LYS:NZ	0.53	2.19	13	1
2:A:284:CYS:HB2	2:A:313:CYS:H	0.53	1.63	18	6
2:A:317:LYS:HD2	2:A:318:SER:N	0.53	2.18	4	2
2:A:262:CYS:O	2:A:291:GLY:HA2	0.53	2.03	19	1
2:A:312:GLN:O	2:A:316:CYS:SG	0.53	2.67	15	2
2:A:289:ARG:HH22	2:A:291:GLY:HA3	0.53	1.62	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:364:TRP:HA	2:A:367:LEU:CG	0.53	2.33	9	1
2:A:346:LEU:CD1	2:A:350:VAL:HG23	0.53	2.34	11	1
2:A:350:VAL:HG23	2:A:352:GLU:N	0.53	2.19	20	2
2:A:292:HIS:O	2:A:296:LEU:HG	0.53	2.03	10	4
2:A:282:VAL:CG2	2:A:291:GLY:O	0.52	2.57	7	13
2:A:343:MET:CB	2:A:350:VAL:HG22	0.52	2.32	12	18
2:A:364:TRP:HA	2:A:367:LEU:H	0.52	1.64	9	1
2:A:303:THR:CG2	2:A:307:LYS:HE2	0.52	2.34	18	2
2:A:314:ILE:CD1	2:A:317:LYS:HE3	0.52	2.34	5	3
2:A:283:SER:HB3	2:A:290:SER:OG	0.52	2.03	17	10
2:A:327:ASN:O	2:A:329:ASP:N	0.52	2.43	19	20
2:A:272:ASN:HB2	2:A:276:GLY:C	0.52	2.24	6	2
2:A:364:TRP:O	2:A:367:LEU:N	0.52	2.42	17	8
2:A:319:CYS:O	2:A:323:GLY:HA2	0.52	2.04	20	16
2:A:341:TYR:CD1	2:A:358:TRP:CZ3	0.52	2.98	12	1
2:A:325:SER:O	2:A:328:ASP:N	0.52	2.43	14	12
2:A:357:SER:O	2:A:358:TRP:HB3	0.52	2.04	17	16
2:A:334:CYS:SG	2:A:336:ASP:HB3	0.52	2.45	20	16
2:A:298:PHE:CE2	2:A:306:VAL:HG21	0.52	2.40	18	4
2:A:313:CYS:SG	2:A:314:ILE:N	0.52	2.82	11	3
2:A:276:GLY:O	2:A:277:ARG:HB2	0.52	2.05	8	3
2:A:306:VAL:HB	2:A:311:TRP:HB2	0.51	1.82	5	5
2:A:361:HIS:O	2:A:365:GLU:HG3	0.51	2.05	16	3
2:A:332:LEU:HD21	2:A:355:GLU:H	0.51	1.65	7	1
2:A:334:CYS:HB3	2:A:341:TYR:OH	0.51	2.05	12	1
2:A:312:GLN:HB2	2:A:317:LYS:HA	0.51	1.82	19	2
2:A:284:CYS:SG	2:A:313:CYS:N	0.51	2.83	9	3
2:A:277:ARG:HB3	2:A:278:PRO:HD2	0.51	1.80	14	5
2:A:285:ALA:HB3	2:A:310:LYS:CG	0.51	2.35	18	1
2:A:298:PHE:CZ	2:A:311:TRP:NE1	0.51	2.78	17	12
2:A:262:CYS:CA	2:A:291:GLY:HA2	0.51	2.35	19	1
2:A:341:TYR:HB2	2:A:346:LEU:CD2	0.51	2.35	19	11
2:A:339:ARG:HD3	2:A:362:LEU:HD12	0.51	1.82	14	3
2:A:269:SER:C	2:A:271:MET:H	0.51	2.08	1	3
2:A:339:ARG:CD	2:A:362:LEU:HD23	0.51	2.35	19	1
2:A:282:VAL:HG11	2:A:306:VAL:HG23	0.51	1.82	13	13
2:A:292:HIS:O	2:A:295:CYS:N	0.51	2.44	7	8
2:A:334:CYS:CB	2:A:360:CYS:HB3	0.51	2.36	19	1
2:A:361:HIS:CD2	2:A:362:LEU:HD13	0.51	2.40	19	1
2:A:268:GLY:O	2:A:270:ASN:N	0.50	2.44	1	1
2:A:322:CYS:CB	2:A:324:THR:HG22	0.50	2.36	1	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:317:LYS:HZ3	2:A:333:PHE:HE2	0.50	1.49	14	3
2:A:331:LEU:N	2:A:342:HIS:HA	0.50	2.21	16	15
2:A:285:ALA:CB	2:A:310:LYS:HD3	0.50	2.37	3	12
2:A:321:LEU:CB	2:A:345:CYS:HB3	0.50	2.37	11	20
