



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2022 – 07:30 PM EST

PDB ID : 2KTB  
Title : Solution Structure of the Second Bromodomain of Human Polybromo in complex with an acetylated peptide from Histone 3  
Authors : Charlop-Powers, Z.; Zhang, Q.; Zeng, L.  
Deposited on : 2010-01-26

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:

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 : 2.27  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

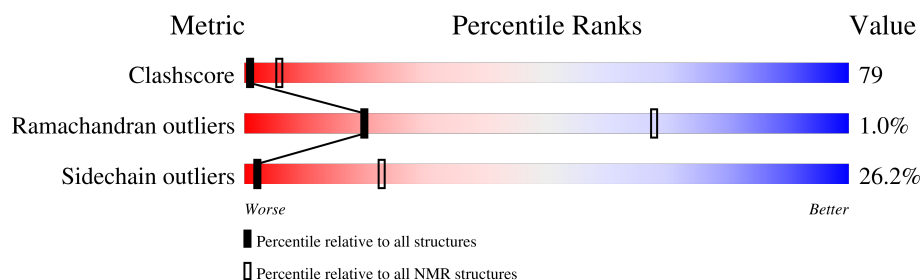
# 1 Overall quality at a glance

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	A	20	100%
2	B	121	12% 54% 10% • 23%

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:181-B:198, B:203-B:210, B:220-B:286 (93)	0.16	5

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

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

The models can be grouped into 4 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2283 atoms, of which 1165 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called H3\_Peptide.

Mol	Chain	Residues	Atoms					Trace
1	A	20	Total	C	H	N	O	0
			331	93	175	35	28	

- Molecule 2 is a protein called Protein polybromo-1.

Mol	Chain	Residues	Atoms						Trace
2	B	121	Total	C	H	N	O	S	0
			1952	617	990	158	184	3	

There is a discrepancy between the modelled and reference sequences:

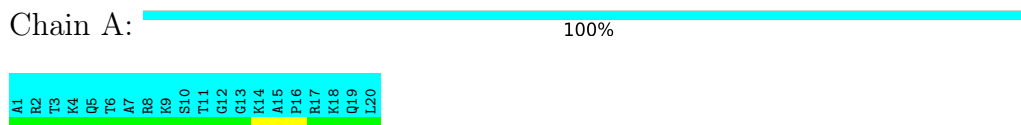
Chain	Residue	Modelled	Actual	Comment	Reference
B	173	SER	-	expression tag	UNP Q86U86

## 4 Residue-property plots

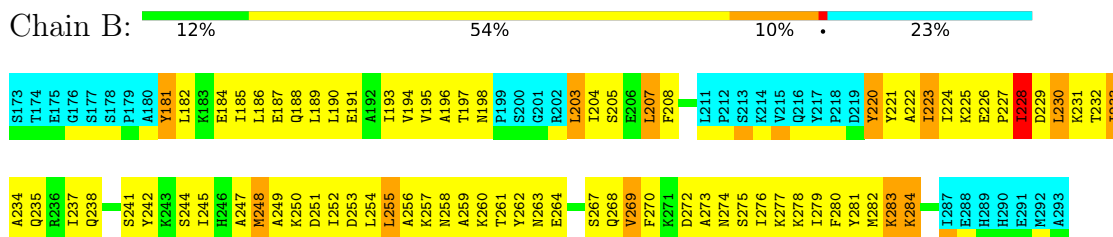
### 4.1 Average score per residue in the NMR ensemble

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: H3\_Peptide



- Molecule 2: Protein polybromo-1

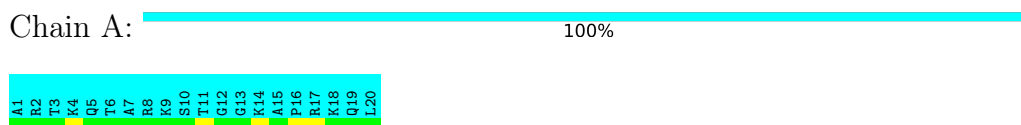


### 4.2 Scores per residue for each member of the ensemble

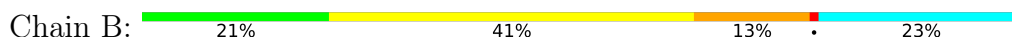
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: H3\_Peptide



- Molecule 2: Protein polybromo-1

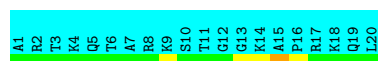




#### 4.2.2 Score per residue for model 2

- Molecule 1: H3\_Peptide

Chain A: 100%



- Molecule 2: Protein polybromo-1

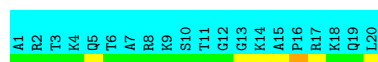
Chain B: 17% 44% 15% 23%



#### 4.2.3 Score per residue for model 3

- Molecule 1: H3\_Peptide

Chain A: 100%



- Molecule 2: Protein polybromo-1

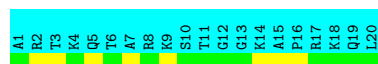
Chain B: 17% 44% 15% 23%



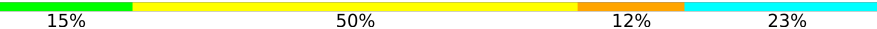
#### 4.2.4 Score per residue for model 4

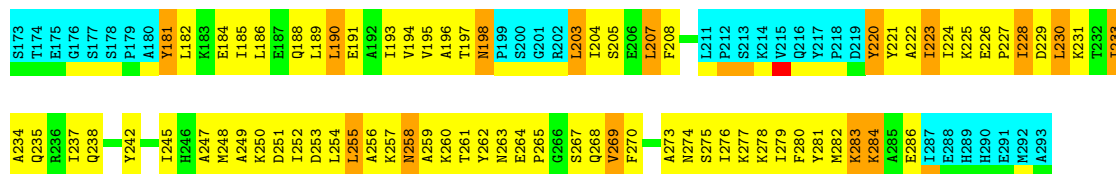
- Molecule 1: H3\_Peptide

Chain A:  100%



- Molecule 2: Protein polybromo-1

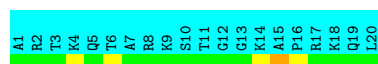
Chain B:  15% 50% 12% 23%




#### 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: H3\_Peptide

Chain A:  100%



- Molecule 2: Protein polybromo-1

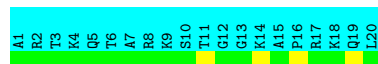
Chain B:  19% 43% 14% 23%




#### 4.2.6 Score per residue for model 6

- Molecule 1: H3\_Peptide

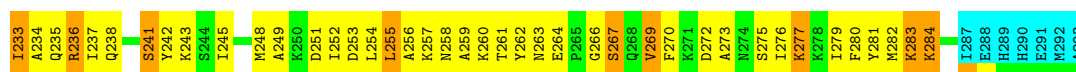
Chain A:  100%



- Molecule 2: Protein polybromo-1

Chain B:  15% 46% 15% 23%

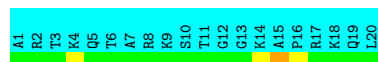




#### 4.2.7 Score per residue for model 7

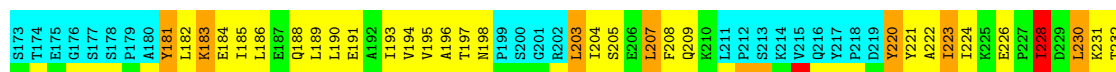
- Molecule 1: H3\_Peptide

Chain A: 100%



- Molecule 2: Protein polybromo-1

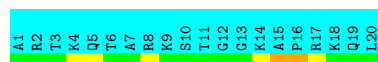
Chain B: 14% 49% 13% 23%



#### 4.2.8 Score per residue for model 8

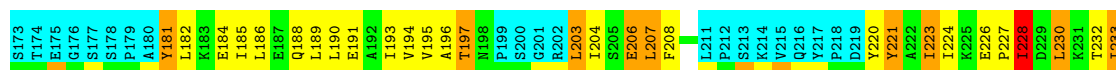
- Molecule 1: H3\_Peptide

Chain A: 100%



- Molecule 2: Protein polybromo-1

Chain B: 22% 39% 15% 23%

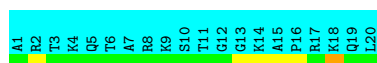


#### 4.2.9 Score per residue for model 9

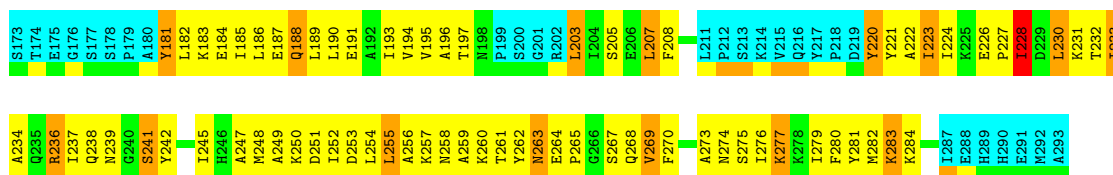
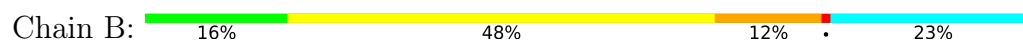
- Molecule 1: H3\_Peptide

Chain A: 100%



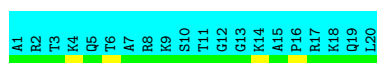


- Molecule 2: Protein polybromo-1

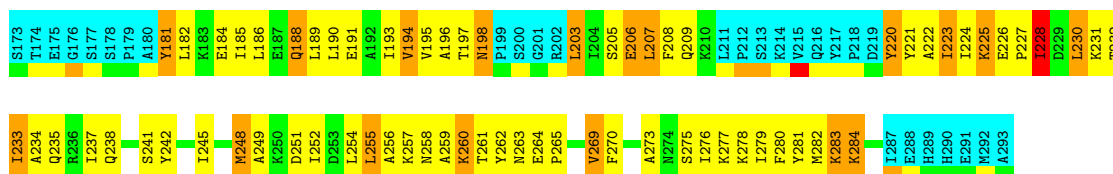
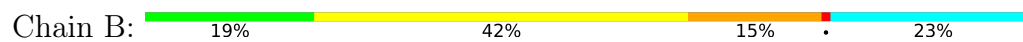


#### 4.2.10 Score per residue for model 10

- Molecule 1: H3\_Peptide

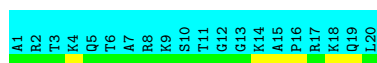


- Molecule 2: Protein polybromo-1

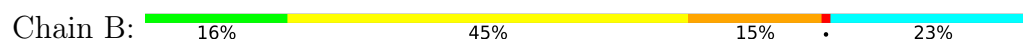


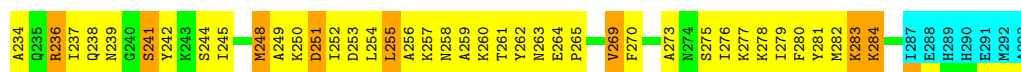
#### 4.2.11 Score per residue for model 11

- Molecule 1: H3\_Peptide



- Molecule 2: Protein polybromo-1

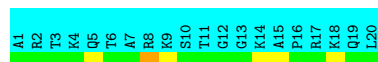




#### 4.2.12 Score per residue for model 12

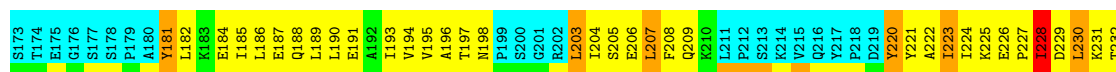
- Molecule 1: H3\_Peptide

Chain A: 100%



- Molecule 2: Protein polybromo-1

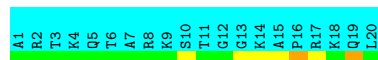
Chain B: 12% 52% 12% 23%



#### 4.2.13 Score per residue for model 13

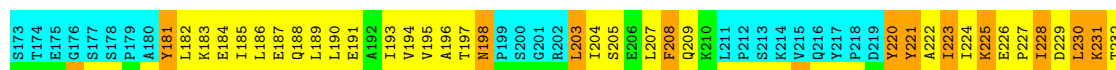
- Molecule 1: H3\_Peptide

Chain A: 100%



- Molecule 2: Protein polybromo-1

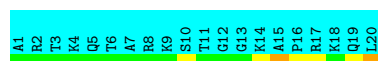
Chain B: 12% 47% 17% 23%



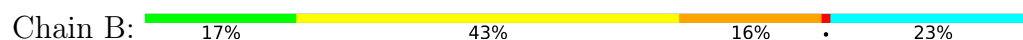
#### 4.2.14 Score per residue for model 14