2:A:341:TYR:CB	2:A:346:LEU:CD2	0.50	2.89	1	10
2:A:280:GLU:O	2:A:281:LEU:O	0.50	2.29	7	1
2:A:314:ILE:O	2:A:314:ILE:HD12	0.50	2.06	13	2
2:A:282:VAL:CG1	2:A:296:LEU:HD11	0.50	2.36	15	2
2:A:359:SER:O	2:A:363:CYS:HB2	0.50	2.07	19	1
2:A:302:MET:HB2	2:A:335:ASP:C	0.50	2.27	2	3
2:A:332:LEU:CG	2:A:343:MET:HG3	0.50	2.33	11	1
2:A:272:ASN:CG	2:A:277:ARG:N	0.50	2.65	13	1
2:A:282:VAL:HG21	2:A:306:VAL:CG2	0.50	2.36	18	2
2:A:272:ASN:ND2	2:A:277:ARG:HA	0.50	2.22	19	1
2:A:269:SER:N	2:A:281:LEU:HD11	0.50	2.22	13	3
2:A:311:TRP:O	2:A:312:GLN:O	0.50	2.30	18	9
2:A:322:CYS:SG	2:A:324:THR:CG2	0.50	3.00	13	2
2:A:332:LEU:CD2	2:A:354:PRO:HG2	0.50	2.37	7	1
2:A:281:LEU:HB3	2:A:290:SER:HB3	0.50	1.82	16	6
2:A:311:TRP:O	2:A:313:CYS:N	0.50	2.45	15	4
2:A:334:CYS:SG	2:A:337:CYS:N	0.50	2.85	16	3
2:A:302:MET:HA	2:A:336:ASP:C	0.50	2.27	11	11
2:A:284:CYS:CB	2:A:313:CYS:H	0.50	2.19	6	5
2:A:302:MET:SD	2:A:335:ASP:HB2	0.49	2.47	6	2
2:A:363:CYS:O	2:A:367:LEU:HB2	0.49	2.06	3	1
2:A:338:ASP:O	2:A:339:ARG:C	0.49	2.50	7	3
2:A:262:CYS:O	2:A:266:LEU:N	0.49	2.45	1	19
2:A:320:ILE:HG21	2:A:341:TYR:CE1	0.49	2.42	20	17
2:A:347:ASN:HB2	2:A:348:PRO:HD3	0.49	1.83	9	6
2:A:339:ARG:HD2	2:A:362:LEU:HD12	0.49	1.83	17	1
2:A:346:LEU:H	2:A:346:LEU:CD2	0.49	2.19	14	7
2:A:306:VAL:HG12	2:A:337:CYS:O	0.49	2.07	15	2
2:A:302:MET:O	2:A:303:THR:C	0.49	2.51	14	7
2:A:324:THR:C	2:A:326:GLU:H	0.49	2.11	2	6
2:A:321:LEU:HD21	2:A:341:TYR:CZ	0.49	2.42	11	6
2:A:302:MET:HG2	2:A:303:THR:N	0.49	2.22	6	1
2:A:271:MET:N	2:A:278:PRO:HA	0.49	2.23	14	3
2:A:280:GLU:O	2:A:307:LYS:HD3	0.49	2.07	13	2
2:A:269:SER:N	2:A:281:LEU:CD1	0.49	2.76	13	3
2:A:314:ILE:HD11	2:A:333:PHE:CD2	0.49	2.43	16	1
2:A:343:MET:CB	2:A:350:VAL:HG13	0.49	2.36	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:327:ASN:C	2:A:329:ASP:N	0.49	2.66	19	19
2:A:305:ALA:HB1	2:A:337:CYS:HB2	0.49	1.85	17	2
2:A:339:ARG:HB2	2:A:360:CYS:SG	0.49	2.48	8	3
2:A:317:LYS:O	2:A:318:SER:C	0.49	2.50	11	1
2:A:277:ARG:O	2:A:279:GLU:N	0.49	2.46	19	2
2:A:270:ASN:HD22	2:A:270:ASN:N	0.49	2.05	15	1
2:A:320:ILE:N	2:A:340:GLY:O	0.49	2.46	12	1
2:A:341:TYR:HB2	2:A:346:LEU:HD22	0.49	1.84	2	5
2:A:283:SER:CA	2:A:290:SER:HA	0.49	2.36	16	1
2:A:275:SER:O	2:A:277:ARG:HD3	0.48	2.08	14	4
2:A:317:LYS:HG2	2:A:318:SER:N	0.48	2.22	14	1
2:A:324:THR:HG21	2:A:326:GLU:HG3	0.48	1.85	5	17
2:A:289:ARG:HD2	2:A:289:ARG:O	0.48	2.08	11	2
2:A:341:TYR:HB3	2:A:346:LEU:HD22	0.48	1.84	11	6