- Molecule 1: H3\_Peptide

Chain A: 100%

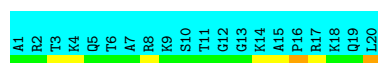


- Molecule 2: Protein polybromo-1

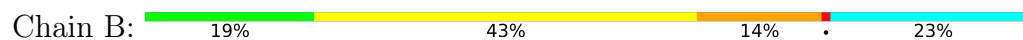


#### 4.2.15 Score per residue for model 15

- Molecule 1: H3\_Peptide

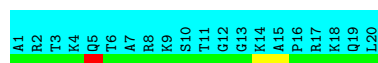


- Molecule 2: Protein polybromo-1

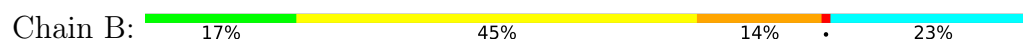


#### 4.2.16 Score per residue for model 16

- Molecule 1: H3\_Peptide



- Molecule 2: Protein polybromo-1

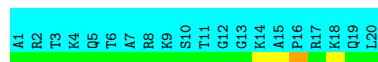




#### 4.2.17 Score per residue for model 17

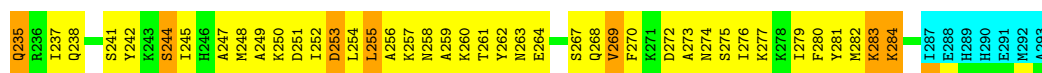
- Molecule 1: H3\_Peptide

Chain A: 100%



- Molecule 2: Protein polybromo-1

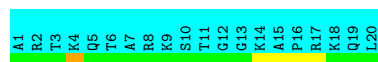
Chain B: 16% 46% 14% 23%



#### 4.2.18 Score per residue for model 18

- Molecule 1: H3\_Peptide

Chain A: 100%



- Molecule 2: Protein polybromo-1

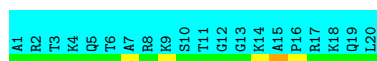
Chain B: 19% 45% 12% 23%



#### 4.2.19 Score per residue for model 19

- Molecule 1: H3\_Peptide

Chain A: 100%



- Molecule 2: Protein polybromo-1

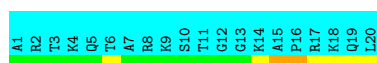
Chain B: 15% 46% 15% • 23%



#### 4.2.20 Score per residue for model 20

- Molecule 1: H3\_Peptide

Chain A: 100%



- Molecule 2: Protein polybromo-1

Chain B: 17% 50% 9% • 23%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *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	structure solution	2.2
CNS	refinement	2.2

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: ALY

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	B	0.47±0.01	0±0/763 ( 0.0± 0.0%)	0.65±0.02	0±0/1027 ( 0.0± 0.0%)
All	All	0.47	0/15260 ( 0.0%)	0.65	1/20540 ( 0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	221	TYR	CB-CG-CD1	-5.37	117.78	121.00	1	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	A	0	0	0	0±0
2	B	751	791	790	122±7
All	All	15020	15820	15800	2446