2:A:314:ILE:HA	2:A:317:LYS:CE	0.48	2.37	6	1
2:A:269:SER:HB2	2:A:281:LEU:H	0.48	1.67	18	2
2:A:285:ALA:HB3	2:A:310:LYS:HB3	0.48	1.85	19	2
2:A:334:CYS:N	2:A:338:ASP:O	0.48	2.47	17	1
2:A:296:LEU:HD13	2:A:298:PHE:CZ	0.48	2.44	19	3
2:A:318:SER:HB2	2:A:325:SER:H	0.48	1.68	10	1
2:A:282:VAL:CG2	2:A:296:LEU:CD1	0.48	2.91	13	10
2:A:324:THR:HG23	2:A:326:GLU:N	0.48	2.24	4	16
2:A:325:SER:O	2:A:326:GLU:C	0.48	2.52	6	14
2:A:332:LEU:CD2	2:A:354:PRO:O	0.48	2.61	17	13
2:A:343:MET:O	2:A:350:VAL:N	0.48	2.47	12	19
2:A:364:TRP:CA	2:A:367:LEU:H	0.48	2.20	9	1
2:A:346:LEU:HD11	2:A:350:VAL:HG23	0.48	1.86	11	1
2:A:342:HIS:C	2:A:344:TYR:N	0.48	2.66	12	20
2:A:268:GLY:O	2:A:271:MET:O	0.48	2.31	17	2
2:A:318:SER:O	2:A:323:GLY:HA2	0.48	2.09	11	1
2:A:317:LYS:NZ	2:A:333:PHE:HE2	0.48	2.06	14	1
2:A:269:SER:C	2:A:271:MET:N	0.48	2.67	1	3
2:A:269:SER:CA	2:A:281:LEU:HG	0.48	2.39	1	1
2:A:366:LEU:O	2:A:366:LEU:HD22	0.48	2.09	14	1
2:A:339:ARG:HD2	2:A:360:CYS:SG	0.48	2.49	20	2
2:A:262:CYS:HB2	2:A:281:LEU:CD2	0.48	2.38	1	14
2:A:364:TRP:CA	2:A:367:LEU:HB2	0.48	2.36	17	2
2:A:331:LEU:HD21	2:A:342:HIS:CE1	0.47	2.44	2	4
2:A:284:CYS:SG	2:A:286:ASP:HB3	0.47	2.48	2	6
2:A:310:LYS:O	2:A:311:TRP:HB3	0.47	2.08	8	10
2:A:320:ILE:CG2	2:A:341:TYR:CE1	0.47	2.97	20	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:334:CYS:C	2:A:336:ASP:H	0.47	2.13	12	11
2:A:282:VAL:CG1	2:A:306:VAL:HG23	0.47	2.40	3	7
2:A:293:PRO:CG	2:A:307:LYS:NZ	0.47	2.77	11	1
2:A:261:TYR:HA	2:A:281:LEU:HD13	0.47	1.85	15	1
2:A:265:CYS:SG	2:A:272:ASN:ND2	0.47	2.87	5	1
2:A:284:CYS:HA	2:A:311:TRP:O	0.47	2.09	19	3
2:A:346:LEU:HB2	2:A:348:PRO:HD2	0.47	1.85	10	6
2:A:331:LEU:HD23	2:A:342:HIS:N	0.47	2.24	12	2
2:A:280:GLU:CG	2:A:307:LYS:HD2	0.47	2.39	18	1
2:A:272:ASN:HA	2:A:292:HIS:CE1	0.47	2.45	7	3
2:A:305:ALA:HB3	2:A:337:CYS:HA	0.47	1.87	10	6
2:A:306:VAL:HG11	2:A:311:TRP:CD1	0.47	2.45	14	2
2:A:314:ILE:HA	2:A:317:LYS:HZ3	0.47	1.69	19	1
2:A:347:ASN:HB3	2:A:348:PRO:HD3	0.47	1.86	6	9
2:A:311:TRP:O	2:A:311:TRP:CE3	0.47	2.68	19	1
2:A:332:LEU:HB2	2:A:341:TYR:O	0.47	2.10	5	1
2:A:263:ASP:HB3	2:A:289:ARG:NE	0.47	2.22	14	1
2:A:272:ASN:CB	2:A:277:ARG:H	0.47	2.23	19	1
2:A:315:GLU:HA	2:A:317:LYS:NZ	0.47	2.25	7	4
2:A:366:LEU:HD22	2:A:366:LEU:O	0.47	2.10	4	3
2:A:314:ILE:C	2:A:316:CYS:N	0.47	2.68	14	1
2:A:346:LEU:CD2	2:A:350:VAL:HG13	0.46	2.40	8	2
2:A:324:THR:HG23	2:A:326:GLU:HB2	0.46	1.87	13	1
2:A:346:LEU:HG	2:A:349:PRO:HA	0.46	1.87	10	14
2:A:277:ARG:N	2:A:277:ARG:HD3	0.46	2.26	12	1