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 79.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:181:TYR:O	2:B:185:ILE:HD13	0.92	1.65	11	20
2:B:189:LEU:HD11	2:B:284:LYS:HD3	0.84	1.49	18	17
2:B:233:ILE:HD13	2:B:252:ILE:HD13	0.83	1.51	7	20
2:B:245:ILE:HD12	2:B:248:MET:SD	0.82	2.13	13	20
2:B:185:ILE:CG2	2:B:189:LEU:HD12	0.81	2.05	13	20
2:B:223:ILE:HG23	2:B:224:ILE:HG12	0.80	1.53	20	20
2:B:208:PHE:CZ	2:B:259:ALA:HB2	0.78	2.13	18	20
2:B:237:ILE:HD11	2:B:248:MET:SD	0.77	2.19	13	20
2:B:189:LEU:HD23	2:B:283:LYS:HG3	0.77	1.52	15	20
2:B:185:ILE:HG23	2:B:189:LEU:HD12	0.77	1.57	18	20
2:B:234:ALA:HA	2:B:237:ILE:HD12	0.76	1.57	11	20
2:B:236:ARG:HG2	2:B:242:TYR:CE2	0.75	2.17	11	4
2:B:224:ILE:HA	2:B:261:THR:HG21	0.74	1.59	20	20
2:B:233:ILE:HG23	2:B:248:MET:HG3	0.73	1.61	9	19
2:B:223:ILE:HG23	2:B:224:ILE:H	0.72	1.43	6	10
2:B:207:LEU:HD22	2:B:207:LEU:H	0.72	1.45	10	9
2:B:263:ASN:HB2	2:B:269:VAL:HG21	0.72	1.62	3	15
2:B:233:ILE:HD11	2:B:251:ASP:C	0.71	2.06	15	20
2:B:263:ASN:HB3	2:B:269:VAL:HG11	0.71	1.60	3	7
2:B:223:ILE:HG23	2:B:224:ILE:N	0.71	2.01	11	20
2:B:189:LEU:HD13	2:B:280:PHE:CZ	0.71	2.21	17	20
2:B:283:LYS:C	2:B:283:LYS:HZ3	0.70	1.90	15	1
2:B:256:ALA:O	2:B:259:ALA:HB3	0.70	1.86	11	20
2:B:189:LEU:CD1	2:B:284:LYS:HD3	0.70	2.17	13	4
2:B:256:ALA:CB	2:B:273:ALA:HB1	0.69	2.16	16	20
2:B:233:ILE:HD13	2:B:252:ILE:CD1	0.69	2.18	2	20
2:B:186:LEU:O	2:B:190:LEU:HB3	0.68	1.88	14	20
2:B:208:PHE:CE1	2:B:259:ALA:HB2	0.68	2.23	17	20
2:B:190:LEU:O	2:B:194:VAL:HG12	0.68	1.89	13	13
2:B:228:ILE:HD11	2:B:233:ILE:N	0.68	2.04	11	20
2:B:230:LEU:H	2:B:230:LEU:HD13	0.68	1.49	12	15
2:B:203:LEU:HD13	2:B:203:LEU:H	0.67	1.49	18	15
2:B:223:ILE:HG21	2:B:262:TYR:CD1	0.67	2.25	3	20
2:B:197:THR:HG22	2:B:203:LEU:N	0.66	2.05	18	20
2:B:193:ILE:HD11	2:B:280:PHE:HA	0.66	1.67	16	20
2:B:184:GLU:O	2:B:188:GLN:HG2	0.66	1.90	15	20
2:B:253:ASP:HA	2:B:277:LYS:HD2	0.66	1.68	6	1
2:B:189:LEU:HD11	2:B:284:LYS:CD	0.65	2.21	18	17
2:B:272:ASP:OD1	2:B:273:ALA:N	0.65	2.29	17	5
2:B:189:LEU:HD13	2:B:280:PHE:CE2	0.65	2.26	3	20
2:B:228:ILE:HD12	2:B:233:ILE:HD12	0.64	1.68	2	20
2:B:255:LEU:HD21	2:B:276:ILE:HD12	0.64	1.69	6	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:245:ILE:HG23	2:B:248:MET:SD	0.64	2.32	15	18
2:B:189:LEU:O	2:B:193:ILE:HD13	0.64	1.93	10	20
2:B:181:TYR:C	2:B:181:TYR:CD1	0.64	2.72	17	20
2:B:182:LEU:HD23	2:B:245:ILE:CD1	0.63	2.23	10	20
2:B:208:PHE:HZ	2:B:259:ALA:HB2	0.63	1.53	10	14
2:B:256:ALA:HA	2:B:273:ALA:HB1	0.63	1.70	13	20
2:B:256:ALA:CA	2:B:273:ALA:HB1	0.63	2.24	13	20
2:B:226:GLU:HB2	2:B:254:LEU:HD22	0.62	1.69	6	16
2:B:224:ILE:HB	2:B:227:PRO:HG3	0.62	1.71	15	18
2:B:189:LEU:HD23	2:B:283:LYS:CG	0.62	2.25	14	20
2:B:269:VAL:HA	2:B:272:ASP:OD2	0.62	1.95	13	6
2:B:263:ASN:HB2	2:B:269:VAL:HG11	0.62	1.72	5	10
2:B:203:LEU:HD13	2:B:203:LEU:N	0.62	2.10	16	4
2:B:281:TYR:HA	2:B:284:LYS:HB2	0.61	1.70	15	3
2:B:236:ARG:CD	2:B:241:SER:HB3	0.61	2.25	6	4
2:B:275:SER:O	2:B:279:ILE:HD13	0.61	1.96	12	20
2:B:236:ARG:HG2	2:B:242:TYR:CD2	0.61	2.31	9	4
2:B:267:SER:HB3	2:B:269:VAL:HG12	0.60	1.70	19	11
2:B:220:TYR:O	2:B:223:ILE:HG22	0.60	1.96	1	10
2:B:207:LEU:HD22	2:B:207:LEU:N	0.60	2.12	1	5
2:B:190:LEU:O	2:B:194:VAL:HG13	0.59	1.98	11	4
2:B:194:VAL:HG23	2:B:209:GLN:HE22	0.58	1.58	20	2
2:B:186:LEU:HD13	2:B:237:ILE:CG2	0.58	2.28	17	16
2:B:193:ILE:HG21	2:B:276:ILE:HG23	0.58	1.73	8	5
2:B:185:ILE:HG21	2:B:245:ILE:HD12	0.58	1.76	9	17
2:B:193:ILE:HB	2:B:230:LEU:HD21	0.58	1.76	1	5
2:B:225:LYS:HG3	2:B:226:GLU:HG3	0.57	1.75	10	3
2:B:193:ILE:CG2	2:B:230:LEU:HD11	0.57	2.29	8	4
2:B:193:ILE:HG22	2:B:230:LEU:HD11	0.57	1.76	8	3
2:B:249:ALA:HB2	2:B:280:PHE:CZ	0.57	2.35	16	20
2:B:256:ALA:HB1	2:B:273:ALA:HB1	0.57	1.75	14	15
2:B:203:LEU:HD23	2:B:206:GLU:CD	0.57	2.19	3	1
2:B:220:TYR:O	2:B:224:ILE:HG12	0.57	2.00	5	20
2:B:245:ILE:HG23	2:B:248:MET:HG2	0.57	1.76	13	1