2:A:289:ARG:NH1	2:A:311:TRP:CH2	0.46	2.83	14	1
2:A:314:ILE:C	2:A:317:LYS:HB3	0.46	2.30	8	3
2:A:326:GLU:HB2	2:A:342:HIS:CE1	0.46	2.45	4	11
2:A:265:CYS:SG	2:A:272:ASN:OD1	0.46	2.73	15	2
2:A:267:GLY:HA3	2:A:273:LYS:HG3	0.46	1.87	18	12
2:A:317:LYS:N	2:A:317:LYS:CD	0.46	2.78	3	1
2:A:332:LEU:HD22	2:A:343:MET:HG3	0.46	1.84	5	1
2:A:261:TYR:CD1	2:A:266:LEU:HA	0.46	2.46	15	5
2:A:316:CYS:C	2:A:318:SER:N	0.46	2.69	11	1
2:A:282:VAL:O	2:A:282:VAL:CG1	0.46	2.64	18	1
2:A:303:THR:O	2:A:307:LYS:CE	0.46	2.63	12	6
2:A:332:LEU:HD13	2:A:343:MET:CG	0.46	2.41	5	1
2:A:303:THR:HG22	2:A:307:LYS:HE3	0.46	1.86	11	1
2:A:296:LEU:O	2:A:297:GLN:OE1	0.46	2.33	14	1
2:A:289:ARG:NH2	2:A:291:GLY:HA3	0.46	2.26	14	1
2:A:313:CYS:O	2:A:317:LYS:N	0.46	2.47	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:342:HIS:C	2:A:344:TYR:H	0.46	2.13	1	20
2:A:346:LEU:CD1	2:A:350:VAL:HG13	0.46	2.40	7	4
2:A:318:SER:O	2:A:319:CYS:O	0.46	2.33	11	1
2:A:334:CYS:SG	2:A:359:SER:HA	0.46	2.51	20	1
2:A:285:ALA:CB	2:A:310:LYS:HA	0.46	2.41	18	1
2:A:364:TRP:O	2:A:365:GLU:C	0.46	2.54	14	3
2:A:299:THR:O	2:A:300:LEU:C	0.45	2.54	2	3
2:A:269:SER:OG	2:A:270:ASN:N	0.45	2.48	18	1
2:A:281:LEU:HD23	2:A:292:HIS:CD2	0.45	2.46	2	8
2:A:262:CYS:SG	2:A:264:PHE:N	0.45	2.87	9	12
2:A:315:GLU:CA	2:A:317:LYS:HZ1	0.45	2.23	15	3
2:A:272:ASN:CG	2:A:276:GLY:HA3	0.45	2.31	8	2
2:A:341:TYR:CE1	2:A:360:CYS:HB2	0.45	2.46	8	2
2:A:275:SER:C	2:A:277:ARG:HD3	0.45	2.32	12	1
2:A:360:CYS:O	2:A:364:TRP:NE1	0.45	2.50	14	2
2:A:319:CYS:C	2:A:320:ILE:HG22	0.45	2.31	11	1
2:A:289:ARG:O	2:A:289:ARG:HD3	0.45	2.11	14	1
2:A:293:PRO:HA	2:A:296:LEU:HB2	0.45	1.88	3	6
2:A:332:LEU:O	2:A:341:TYR:CD1	0.45	2.70	12	1
2:A:284:CYS:SG	2:A:286:ASP:HB2	0.45	2.51	14	1
2:A:284:CYS:HB3	2:A:288:GLY:HA3	0.45	1.88	16	1
2:A:320:ILE:HD11	2:A:362:LEU:HD21	0.45	1.87	16	1
2:A:320:ILE:CG2	2:A:340:GLY:O	0.45	2.64	12	3
2:A:302:MET:O	2:A:305:ALA:N	0.45	2.50	14	4
2:A:314:ILE:HA	2:A:317:LYS:HB2	0.45	1.88	1	2
2:A:320:ILE:CG2	2:A:341:TYR:CD1	0.45	3.00	9	10
2:A:346:LEU:CD2	2:A:346:LEU:H	0.45	2.23	10	5
2:A:314:ILE:C	2:A:317:LYS:HE3	0.45	2.32	15	2
2:A:341:TYR:CB	2:A:346:LEU:CD1	0.45	2.95	9	2
2:A:325:SER:O	2:A:328:ASP:HB3	0.45	2.12	9	1
2:A:303:THR:CG2	2:A:307:LYS:NZ	0.45	2.79	13	2
2:A:346:LEU:N	2:A:346:LEU:CD2	0.45	2.79	19	4
2:A:356:GLY:O	2:A:357:SER:HB2	0.45	2.11	8	2
2:A:320:ILE:CG2	2:A:341:TYR:CE2	0.45	3.00	12	1
2:A:300:LEU:O	2:A:303:THR:HB	0.45	2.12	2	2