2:B:190:LEU:HD13	2:B:234:ALA:HB2	0.57	1.77	4	1
2:B:237:ILE:HG12	2:B:245:ILE:HD11	0.57	1.76	13	17
2:B:191:GLU:O	2:B:195:VAL:HG13	0.57	2.00	9	17
2:B:208:PHE:O	2:B:229:ASP:HB2	0.57	1.99	16	6
2:B:220:TYR:O	2:B:224:ILE:CG1	0.56	2.53	10	20
2:B:225:LYS:HG3	2:B:226:GLU:HG2	0.56	1.76	13	1
2:B:269:VAL:HG13	2:B:270:PHE:HD1	0.56	1.61	3	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:245:ILE:CG2	2:B:284:LYS:HE2	0.56	2.31	3	2
2:B:230:LEU:N	2:B:255:LEU:HD12	0.56	2.16	12	20
2:B:193:ILE:O	2:B:196:ALA:HB3	0.56	2.01	20	20
2:B:206:GLU:HA	2:B:209:GLN:HG2	0.56	1.78	12	2
2:B:208:PHE:CZ	2:B:273:ALA:HB2	0.55	2.35	5	13
2:B:223:ILE:CG2	2:B:224:ILE:H	0.55	2.14	16	10
2:B:274:ASN:HA	2:B:277:LYS:HE3	0.55	1.78	14	3
2:B:197:THR:HG22	2:B:203:LEU:HD13	0.55	1.79	19	18
2:B:230:LEU:HD22	2:B:231:LYS:N	0.55	2.17	19	13
2:B:242:TYR:CZ	2:B:248:MET:HA	0.55	2.36	11	4
2:B:223:ILE:CG2	2:B:224:ILE:N	0.55	2.69	2	20
2:B:181:TYR:HE1	2:B:245:ILE:H	0.55	1.45	11	17
2:B:190:LEU:O	2:B:194:VAL:HG23	0.55	2.02	14	3
2:B:230:LEU:HD12	2:B:255:LEU:HD11	0.55	1.79	20	8
2:B:197:THR:HA	2:B:203:LEU:HA	0.55	1.78	10	20
2:B:245:ILE:HG22	2:B:284:LYS:HE3	0.54	1.79	12	13
2:B:249:ALA:HB2	2:B:280:PHE:CE1	0.54	2.37	16	20
2:B:188:GLN:HB3	2:B:283:LYS:HE2	0.54	1.79	3	18
2:B:224:ILE:HD12	2:B:258:ASN:HB2	0.54	1.79	7	8
2:B:236:ARG:HD3	2:B:241:SER:HB3	0.54	1.79	14	3
2:B:228:ILE:HD12	2:B:233:ILE:CD1	0.54	2.33	7	20
2:B:233:ILE:HG21	2:B:252:ILE:HD11	0.54	1.78	9	19
2:B:272:ASP:CG	2:B:273:ALA:N	0.54	2.61	14	2
2:B:203:LEU:N	2:B:203:LEU:HD13	0.54	2.18	12	16
2:B:181:TYR:O	2:B:185:ILE:CD1	0.54	2.52	5	12
2:B:236:ARG:HG3	2:B:241:SER:CB	0.54	2.33	6	4
2:B:278:LYS:O	2:B:282:MET:HG3	0.54	2.02	5	10
2:B:228:ILE:H	2:B:258:ASN:ND2	0.54	2.01	18	6
2:B:204:ILE:HD12	2:B:276:ILE:HG12	0.53	1.80	14	16
2:B:252:ILE:HG13	2:B:280:PHE:CE2	0.53	2.38	9	20
2:B:204:ILE:HA	2:B:272:ASP:HB2	0.53	1.78	13	4
2:B:193:ILE:CG2	2:B:276:ILE:HG23	0.53	2.33	1	10
2:B:237:ILE:HD11	2:B:248:MET:HG3	0.53	1.79	14	12
2:B:233:ILE:HG23	2:B:248:MET:CG	0.53	2.34	7	19
2:B:231:LYS:HE3	2:B:235:GLN:HE21	0.53	1.63	17	1
2:B:282:MET:HG3	2:B:283:LYS:N	0.53	2.18	17	6
2:B:206:GLU:OE2	2:B:207:LEU:HD11	0.52	2.03	18	1
2:B:237:ILE:HG13	2:B:242:TYR:HD2	0.52	1.64	9	10
2:B:263:ASN:CB	2:B:269:VAL:HG21	0.52	2.34	3	4
2:B:203:LEU:HD22	2:B:203:LEU:H	0.52	1.65	11	9
2:B:237:ILE:HG12	2:B:245:ILE:CD1	0.52	2.34	15	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:231:LYS:NZ	2:B:235:GLN:NE2	0.52	2.58	16	8
2:B:269:VAL:HG13	2:B:270:PHE:CD1	0.52	2.40	3	19
2:B:190:LEU:HD23	2:B:230:LEU:O	0.52	2.05	3	10
2:B:223:ILE:HG21	2:B:262:TYR:HD1	0.51	1.65	13	17
2:B:220:TYR:CD1	2:B:224:ILE:HG13	0.51	2.40	11	20
2:B:279:ILE:O	2:B:282:MET:HG3	0.51	2.05	2	2
2:B:259:ALA:HB1	2:B:269:VAL:HG23	0.51	1.82	9	2
2:B:186:LEU:O	2:B:190:LEU:CB	0.51	2.58	8	20
2:B:245:ILE:CG2	2:B:284:LYS:CE	0.51	2.89	3	2
2:B:189:LEU:CD1	2:B:245:ILE:HG21	0.51	2.34	16	17
2:B:264:GLU:O	2:B:267:SER:HB2	0.51	2.06	17	3
2:B:257:LYS:O	2:B:260:LYS:HG3	0.51	2.05	8	4
2:B:185:ILE:HG21	2:B:245:ILE:CD1	0.51	2.36	20	19
2:B:223:ILE:CG2	2:B:224:ILE:HG12	0.50	2.36	12	16
2:B:268:GLN:NE2	2:B:268:GLN:H	0.50	2.03	14	1
2:B:283:LYS:HE3	2:B:283:LYS:O	0.50	2.06	3	9
2:B:185:ILE:HG23	2:B:189:LEU:HB2	0.50	1.82	4	18
2:B:252:ILE:O	2:B:255:LEU:HB3	0.50	2.07	13	20
2:B:224:ILE:HD12	2:B:258:ASN:HB3	0.50	1.84	18	8
2:B:237:ILE:HD11	2:B:248:MET:CG	0.50	2.37	14	10
2:B:245:ILE:HG22	2:B:284:LYS:CE	0.50	2.36	14	13
2:B:230:LEU:HD13	2:B:230:LEU:N	0.50	2.22	12	13
2:B:270:PHE:CD1	2:B:270:PHE:N	0.50	2.80	8	20
2:B:226:GLU:CB	2:B:254:LEU:HD22	0.50	2.37	9	6
2:B:248:MET:O	2:B:252:ILE:HG12	0.50	2.07	13	2
2:B:255:LEU:HD23	2:B:256:ALA:N	0.49	2.22	17	11
2:B:234:ALA:HA	2:B:237:ILE:CD1	0.49	2.37	12	14
2:B:189:LEU:HD21	2:B:284:LYS:HG2	0.49	1.85	9	3
2:B:203:LEU:N	2:B:203:LEU:HD22	0.49	2.22	18	4
2:B:271:LYS:NZ	2:B:271:LYS:HB3	0.49	2.22	15	1
2:B:283:LYS:NZ	2:B:283:LYS:O	0.49	2.45	15	1
2:B:182:LEU:HD23	2:B:245:ILE:HG12	0.49	1.83	7	3
2:B:230:LEU:H	2:B:230:LEU:CD1	0.49	2.21	12	9
2:B:185:ILE:HG23	2:B:189:LEU:CD1	0.49	2.36	13	2
2:B:194:VAL:HA	2:B:205:SER:OG	0.49	2.07	6	12
2:B:198:ASN:ND2	2:B:204:ILE:HG22	0.49	2.23	13	2
2:B:226:GLU:HB3	2:B:254:LEU:HD13	0.49	1.85	17	5
2:B:193:ILE:HD11	2:B:280:PHE:CA	0.49	2.37	16	6
2:B:248:MET:CE	2:B:280:PHE:HE2	0.49	2.21	20	20
2:B:207:LEU:HG	2:B:263:ASN:ND2	0.49	2.23	3	1
2:B:221:TYR:CE1	2:B:227:PRO:HB2	0.49	2.43	20	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:248:MET:HE2	2:B:252:ILE:HD11	0.48	1.84	20	7
2:B:257:LYS:O	2:B:260:LYS:HG2	0.48	2.08	11	13
2:B:186:LEU:HD11	2:B:234:ALA:O	0.48	2.09	11	11
2:B:204:ILE:CA	2:B:272:ASP:HB2	0.48	2.38	6	4
2:B:229:ASP:OD2	2:B:231:LYS:HB3	0.48	2.09	15	5
2:B:183:LYS:O	2:B:186:LEU:HB3	0.48	2.09	7	4
2:B:264:GLU:HG2	2:B:265:PRO:HD2	0.48	1.86	11	9
2:B:208:PHE:HB2	2:B:230:LEU:CD1	0.48	2.39	10	4
2:B:224:ILE:HG22	2:B:225:LYS:N	0.48	2.24	17	3
2:B:279:ILE:O	2:B:282:MET:HG2	0.47	2.09	9	6
2:B:283:LYS:O	2:B:283:LYS:HE3	0.47	2.09	1	8
2:B:204:ILE:HG22	2:B:272:ASP:HB2	0.47	1.86	7	2
2:B:274:ASN:N	2:B:274:ASN:HD22	0.47	2.08	7	2
2:B:223:ILE:HG21	2:B:262:TYR:CE1	0.47	2.44	17	11
2:B:183:LYS:HD3	2:B:183:LYS:C	0.47	2.30	11	6
2:B:188:GLN:NE2	2:B:188:GLN:HA	0.47	2.24	3	2
2:B:203:LEU:H	2:B:203:LEU:HD22	0.47	1.69	5	8
2:B:207:LEU:HG	2:B:263:ASN:OD1	0.47	2.09	6	2
2:B:203:LEU:H	2:B:203:LEU:HD13	0.47	1.69	11	4
2:B:279:ILE:HG13	2:B:282:MET:HE3	0.47	1.85	1	3
2:B:189:LEU:HD12	2:B:245:ILE:HG21	0.47	1.84	17	2
2:B:186:LEU:HD13	2:B:237:ILE:HG21	0.47	1.86	17	1
2:B:182:LEU:HB3	2:B:237:ILE:HG23	0.47	1.87	20	1
2:B:232:THR:HA	2:B:235:GLN:HB2	0.47	1.86	8	9
2:B:281:TYR:HA	2:B:284:LYS:HB3	0.47	1.85	16	3
2:B:260:LYS:HA	2:B:270:PHE:CZ	0.47	2.44	5	16
2:B:280:PHE:C	2:B:280:PHE:CD1	0.47	2.89	14	7
2:B:253:ASP:O	2:B:257:LYS:HG2	0.46	2.10	13	5
2:B:228:ILE:HD13	2:B:229:ASP:N	0.46	2.25	13	4
2:B:208:PHE:CD2	2:B:276:ILE:HD12	0.46	2.46	17	4
2:B:233:ILE:HD11	2:B:252:ILE:N	0.46	2.26	2	15
2:B:221:TYR:CD1	2:B:227:PRO:HG2	0.46	2.46	15	1
2:B:204:ILE:HA	2:B:272:ASP:OD2	0.46	2.11	3	1
2:B:242:TYR:C	2:B:244:SER:H	0.46	2.13	1	6
2:B:270:PHE:N	2:B:270:PHE:HD1	0.46	2.09	19	9
2:B:189:LEU:CD2	2:B:284:LYS:HG2	0.46	2.41	9	3
2:B:253:ASP:CG	2:B:277:LYS:HD3	0.46	2.31	16	5
2:B:228:ILE:CD1	2:B:232:THR:HB	0.45	2.40	13	5
2:B:233:ILE:HD11	2:B:251:ASP:CB	0.45	2.42	9	9
2:B:227:PRO:HA	2:B:258:ASN:CG	0.45	2.31	3	2
2:B:236:ARG:CG	2:B:241:SER:HB3	0.45	2.41	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:205:SER:O	2:B:209:GLN:N	0.45	2.50	6	8
2:B:188:GLN:HB3	2:B:283:LYS:HE3	0.45	1.88	15	1
2:B:204:ILE:HA	2:B:272:ASP:HB3	0.45	1.88	3	3
2:B:228:ILE:O	2:B:255:LEU:HA	0.45	2.11	8	4
2:B:268:GLN:HE21	2:B:268:GLN:HA	0.45	1.71	5	1
2:B:270:PHE:HD1	2:B:270:PHE:N	0.45	2.09	14	9
2:B:249:ALA:O	2:B:252:ILE:HB	0.45	2.12	15	13
2:B:207:LEU:N	2:B:207:LEU:HD13	0.45	2.27	17	2
2:B:194:VAL:HG23	2:B:209:GLN:NE2	0.45	2.27	20	2
2:B:236:ARG:HA	2:B:239:ASN:HB3	0.45	1.88	11	3
2:B:221:TYR:CE1	2:B:227:PRO:HG2	0.45	2.47	15	1
2:B:280:PHE:CD1	2:B:280:PHE:C	0.45	2.90	11	8
2:B:189:LEU:HA	2:B:283:LYS:HG2	0.45	1.88	18	3
2:B:245:ILE:HG23	2:B:248:MET:CG	0.45	2.42	13	1
2:B:193:ILE:HD12	2:B:193:ILE:N	0.45	2.27	14	8
2:B:194:VAL:HG12	2:B:230:LEU:HG	0.44	1.89	5	1
2:B:274:ASN:O	2:B:277:LYS:HG2	0.44	2.12	20	9
2:B:224:ILE:HD11	2:B:262:TYR:HB2	0.44	1.90	9	5
2:B:236:ARG:HA	2:B:239:ASN:HB2	0.44	1.90	12	1
2:B:182:LEU:HD23	2:B:245:ILE:HD11	0.44	1.89	10	4
2:B:207:LEU:HB2	2:B:208:PHE:CE1	0.44	2.48	16	2
2:B:205:SER:HA	2:B:276:ILE:HD11	0.44	1.89	10	2
2:B:278:LYS:O	2:B:282:MET:HG2	0.44	2.11	7	2
2:B:226:GLU:O	2:B:258:ASN:OD1	0.44	2.36	3	1
2:B:280:PHE:O	2:B:284:LYS:HG2	0.44	2.13	20	2
2:B:236:ARG:NE	2:B:242:TYR:CD1	0.44	2.85	6	1
2:B:233:ILE:O	2:B:237:ILE:HD12	0.44	2.12	13	1
2:B:185:ILE:HG12	2:B:245:ILE:HG13	0.44	1.88	3	2
2:B:190:LEU:O	2:B:190:LEU:HD22	0.44	2.13	7	4