2:A:319:CYS:HB2	2:A:331:LEU:HD21	0.45	1.88	12	11
2:A:279:GLU:O	2:A:280:GLU:HB2	0.45	2.11	19	2
2:A:262:CYS:HB2	2:A:281:LEU:HD23	0.45	1.88	1	2
2:A:282:VAL:CG2	2:A:306:VAL:HG23	0.45	2.41	18	1
2:A:332:LEU:HD11	2:A:350:VAL:HG11	0.45	1.89	17	1
2:A:327:ASN:N	2:A:327:ASN:HD22	0.44	2.10	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:284:CYS:C	2:A:286:ASP:H	0.44	2.16	10	2
2:A:262:CYS:C	2:A:264:PHE:N	0.44	2.71	15	2
2:A:291:GLY:O	2:A:296:LEU:HD11	0.44	2.12	10	1
2:A:317:LYS:CE	2:A:333:PHE:CE2	0.44	3.00	14	3
2:A:264:PHE:CE1	2:A:289:ARG:NH2	0.44	2.86	14	1
2:A:334:CYS:HB2	2:A:360:CYS:HB3	0.44	1.89	19	1
2:A:320:ILE:HD13	2:A:341:TYR:CE1	0.44	2.48	13	5
2:A:332:LEU:CD2	2:A:346:LEU:HD11	0.44	2.42	5	1
2:A:263:ASP:N	2:A:290:SER:O	0.44	2.49	13	1
2:A:317:LYS:CE	2:A:333:PHE:HE2	0.44	2.25	14	1
2:A:317:LYS:CG	2:A:318:SER:N	0.44	2.80	14	4
2:A:273:LYS:C	2:A:275:SER:N	0.44	2.71	7	3
2:A:364:TRP:CD1	2:A:367:LEU:HD22	0.44	2.47	19	3
2:A:350:VAL:CG1	2:A:353:PRO:HG2	0.44	2.42	11	1
2:A:262:CYS:O	2:A:264:PHE:CD1	0.44	2.67	19	1
2:A:312:GLN:O	2:A:313:CYS:C	0.44	2.56	15	6
2:A:366:LEU:HD13	2:A:366:LEU:O	0.44	2.13	8	3
2:A:333:PHE:CD2	2:A:333:PHE:N	0.44	2.85	8	1
2:A:363:CYS:O	2:A:367:LEU:HG	0.44	2.13	9	1
2:A:332:LEU:HD22	2:A:354:PRO:O	0.44	2.13	11	1
2:A:351:ALA:C	2:A:352:GLU:CG	0.44	2.86	8	17
2:A:280:GLU:HB3	2:A:307:LYS:HD3	0.44	1.89	6	2
2:A:265:CYS:SG	2:A:274:LYS:HG3	0.44	2.52	9	2
2:A:317:LYS:NZ	2:A:338:ASP:OD2	0.44	2.50	10	1
2:A:262:CYS:C	2:A:264:PHE:H	0.44	2.15	15	4
2:A:347:ASN:C	2:A:349:PRO:CD	0.43	2.86	5	18
2:A:330:GLN:O	2:A:343:MET:HG3	0.43	2.13	7	4
2:A:343:MET:HG2	2:A:350:VAL:HB	0.43	1.89	11	1
2:A:284:CYS:HA	2:A:312:GLN:HA	0.43	1.90	6	1
2:A:283:SER:OG	2:A:288:GLY:C	0.43	2.57	13	2
2:A:272:ASN:C	2:A:272:ASN:HD22	0.43	2.15	12	1
2:A:341:TYR:CD1	2:A:358:TRP:HZ3	0.43	2.31	12	1
2:A:325:SER:O	2:A:328:ASP:OD1	0.43	2.36	13	2
2:A:289:ARG:HH12	2:A:291:GLY:HA3	0.43	1.74	14	1
2:A:262:CYS:SG	2:A:262:CYS:O	0.43	2.76	19	1
2:A:282:VAL:C	2:A:290:SER:HA	0.43	2.34	16	1
2:A:339:ARG:NH1	2:A:362:LEU:HB2	0.43	2.28	1	1
2:A:273:LYS:O	2:A:274:LYS:HB2	0.43	2.14	6	5
2:A:322:CYS:HB3	2:A:324:THR:HG22	0.43	1.91	4	5
2:A:320:ILE:O	2:A:320:ILE:HG13	0.43	2.14	8	3
2:A:328:ASP:HB3	2:A:331:LEU:HD12	0.43	1.90	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:284:CYS:HB3	2:A:288:GLY:N	0.43	2.28	16	1
2:A:267:GLY:CA	2:A:273:LYS:HG3	0.43	2.43	9	4
2:A:306:VAL:CG1	2:A:311:TRP:CD1	0.43	3.02	12	4