2:B:263:ASN:HB3	2:B:269:VAL:HG21	0.44	1.89	7	1
2:B:272:ASP:OD1	2:B:272:ASP:C	0.44	2.56	14	2
2:B:254:LEU:O	2:B:258:ASN:ND2	0.44	2.51	8	1
2:B:247:ALA:O	2:B:250:LYS:HG2	0.43	2.13	7	11
2:B:198:ASN:ND2	2:B:272:ASP:OD1	0.43	2.51	3	1
2:B:206:GLU:OE2	2:B:207:LEU:CD1	0.43	2.65	18	1
2:B:236:ARG:HD2	2:B:242:TYR:CE1	0.43	2.48	9	3
2:B:182:LEU:HD23	2:B:245:ILE:CG1	0.43	2.43	2	2
2:B:252:ILE:HG13	2:B:280:PHE:CD2	0.43	2.48	13	12
2:B:232:THR:O	2:B:235:GLN:HB2	0.43	2.14	13	2
2:B:194:VAL:HG23	2:B:230:LEU:HD22	0.43	1.89	17	1
2:B:223:ILE:HD13	2:B:223:ILE:O	0.43	2.13	12	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:223:ILE:CD1	2:B:261:THR:HG22	0.43	2.44	3	3
2:B:263:ASN:CB	2:B:269:VAL:HG11	0.43	2.44	10	2
2:B:237:ILE:HG13	2:B:242:TYR:CD2	0.43	2.48	14	2
2:B:185:ILE:CG2	2:B:248:MET:SD	0.43	3.07	9	6
2:B:185:ILE:HG21	2:B:248:MET:SD	0.43	2.54	3	1
2:B:204:ILE:O	2:B:272:ASP:OD1	0.43	2.37	7	2
2:B:245:ILE:HG21	2:B:284:LYS:HE2	0.43	1.89	3	2
2:B:187:GLU:O	2:B:191:GLU:CB	0.43	2.66	9	2
2:B:181:TYR:CE1	2:B:245:ILE:HB	0.43	2.49	3	1
2:B:236:ARG:CG	2:B:241:SER:CB	0.43	2.97	6	1
2:B:190:LEU:HD21	2:B:230:LEU:HD23	0.43	1.91	10	1
2:B:197:THR:CG2	2:B:203:LEU:HD13	0.42	2.44	3	1
2:B:229:ASP:OD1	2:B:231:LYS:HE3	0.42	2.14	16	2
2:B:208:PHE:O	2:B:209:GLN:C	0.42	2.58	12	1
2:B:204:ILE:CB	2:B:272:ASP:HB2	0.42	2.44	16	1
2:B:257:LYS:HA	2:B:257:LYS:HE2	0.42	1.92	15	2
2:B:231:LYS:HZ2	2:B:235:GLN:NE2	0.42	2.12	6	1
2:B:245:ILE:HG23	2:B:248:MET:HB3	0.42	1.92	7	1
2:B:242:TYR:OH	2:B:251:ASP:CG	0.42	2.58	9	1
2:B:197:THR:C	2:B:204:ILE:HG23	0.42	2.35	13	1
2:B:203:LEU:H	2:B:203:LEU:CD1	0.42	2.19	18	1
2:B:274:ASN:HA	2:B:277:LYS:CD	0.42	2.44	9	1
2:B:208:PHE:CE1	2:B:259:ALA:CB	0.42	3.00	16	1
2:B:208:PHE:HZ	2:B:273:ALA:HB2	0.42	1.75	9	5
2:B:233:ILE:HG22	2:B:234:ALA:N	0.42	2.29	2	4
2:B:274:ASN:HA	2:B:277:LYS:HD3	0.42	1.91	9	1
2:B:183:LYS:C	2:B:183:LYS:CD	0.42	2.89	7	2
2:B:256:ALA:HB3	2:B:277:LYS:HE2	0.42	1.90	11	1
2:B:242:TYR:C	2:B:244:SER:N	0.42	2.73	17	4
2:B:193:ILE:CG2	2:B:276:ILE:HD13	0.42	2.45	17	1
2:B:264:GLU:HG2	2:B:266:GLY:H	0.41	1.75	6	1
2:B:192:ALA:O	2:B:196:ALA:HB2	0.41	2.15	6	1
2:B:269:VAL:O	2:B:272:ASP:OD1	0.41	2.38	5	2
2:B:207:LEU:N	2:B:207:LEU:CD2	0.41	2.83	1	1
2:B:203:LEU:HB2	2:B:206:GLU:HB2	0.41	1.92	3	1
2:B:181:TYR:OH	2:B:246:HIS:CD2	0.41	2.74	7	1
2:B:268:GLN:HB3	2:B:272:ASP:OD1	0.41	2.16	8	1
2:B:273:ALA:O	2:B:276:ILE:HB	0.41	2.15	8	1
2:B:264:GLU:HG2	2:B:265:PRO:CD	0.41	2.46	9	3
2:B:183:LYS:O	2:B:186:LEU:CB	0.41	2.69	20	1
2:B:181:TYR:C	2:B:181:TYR:HD1	0.41	2.18	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:258:ASN:C	2:B:258:ASN:ND2	0.41	2.74	12	1
2:B:228:ILE:O	2:B:228:ILE:HG23	0.41	2.16	16	2
2:B:238:GLN:HE21	2:B:239:ASN:N	0.41	2.13	2	2
2:B:204:ILE:C	2:B:276:ILE:HD11	0.41	2.36	4	1
2:B:245:ILE:HG22	2:B:284:LYS:HE2	0.41	1.93	20	1
2:B:245:ILE:HD13	2:B:245:ILE:HA	0.41	1.71	3	2
2:B:258:ASN:ND2	2:B:258:ASN:N	0.41	2.67	8	1
2:B:210:LYS:HA	2:B:229:ASP:OD2	0.41	2.15	16	1
2:B:258:ASN:N	2:B:258:ASN:ND2	0.41	2.68	5	1
2:B:236:ARG:NE	2:B:241:SER:HB3	0.41	2.31	6	1
2:B:221:TYR:CG	2:B:227:PRO:HG2	0.41	2.51	8	1
2:B:185:ILE:HG21	2:B:189:LEU:HD12	0.41	1.87	13	1
2:B:207:LEU:H	2:B:207:LEU:CD2	0.40	2.24	10	1
2:B:191:GLU:HA	2:B:194:VAL:HG12	0.40	1.91	20	1
2:B:205:SER:HB2	2:B:230:LEU:HD13	0.40	1.93	17	1
2:B:204:ILE:HG22	2:B:272:ASP:HA	0.40	1.93	18	1
2:B:228:ILE:H	2:B:258:ASN:HD21	0.40	1.58	18	1
2:B:245:ILE:HG21	2:B:284:LYS:CE	0.40	2.47	3	1
2:B:228:ILE:HG23	2:B:228:ILE:O	0.40	2.17	5	1
2:B:242:TYR:CE2	2:B:248:MET:HA	0.40	2.51	9	1
2:B:235:GLN:HA	2:B:238:GLN:HE21	0.40	1.76	18	1
2:B:188:GLN:HA	2:B:188:GLN:NE2	0.40	2.32	4	1
2:B:184:GLU:CD	2:B:188:GLN:HG2	0.40	2.37	10	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	0	-	-	-	-	
2	B	93/121 (77%)	87±2 (93±2%)	5±2 (6±2%)	1±0 (1±0%)	20	68
All	All	1860/2820 (66%)	1737 (93%)	104 (6%)	19 (1%)	20	68