2:A:262:CYS:SG	2:A:265:CYS:N	0.43	2.92	7	2
2:A:314:ILE:CD1	2:A:317:LYS:HG2	0.43	2.42	8	2
2:A:332:LEU:HD21	2:A:354:PRO:O	0.43	2.14	17	1
2:A:303:THR:O	2:A:307:LYS:HB2	0.43	2.14	13	1
2:A:351:ALA:O	2:A:352:GLU:HB3	0.43	2.13	20	1
2:A:270:ASN:HD22	2:A:270:ASN:H	0.43	1.57	15	1
2:A:261:TYR:CE1	2:A:266:LEU:HD22	0.43	2.48	1	5
2:A:262:CYS:O	2:A:264:PHE:N	0.43	2.52	2	1
2:A:261:TYR:C	2:A:290:SER:HB2	0.43	2.33	15	2
2:A:264:PHE:N	2:A:264:PHE:CD1	0.43	2.87	7	1
2:A:331:LEU:HA	2:A:342:HIS:HA	0.43	1.91	19	3
2:A:302:MET:SD	2:A:335:ASP:CB	0.43	3.06	13	1
2:A:269:SER:CB	2:A:281:LEU:H	0.43	2.27	18	1
2:A:314:ILE:HD13	2:A:317:LYS:HE2	0.43	1.90	19	1
2:A:282:VAL:HG11	2:A:296:LEU:CD1	0.43	2.44	15	2
2:A:327:ASN:ND2	2:A:344:TYR:OH	0.42	2.52	12	6
2:A:269:SER:O	2:A:270:ASN:ND2	0.42	2.52	5	1
2:A:317:LYS:NZ	2:A:331:LEU:CD1	0.42	2.82	20	1
2:A:269:SER:H	2:A:281:LEU:CG	0.42	2.27	1	1
2:A:330:GLN:O	2:A:343:MET:CG	0.42	2.67	15	8
2:A:272:ASN:ND2	2:A:292:HIS:ND1	0.42	2.67	11	1
2:A:317:LYS:NZ	2:A:333:PHE:CE2	0.42	2.86	14	1
2:A:272:ASN:HD22	2:A:275:SER:H	0.42	1.56	3	1
2:A:316:CYS:O	2:A:317:LYS:C	0.42	2.58	3	2
2:A:317:LYS:HZ3	2:A:331:LEU:HD12	0.42	1.74	4	2
2:A:346:LEU:HG	2:A:358:TRP:HZ2	0.42	1.74	8	1
2:A:362:LEU:HD22	2:A:362:LEU:N	0.42	2.30	16	1
2:A:364:TRP:C	2:A:367:LEU:H	0.42	2.18	9	1
2:A:292:HIS:O	2:A:294:THR:N	0.42	2.53	6	1
2:A:314:ILE:HD12	2:A:317:LYS:CB	0.42	2.44	13	1
2:A:359:SER:HB2	2:A:363:CYS:SG	0.42	2.55	20	1
2:A:262:CYS:SG	2:A:264:PHE:CB	0.42	3.06	1	3
2:A:320:ILE:HG23	2:A:321:LEU:HD23	0.42	1.91	3	5
2:A:332:LEU:HD22	2:A:343:MET:HG2	0.42	1.87	5	1
2:A:335:ASP:OD2	2:A:357:SER:HA	0.42	2.14	7	1
2:A:351:ALA:O	2:A:352:GLU:CD	0.42	2.58	11	1
2:A:273:LYS:O	2:A:274:LYS:CB	0.42	2.67	13	1
2:A:271:MET:SD	2:A:278:PRO:HD3	0.42	2.54	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:291:GLY:HA3	2:A:296:LEU:HD21	0.42	1.92	11	1
2:A:312:GLN:O	2:A:313:CYS:SG	0.42	2.77	12	1
2:A:331:LEU:HG	2:A:342:HIS:CD2	0.42	2.49	13	1
2:A:285:ALA:HB1	2:A:310:LYS:HD3	0.42	1.92	19	1
2:A:296:LEU:O	2:A:297:GLN:HB2	0.42	2.15	3	2
2:A:339:ARG:CD	2:A:362:LEU:HD12	0.42	2.45	3	2
2:A:317:LYS:HZ1	2:A:338:ASP:CG	0.42	2.18	10	1
2:A:316:CYS:O	2:A:318:SER:N	0.42	2.52	11	1
2:A:334:CYS:O	2:A:338:ASP:CA	0.42	2.68	18	1
2:A:346:LEU:CD2	2:A:346:LEU:N	0.41	2.79	3	1
2:A:284:CYS:HB2	2:A:313:CYS:N	0.41	2.30	16	1
2:A:350:VAL:CG2	2:A:353:PRO:HB2	0.41	2.45	17	1
2:A:262:CYS:N	2:A:281:LEU:CD2	0.41	2.81	13	2
2:A:302:MET:CG	2:A:303:THR:N	0.41	2.83	6	1
2:A:281:LEU:O	2:A:282:VAL:HG13	0.41	2.14	7	1
2:A:311:TRP:CZ2	2:A:313:CYS:HA	0.41	2.50	14	2
2:A:269:SER:HB2	2:A:281:LEU:N	0.41	2.30	15	1
2:A:341:TYR:OH	2:A:361:HIS:CG	0.41	2.74	8	1
2:A:319:CYS:SG	2:A:341:TYR:HA	0.41	2.56	12	1
2:A:350:VAL:CG2	2:A:352:GLU:H	0.41	2.20	17	1
2:A:300:LEU:O	2:A:301:ASN:C	0.41	2.58	12	2
2:A:318:SER:HB3	2:A:325:SER:HB3	0.41	1.93	13	1
2:A:272:ASN:CB	2:A:277:ARG:O	0.41	2.69	15	2
2:A:317:LYS:NZ	2:A:331:LEU:HD12	0.41	2.31	20	1
2:A:337:CYS:SG	2:A:339:ARG:NH1	0.41	2.93	1	1
2:A:314:ILE:HA	2:A:317:LYS:HB3	0.41	1.91	5	1
2:A:310:LYS:CG	2:A:312:GLN:HG3	0.41	2.45	18	1
2:A:270:ASN:C	2:A:278:PRO:HA	0.41	2.36	14	3
2:A:314:ILE:C	2:A:317:LYS:NZ	0.41	2.74	5	1
2:A:282:VAL:HG11	2:A:293:PRO:HG3	0.41	1.93	11	1
2:A:314:ILE:C	2:A:317:LYS:CE	0.41	2.89	15	1
2:A:312:GLN:O	2:A:313:CYS:O	0.41	2.38	15	3
2:A:339:ARG:O	2:A:341:TYR:CE1	0.41	2.74	12	1
2:A:302:MET:SD	2:A:338:ASP:HB2	0.41	2.56	2	1
2:A:306:VAL:CB	2:A:311:TRP:HB2	0.41	2.46	2	1
2:A:325:SER:O	2:A:328:ASP:OD2	0.41	2.39	18	2
2:A:310:LYS:C	2:A:312:GLN:H	0.41	2.19	18	2
2:A:364:TRP:O	2:A:367:LEU:CB	0.41	2.69	17	1
2:A:299:THR:O	2:A:303:THR:OG1	0.41	2.33	18	1
2:A:314:ILE:CD1	2:A:317:LYS:HD3	0.41	2.42	19	1
2:A:337:CYS:SG	2:A:339:ARG:NE	0.41	2.94	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:330:GLN:HG3	2:A:344:TYR:CE1	0.41	2.51	7	1
2:A:275:SER:HB3	2:A:277:ARG:HH11	0.41	1.75	9	1
2:A:262:CYS:CB	2:A:281:LEU:CD2	0.40	2.99	1	1
2:A:277:ARG:N	2:A:277:ARG:CD	0.40	2.84	13	1
2:A:356:GLY:O	2:A:357:SER:O	0.40	2.39	16	1
2:A:359:SER:OG	2:A:360:CYS:N	0.40	2.54	6	1
2:A:289:ARG:NH1	2:A:289:ARG:HB3	0.40	2.31	12	1
2:A:324:THR:C	2:A:326:GLU:N	0.40	2.75	13	1
2:A:277:ARG:HB3	2:A:278:PRO:CD	0.40	2.46	14	1
2:A:341:TYR:OH	2:A:361:HIS:ND1	0.40	2.54	16	1
2:A:352:GLU:CG	2:A:353:PRO:CD	0.40	2.99	20	1
2:A:272:ASN:HD22	2:A:275:SER:N	0.40	2.15	3	1
2:A:273:LYS:C	2:A:275:SER:H	0.40	2.19	4	1
2:A:354:PRO:CG	2:A:358:TRP:CD1	0.40	3.04	9	1
2:A:272:ASN:H	2:A:277:ARG:C	0.40	2.18	15	1
2:A:343:MET:HG2	2:A:350:VAL:CG2	0.40	2.44	14	1
2:A:311:TRP:O	2:A:312:GLN:C	0.40	2.59	15	1
2:A:262:CYS:H	2:A:281:LEU:CD2	0.40	2.30	1	1
2:A:281:LEU:HA	2:A:291:GLY:O	0.40	2.17	1	1
2:A:314:ILE:CG1	2:A:317:LYS:HE3	0.40	2.47	5	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	0	-	-	-	-
2	A	107/114 (94%)	62±3 (57±3%)	26±4 (24±3%)	19±3 (18±2%)	0   3
All	All	2140/2680 (80%)	1230 (57%)	522 (24%)	388 (18%)	0   3

All 44 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	326	GLU	20

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Mol	Chain	Res	Type	Models (Total)
2	A	328	ASP	20
2	A	337	CYS	20
2	A	343	MET	20
2	A	348	PRO	20
2	A	352	GLU	20
2	A	353	PRO	20
2	A	357	SER	20
2	A	318	SER	19
2	A	358	TRP	19
2	A	281	LEU	18
2	A	338	ASP	17
2	A	312	GLN	16
2	A	354	PRO	15
2	A	346	LEU	13
2	A	313	CYS	13
2	A	280	GLU	10
2	A	355	GLU	10
2	A	271	MET	10
2	A	314	ILE	7
2	A	278	PRO	7
2	A	339	ARG	7
2	A	310	LYS	6
2	A	315	GLU	5
2	A	334	CYS	5
2	A	273	LYS	4
2	A	279	GLU	3
2	A	293	PRO	3
2	A	268	GLY	2
2	A	269	SER	2
2	A	263	ASP	2
2	A	317	LYS	2
2	A	261	TYR	2
2	A	270	ASN	1
2	A	282	VAL	1
2	A	356	GLY	1
2	A	277	ARG	1
2	A	303	THR	1
2	A	319	CYS	1
2	A	320	ILE	1
2	A	275	SER	1
2	A	287	CYS	1
2	A	311	TRP	1

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Mol	Chain	Res	Type	Models (Total)
2	A	262	CYS	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	0	-	-	-	
2	A	96/101 (95%)	70±3 (73±3%)	26±3 (27±3%)	1	20
All	All	1920/2220 (86%)	1400 (73%)	520 (27%)	1	20

All 55 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	261	TYR	20
2	A	262	CYS	20
2	A	309	TYR	20
2	A	320	ILE	20
2	A	321	LEU	20
2	A	326	GLU	20
2	A	343	MET	20
2	A	346	LEU	20
2	A	263	ASP	19
2	A	350	VAL	19
2	A	352	GLU	19
2	A	353	PRO	19
2	A	354	PRO	19
2	A	364	TRP	19
2	A	314	ILE	17
2	A	328	ASP	17
2	A	300	LEU	17
2	A	317	LYS	17
2	A	282	VAL	16
2	A	273	LYS	15
2	A	367	LEU	15
2	A	335	ASP	12
2	A	271	MET	10

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Mol	Chain	Res	Type	Models (Total)
2	A	277	ARG	10
2	A	365	GLU	10
2	A	299	THR	9
2	A	334	CYS	9
2	A	289	ARG	6
2	A	310	LYS	5
2	A	302	MET	5
2	A	270	ASN	5
2	A	359	SER	5
2	A	313	CYS	4
2	A	363	CYS	4
2	A	283	SER	4
2	A	333	PHE	3
2	A	286	ASP	3
2	A	290	SER	2
2	A	327	ASN	2
2	A	280	GLU	2
2	A	269	SER	2
2	A	341	TYR	2
2	A	275	SER	2
2	A	284	CYS	2
2	A	287	CYS	2
2	A	312	GLN	2
2	A	337	CYS	2
2	A	355	GLU	1
2	A	318	SER	1
2	A	272	ASN	1
2	A	297	GLN	1
2	A	339	ARG	1
2	A	316	CYS	1
2	A	362	LEU	1
2	A	366	LEU	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	SAC	B	1	1	7,8,9	0.67±0.03	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	SAC	B	1	1	7,9,11	1.18±0.05	0±0 (2±5%)

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	SAC	B	1	1	-	0±0,7,8,10	-

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	1	SAC	OAC-C1A-C2A	3.12	116.50	122.05	14	3

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides 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