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.



Mol	Chain	Res	Type	Models (Total)
2	B	228	ILE	18
2	B	244	SER	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	0	-	-	-	
2	B	81/105 (77%)	60±2 (74±3%)	21±2 (26±3%)	2	23
All	All	1620/2380 (68%)	1196 (74%)	424 (26%)	2	23

All 51 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	B	181	TYR	20
2	B	203	LEU	20
2	B	223	ILE	20
2	B	228	ILE	20
2	B	230	LEU	20
2	B	233	ILE	20
2	B	238	GLN	20
2	B	255	LEU	20
2	B	269	VAL	20
2	B	283	LYS	20
2	B	284	LYS	19
2	B	207	LEU	17
2	B	220	TYR	17
2	B	241	SER	17
2	B	267	SER	13
2	B	187	GLU	12
2	B	253	ASP	12
2	B	248	MET	10
2	B	198	ASN	8
2	B	221	TYR	7
2	B	188	GLN	7
2	B	225	LYS	6
2	B	258	ASN	6

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Mol	Chain	Res	Type	Models (Total)
2	B	263	ASN	6
2	B	281	TYR	6
2	B	277	LYS	5
2	B	260	LYS	5
2	B	194	VAL	4
2	B	231	LYS	4
2	B	236	ARG	4
2	B	272	ASP	3
2	B	208	PHE	3
2	B	235	GLN	3
2	B	206	GLU	3
2	B	183	LYS	2
2	B	268	GLN	2
2	B	274	ASN	2
2	B	250	LYS	2
2	B	282	MET	2
2	B	229	ASP	2
2	B	251	ASP	2
2	B	244	SER	2
2	B	257	LYS	2
2	B	227	PRO	2
2	B	190	LEU	1
2	B	286	GLU	1
2	B	243	LYS	1
2	B	197	THR	1
2	B	275	SER	1
2	B	271	LYS	1
2	B	270	PHE	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	A	14	1	10,11,12	0.64±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	ALY	A	14	1	7,12,14	0.93±0.06	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	A	14	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 monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided