Full wwPDB NMR Structure Validation Report (i)

Nov 6, 2023 – 10:15 AM EST

PDB ID	:	2KWJ
Title	:	Solution structures of the double PHD fingers of human transcriptional protein DPF3 bound to a histone peptide containing acetylation at lysine 14
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Deposited on	:	2010-04-12

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

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

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

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

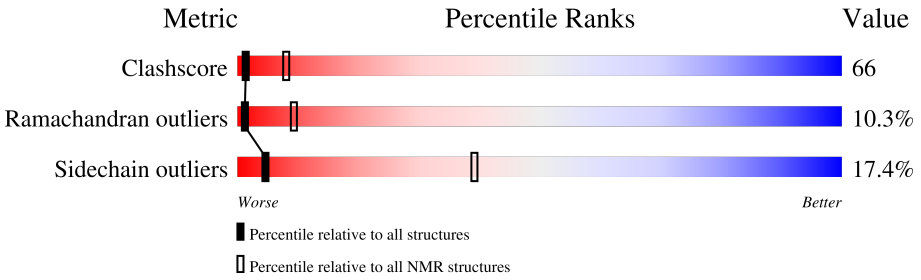
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	B	20	5% 40% 10% 45%
2	A	114	25% 52% 14% • 9%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:1-B:4, B:9-B:13, B:15-B:16, A:260-A:363 (115)	0.59	1

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

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

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

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2025 atoms, of which 985 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Histone peptide.

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

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	A	114	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	
			Total	Zn
3	A	4	4	4

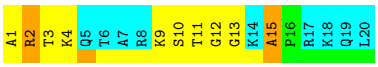
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

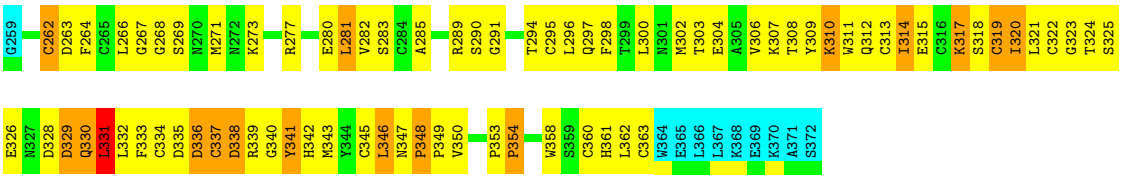
• Molecule 1: Histone peptide

Chain B: 5% 40% 10% 45%



• Molecule 2: Zinc finger protein DPF3

Chain A: 25% 52% 14% • 9%



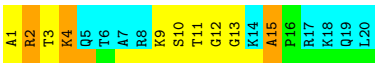
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

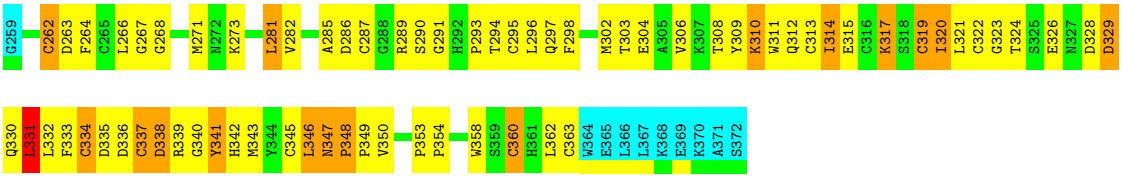
• Molecule 1: Histone peptide

Chain B: 5% 35% 15% 45%



• Molecule 2: Zinc finger protein DPF3

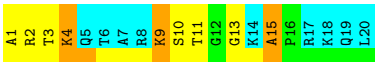
Chain A: 30% 46% 14% • 9%



4.2.2 Score per residue for model 2

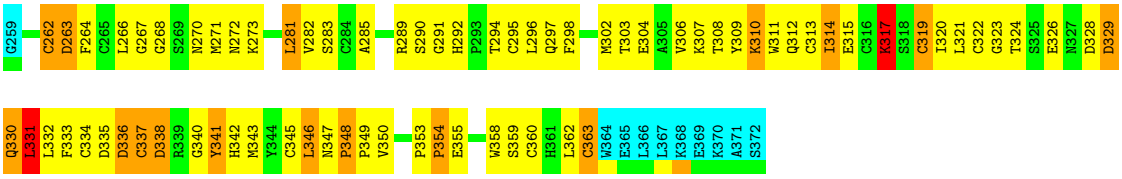
- Molecule 1: Histone peptide

Chain B: 10% 30% 15% 45%



- Molecule 2: Zinc finger protein DPF3

Chain A: 27% 48% 14% • 9%



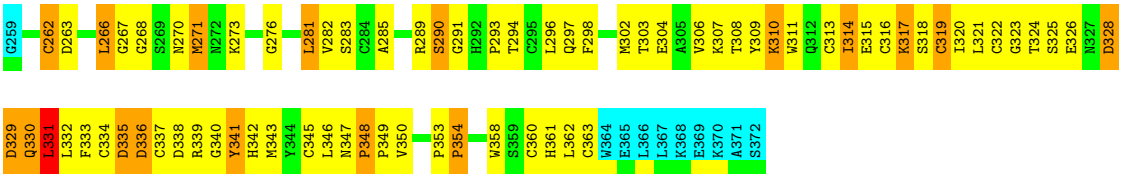
4.2.3 Score per residue for model 3

- Molecule 1: Histone peptide

Chain B: 10% 40% 5% 45%

- Molecule 2: Zinc finger protein DPF3

Chain A: 27% 48% 15% • 9%



4.2.4 Score per residue for model 4

- Molecule 1: Histone peptide

Chain B: 5% 45% 5% 45%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15 P16 R17 K18 Q19 L20

- Molecule 2: Zinc finger protein DPF3

Chain A: 24% 49% 18% • 9%

G259 C262 D263 F264 C265 L266 G267 G268 S269 N270 M271 N272 K273 R277 P278 E279 E280 L281 V282 S283 C284 A285 R289 S290 G291 T294 C295 L296 Q297 F298 T299 L300 M301 M302 T303 E304 A305 V306 K307 T308 Y309 K310 W311 Q312 C313 I314 E315 C316 K317 S318 C319 I320 L321 C322 G323 T324

S325 E326 N327 D328 D329 Q330 L331 L332 F333 C334 D335 D336 C337 D338 R339 G340 Y341 H342 M343 Y344 C345 L346 N347 P348 P349 V350 P353 P354 W358 S359 C360 H361 L362 C363 W364 E365 L366 L367 K368 E369 K370 A371 S372

4.2.5 Score per residue for model 5

- Molecule 1: Histone peptide

Chain B: 15% 35% 5% 45%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15 P16 R17 K18 Q19 L20

- Molecule 2: Zinc finger protein DPF3

Chain A: 27% 46% 16% • 9%

G259 C262 D263 F264 C265 L266 G267 G268 M271 N272 K273 G276 L281 V282 S283 C284 A285 R289 S290 G291 T294 C295 L296 Q297 F298 T299 L300 M301 M302 T303 E304 A305 V306 K307 T308 Y309 K310 W311 Q312 C313 I314 E315 C316 K317 S318 C319 I320 L321 C322 G323 T324 S325 E326 N327

D328 D329 Q330 L331 L332 F333 C334 D335 D336 C337 D338 R339 G340 Y341 H342 M343 Y344 C345 L346 N347 P348 P349 V350 P353 P354 E355 W358 S359 C360 H361 L362 C363 W364 E365 L366 L367 K368 E369 K370 A371 S372

4.2.6 Score per residue for model 6

- Molecule 1: Histone peptide

Chain B: 10% 40% 5% 45%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15 P16 R17 K18 Q19 L20

- Molecule 2: Zinc finger protein DPF3

Chain A: 28% 47% 15% • 9%

G259 C262 D263 F264 C265 L266 G267 G268 S269 N270 M271 N272 K273 G276 E279 E280 L281 V282 S283 R289 S290 G291 H292 P293 T294 C295 L296 Q297 F298 M302 T303 E304 A305 V306 K307 T308 Y309 K310 W311 Q312 C313 I314 E315 C316 K317 S318 C319 I320 L321 C322 G323 T324 S325 E326 N327

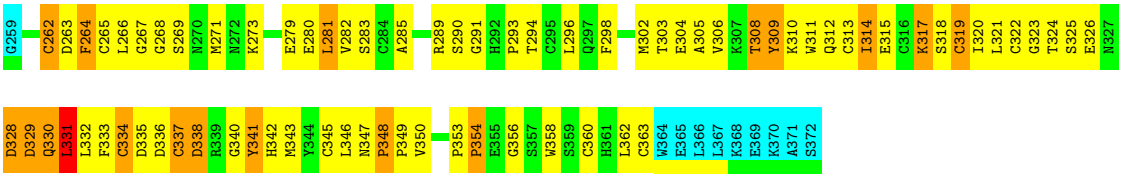
4.2.7 Score per residue for model 7

- Molecule 1: Histone peptide

Chain B: 15% 35% 5% 45%

- Molecule 2: Zinc finger protein DPF3

Chain A: 26% 49% 15% • 9%



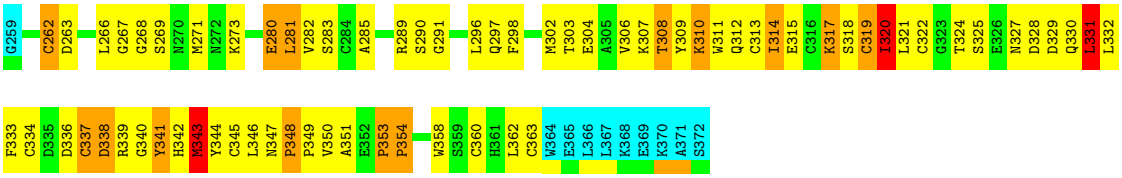
4.2.8 Score per residue for model 8

- Molecule 1: Histone peptide

Chain B: 10% 30% 15% 45%

- Molecule 2: Zinc finger protein DPF3

Chain A: 30% 46% 12% • 9%

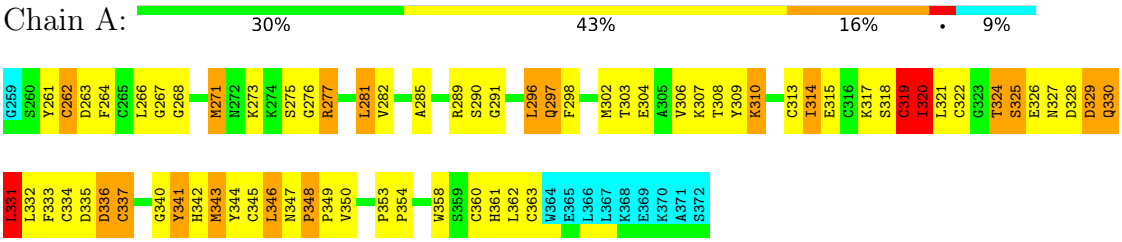


4.2.9 Score per residue for model 9

- Molecule 1: Histone peptide

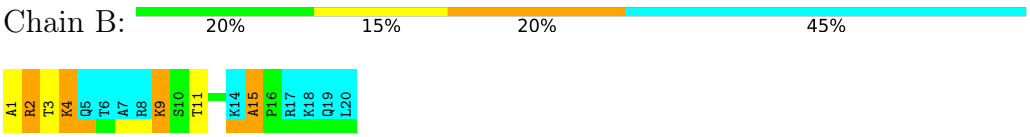
Chain B: 10% 30% 15% 45%

• Molecule 2: Zinc finger protein DPF3

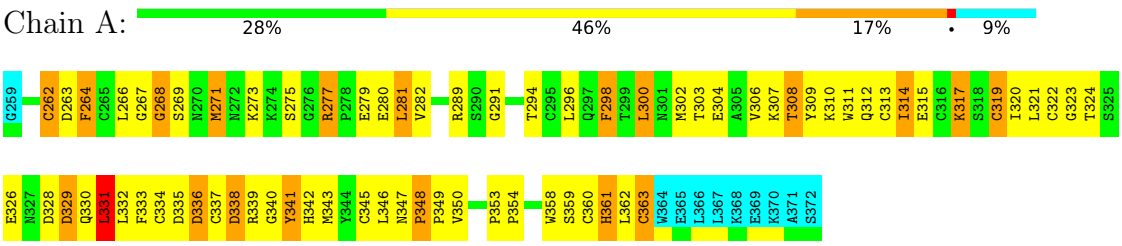


4.2.10 Score per residue for model 10

• Molecule 1: Histone peptide

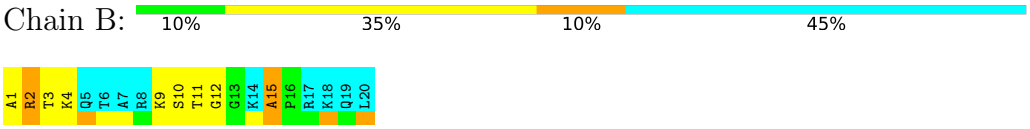


• Molecule 2: Zinc finger protein DPF3

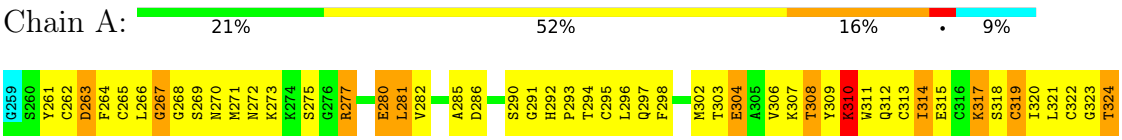


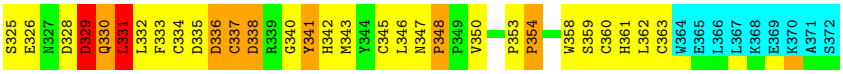
4.2.11 Score per residue for model 11

• Molecule 1: Histone peptide



• Molecule 2: Zinc finger protein DPF3





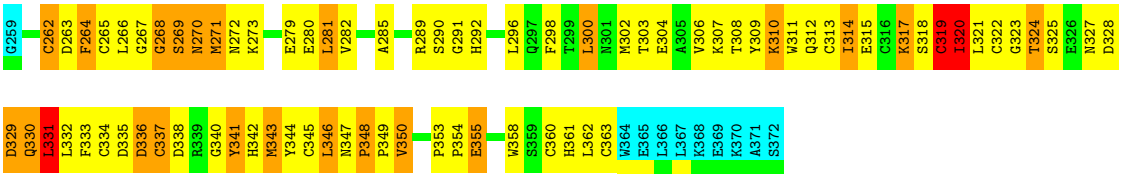
4.2.12 Score per residue for model 12

- Molecule 1: Histone peptide

Chain B: 15% 35% 5% 45%

- Molecule 2: Zinc finger protein DPF3

Chain A: 24% 46% 19% • 9%



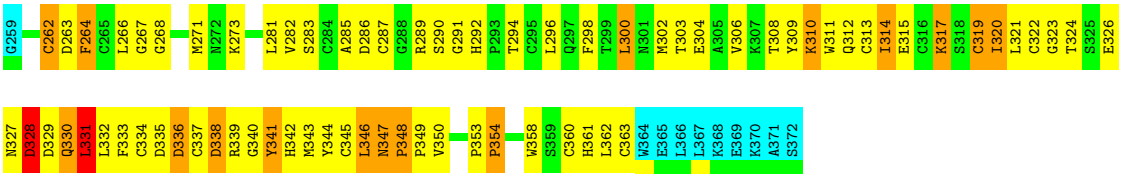
4.2.13 Score per residue for model 13

- Molecule 1: Histone peptide

Chain B: 10% 30% 15% 45%

- Molecule 2: Zinc finger protein DPF3

Chain A: 27% 48% 14% • 9%



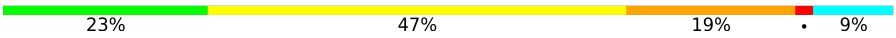
4.2.14 Score per residue for model 14

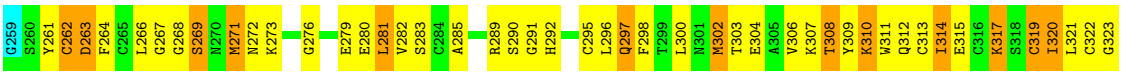
- Molecule 1: Histone peptide

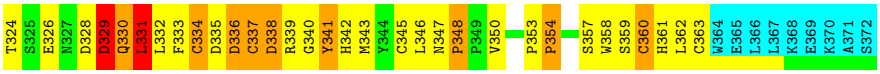
Chain B: 15% 25% 15% 45%

• Molecule 2: Zinc finger protein DPF3

Chain A:



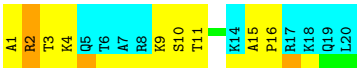




4.2.15 Score per residue for model 15

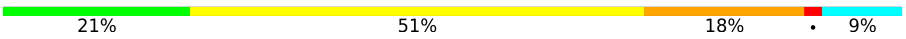
• Molecule 1: Histone peptide

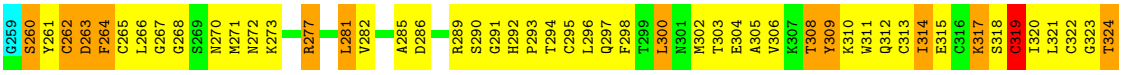
Chain B:

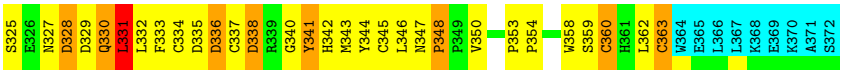


• Molecule 2: Zinc finger protein DPF3

Chain A:



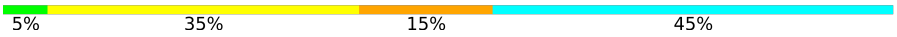




4.2.16 Score per residue for model 16

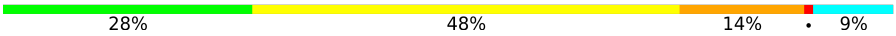
• Molecule 1: Histone peptide

Chain B:



• Molecule 2: Zinc finger protein DPF3

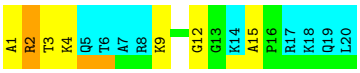
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: Histone peptide

Chain B: 20% 30% 5% 45%



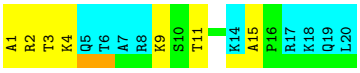
- Molecule 2: Zinc finger protein DPF3

Chain A: 27% 47% 14% • 9%

4.2.18 Score per residue for model 18

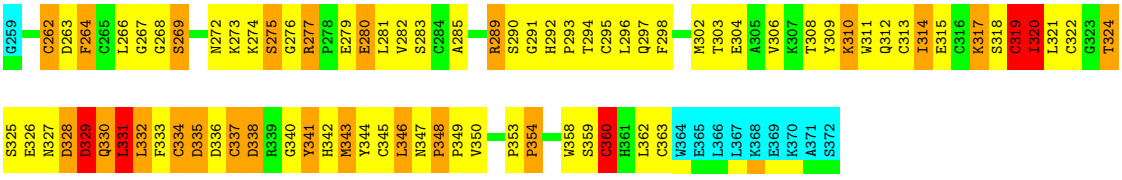
- Molecule 1: Histone peptide

Chain B: 20% 35% 45%



- Molecule 2: Zinc finger protein DPF3

Chain A: 21% 46% 20% • 9%



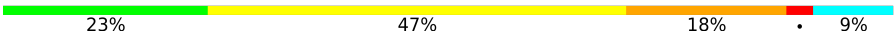
4.2.19 Score per residue for model 19

- Molecule 1: Histone peptide

Chain B: 5% 35% 15% 45%

• Molecule 2: Zinc finger protein DPF3

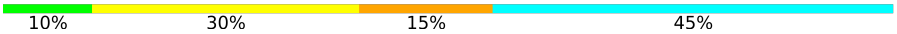
Chain A:



4.2.20 Score per residue for model 20

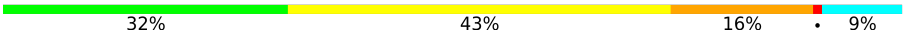
• Molecule 1: Histone peptide

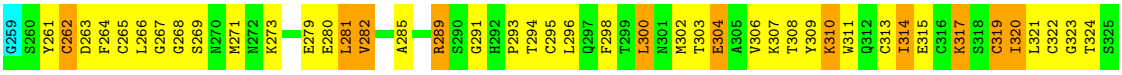
Chain B:

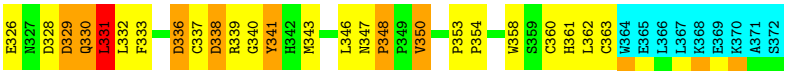


• Molecule 2: Zinc finger protein DPF3

Chain A:







5 Refinement protocol and experimental data overview (i)

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: ALY, ZN

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

There are no bond-length outliers.

There are no bond-angle outliers.

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	74	83	83	25±3
2	A	798	725	724	108±9
All	All	17520	16160	16140	2208

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 66.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:9:LYS:HG3	2:A:314:ILE:HG21	0.99	1.34	11	12
2:A:346:LEU:HD12	2:A:350:VAL:HG23	0.88	1.46	17	16
2:A:346:LEU:HD12	2:A:350:VAL:HG12	0.85	1.46	19	4
2:A:322:CYS:SG	2:A:324:THR:HG22	0.84	2.13	16	6
2:A:332:LEU:HD11	2:A:350:VAL:HG11	0.81	1.53	20	4
1:B:3:THR:HG22	2:A:332:LEU:CD1	0.80	2.06	6	2
2:A:330:GLN:HE22	2:A:343:MET:H	0.79	1.20	13	1
2:A:336:ASP:HB3	2:A:363:CYS:SG	0.79	2.18	13	4
2:A:262:CYS:SG	2:A:264:PHE:CD2	0.78	2.77	15	6
2:A:282:VAL:HG22	2:A:291:GLY:O	0.75	1.80	13	20
1:B:4:LYS:HB3	2:A:328:ASP:O	0.74	1.82	9	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:334:CYS:HB2	2:A:360:CYS:HB3	0.74	1.60	7	14
2:A:343:MET:CB	2:A:350:VAL:HG13	0.73	2.14	19	4
2:A:314:ILE:HG22	2:A:315:GLU:N	0.73	1.99	17	19
1:B:4:LYS:HG2	2:A:328:ASP:HB3	0.73	1.58	3	6
2:A:343:MET:CA	2:A:350:VAL:HG13	0.72	2.14	16	4
2:A:330:GLN:NE2	2:A:343:MET:H	0.72	1.81	13	1
2:A:303:THR:O	2:A:306:VAL:HG22	0.71	1.85	1	20
2:A:342:HIS:HB2	2:A:345:CYS:SG	0.71	2.25	9	18
2:A:267:GLY:HA2	2:A:273:LYS:HE3	0.70	1.63	4	17
2:A:350:VAL:HG11	2:A:354:PRO:HD3	0.70	1.62	8	11
1:B:4:LYS:HZ1	2:A:315:GLU:HA	0.70	1.45	4	11
1:B:4:LYS:NZ	2:A:315:GLU:HA	0.69	2.02	7	18
2:A:319:CYS:HA	2:A:340:GLY:O	0.69	1.88	18	20
1:B:4:LYS:HG2	2:A:328:ASP:HB2	0.68	1.64	2	4
2:A:267:GLY:HA2	2:A:273:LYS:HE2	0.67	1.67	13	3
2:A:359:SER:OG	2:A:363:CYS:SG	0.67	2.53	15	1
1:B:2:ARG:HB2	2:A:333:PHE:CD2	0.67	2.25	8	2
2:A:330:GLN:HE22	2:A:343:MET:N	0.67	1.87	13	1
2:A:264:PHE:CZ	2:A:296:LEU:HG	0.67	2.25	18	6
2:A:314:ILE:HG22	2:A:315:GLU:OE1	0.66	1.90	4	1
2:A:302:MET:O	2:A:306:VAL:HG13	0.66	1.90	19	20
2:A:282:VAL:HG11	2:A:306:VAL:HG21	0.65	1.68	5	18
2:A:337:CYS:SG	2:A:339:ARG:HG3	0.65	2.32	20	3
2:A:330:GLN:NE2	2:A:343:MET:SD	0.65	2.69	13	1
1:B:3:THR:HG21	2:A:353:PRO:HG3	0.65	1.66	6	19
1:B:3:THR:HG22	2:A:332:LEU:HD23	0.65	1.69	13	17
2:A:343:MET:CG	2:A:350:VAL:HB	0.65	2.22	8	1
1:B:15:ALA:HB3	2:A:289:ARG:NH2	0.64	2.07	16	1
2:A:292:HIS:HB2	2:A:295:CYS:SG	0.64	2.33	11	2
2:A:337:CYS:SG	2:A:362:LEU:HD23	0.64	2.31	14	1
1:B:4:LYS:HE3	2:A:314:ILE:O	0.63	1.92	3	19
2:A:343:MET:HA	2:A:350:VAL:HG13	0.63	1.70	16	3
1:B:4:LYS:HB2	2:A:331:LEU:O	0.63	1.94	13	3
2:A:332:LEU:HD23	2:A:346:LEU:HD11	0.63	1.70	6	2
2:A:343:MET:HB3	2:A:350:VAL:HG13	0.63	1.70	19	3
1:B:4:LYS:HE2	2:A:314:ILE:HG23	0.62	1.71	4	19
1:B:3:THR:CG2	2:A:353:PRO:HG3	0.62	2.25	19	3
2:A:321:LEU:HD21	2:A:341:TYR:CE2	0.62	2.30	2	18
2:A:262:CYS:O	2:A:266:LEU:N	0.62	2.32	10	6
2:A:269:SER:HB2	2:A:280:GLU:HA	0.62	1.71	18	8
1:B:9:LYS:CG	2:A:314:ILE:HG21	0.62	2.18	11	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:1:ALA:HB1	2:A:332:LEU:HD22	0.61	1.71	19	1
2:A:330:GLN:HE22	2:A:343:MET:CB	0.61	2.08	13	1
2:A:360:CYS:N	2:A:363:CYS:SG	0.61	2.73	10	1
2:A:334:CYS:SG	2:A:339:ARG:N	0.61	2.73	16	3
1:B:12:GLY:HA2	2:A:314:ILE:N	0.61	2.11	16	1
2:A:346:LEU:HD23	2:A:346:LEU:N	0.61	2.11	9	18
2:A:332:LEU:CD1	2:A:350:VAL:HG11	0.61	2.25	16	4
1:B:9:LYS:HE3	2:A:315:GLU:OE2	0.61	1.95	17	1
2:A:319:CYS:SG	2:A:321:LEU:HB2	0.61	2.36	8	20
2:A:314:ILE:O	2:A:317:LYS:HB3	0.61	1.96	11	4
1:B:4:LYS:HG3	2:A:328:ASP:HB2	0.61	1.71	8	1
2:A:346:LEU:CD1	2:A:350:VAL:HG12	0.60	2.25	19	3
1:B:13:GLY:HA2	2:A:263:ASP:HB3	0.60	1.72	20	1
1:B:9:LYS:HB2	1:B:9:LYS:NZ	0.60	2.11	17	1
1:B:13:GLY:N	2:A:313:CYS:HB2	0.60	2.10	16	1
2:A:304:GLU:O	2:A:308:THR:HG22	0.60	1.96	17	19
2:A:262:CYS:SG	2:A:264:PHE:HD2	0.60	2.18	15	6
2:A:298:PHE:CD2	2:A:302:MET:SD	0.60	2.95	14	1
2:A:341:TYR:CZ	2:A:360:CYS:HB2	0.60	2.31	13	19
2:A:303:THR:O	2:A:307:LYS:HD3	0.60	1.97	9	11
2:A:314:ILE:O	2:A:317:LYS:HB2	0.60	1.97	13	5
1:B:1:ALA:HB3	2:A:354:PRO:HD2	0.59	1.73	8	9
1:B:2:ARG:HB3	2:A:333:PHE:HB2	0.59	1.73	7	16
2:A:360:CYS:SG	2:A:361:HIS:N	0.59	2.75	10	1
2:A:330:GLN:C	2:A:330:GLN:HE21	0.59	2.01	13	1
2:A:330:GLN:NE2	2:A:343:MET:HB2	0.59	2.12	15	2
1:B:11:THR:HG23	2:A:296:LEU:HA	0.59	1.73	7	9
1:B:4:LYS:HB3	2:A:331:LEU:HB3	0.59	1.75	2	3
2:A:264:PHE:HB2	2:A:295:CYS:HB3	0.59	1.75	16	7
2:A:282:VAL:CG1	2:A:306:VAL:HG21	0.59	2.28	5	8
2:A:334:CYS:SG	2:A:335:ASP:N	0.59	2.76	11	15
2:A:332:LEU:HG	2:A:343:MET:HG3	0.59	1.74	19	17
1:B:3:THR:HG22	2:A:332:LEU:CD2	0.59	2.27	3	17
2:A:328:ASP:O	2:A:330:GLN:N	0.58	2.35	6	17
2:A:264:PHE:CE1	2:A:296:LEU:HD12	0.58	2.33	9	1
2:A:321:LEU:HD21	2:A:341:TYR:CD2	0.58	2.34	17	20
2:A:275:SER:HB3	2:A:277:ARG:HE	0.58	1.57	11	5
1:B:4:LYS:HG3	1:B:9:LYS:NZ	0.58	2.13	17	1
2:A:262:CYS:SG	2:A:263:ASP:N	0.58	2.76	20	1
2:A:285:ALA:HB1	2:A:310:LYS:HD3	0.58	1.75	18	17
1:B:12:GLY:C	2:A:313:CYS:HB2	0.58	2.19	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:336:ASP:CB	2:A:363:CYS:SG	0.58	2.92	18	12
1:B:1:ALA:HB2	2:A:354:PRO:CD	0.58	2.29	7	2
2:A:264:PHE:CD2	2:A:295:CYS:HB2	0.57	2.34	15	1
1:B:9:LYS:O	1:B:9:LYS:CG	0.57	2.52	14	3
1:B:1:ALA:HB1	2:A:354:PRO:HD2	0.57	1.76	10	5
2:A:340:GLY:C	2:A:341:TYR:HD1	0.57	2.03	18	20
2:A:328:ASP:O	2:A:331:LEU:N	0.57	2.38	17	13
2:A:262:CYS:O	2:A:266:LEU:HA	0.56	2.00	16	17
2:A:282:VAL:CG2	2:A:296:LEU:HD11	0.56	2.30	19	10
2:A:263:ASP:OD2	2:A:264:PHE:CE2	0.56	2.58	11	2
1:B:2:ARG:HD3	1:B:10:SER:HB2	0.56	1.77	9	1
2:A:314:ILE:O	2:A:315:GLU:HB2	0.56	2.00	19	1
1:B:4:LYS:HE3	2:A:314:ILE:C	0.56	2.20	2	9
2:A:269:SER:N	2:A:281:LEU:HD11	0.56	2.14	12	9
2:A:282:VAL:HG21	2:A:296:LEU:CD1	0.56	2.31	15	8
2:A:314:ILE:CG2	2:A:315:GLU:N	0.56	2.68	17	15
2:A:346:LEU:CD1	2:A:350:VAL:HG23	0.56	2.30	8	16
1:B:11:THR:HB	2:A:314:ILE:HG13	0.56	1.78	6	2
1:B:1:ALA:HB2	2:A:354:PRO:HB2	0.56	1.76	15	8
2:A:293:PRO:HA	2:A:296:LEU:HD12	0.56	1.76	19	4
2:A:343:MET:HG3	2:A:350:VAL:HB	0.56	1.78	8	1
2:A:304:GLU:O	2:A:308:THR:HG23	0.56	2.00	11	1
2:A:322:CYS:SG	2:A:324:THR:CG2	0.55	2.94	17	5
2:A:263:ASP:N	2:A:290:SER:O	0.55	2.39	4	5
1:B:9:LYS:HG2	2:A:314:ILE:HG21	0.55	1.78	19	2
2:A:291:GLY:HA3	2:A:296:LEU:HD11	0.55	1.77	9	1
2:A:331:LEU:HD12	2:A:331:LEU:C	0.55	2.21	13	20
2:A:327:ASN:C	2:A:329:ASP:H	0.55	2.04	15	2
2:A:320:ILE:HG21	2:A:339:ARG:NE	0.55	2.16	1	1
2:A:337:CYS:SG	2:A:362:LEU:HD12	0.55	2.41	1	11
2:A:347:ASN:HB2	2:A:348:PRO:HD3	0.55	1.78	16	19
2:A:268:GLY:HA2	2:A:281:LEU:HD11	0.55	1.79	15	18
2:A:303:THR:HG22	2:A:307:LYS:HD2	0.55	1.79	2	1
1:B:11:THR:HG23	2:A:296:LEU:O	0.55	2.01	14	3
1:B:4:LYS:HB2	2:A:328:ASP:O	0.55	2.02	19	1
2:A:336:ASP:HB2	2:A:363:CYS:SG	0.55	2.42	14	6
2:A:337:CYS:O	2:A:338:ASP:HB3	0.55	2.02	4	10
2:A:298:PHE:CB	2:A:302:MET:HG2	0.55	2.32	14	1
2:A:334:CYS:SG	2:A:336:ASP:N	0.55	2.79	3	8
2:A:319:CYS:O	2:A:323:GLY:N	0.54	2.40	5	17
1:B:4:LYS:HD2	2:A:333:PHE:CE1	0.54	2.37	13	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:269:SER:HA	2:A:279:GLU:O	0.54	2.01	12	8
2:A:298:PHE:HB3	2:A:302:MET:CG	0.54	2.32	14	1
1:B:9:LYS:O	1:B:9:LYS:HG2	0.54	2.02	1	8
2:A:312:GLN:O	2:A:317:LYS:HD3	0.54	2.01	10	2
1:B:11:THR:HB	2:A:314:ILE:HD11	0.54	1.80	18	6
2:A:264:PHE:CD2	2:A:295:CYS:CB	0.54	2.90	15	1
1:B:4:LYS:HZ2	2:A:328:ASP:HB3	0.54	1.62	19	1
2:A:321:LEU:HD11	2:A:341:TYR:CD2	0.54	2.38	19	11
2:A:341:TYR:HH	2:A:361:HIS:CE1	0.54	2.20	19	5
2:A:298:PHE:HB3	2:A:302:MET:HG2	0.54	1.79	14	1
2:A:328:ASP:C	2:A:330:GLN:H	0.54	2.06	4	15
2:A:264:PHE:CE2	2:A:296:LEU:HG	0.54	2.38	10	4
1:B:2:ARG:HB2	2:A:333:PHE:HD2	0.54	1.63	10	2
2:A:283:SER:HA	2:A:289:ARG:O	0.54	2.02	18	11
1:B:4:LYS:NZ	2:A:315:GLU:HG3	0.54	2.18	4	1
2:A:332:LEU:HD12	2:A:346:LEU:HD11	0.54	1.80	19	14
2:A:322:CYS:O	2:A:324:THR:HG23	0.53	2.02	3	9
1:B:13:GLY:O	2:A:263:ASP:HB3	0.53	2.03	1	3
2:A:337:CYS:O	2:A:338:ASP:CB	0.53	2.55	14	13
2:A:303:THR:O	2:A:307:LYS:HD2	0.53	2.02	2	1
2:A:262:CYS:O	2:A:266:LEU:HG	0.53	2.04	20	2
1:B:1:ALA:HB2	2:A:358:TRP:HB2	0.53	1.78	14	12
1:B:10:SER:HB2	2:A:297:GLN:NE2	0.53	2.19	1	3
1:B:15:ALA:CB	2:A:266:LEU:HD21	0.53	2.32	2	9
2:A:298:PHE:HA	2:A:302:MET:SD	0.53	2.44	11	15
2:A:298:PHE:CE2	2:A:306:VAL:HG11	0.53	2.39	8	9
1:B:12:GLY:N	2:A:314:ILE:HD12	0.53	2.19	1	4
2:A:330:GLN:O	2:A:343:MET:SD	0.53	2.67	15	13
2:A:331:LEU:HD11	2:A:340:GLY:C	0.53	2.24	15	11
2:A:347:ASN:C	2:A:349:PRO:HD3	0.53	2.24	13	9
2:A:302:MET:SD	2:A:337:CYS:O	0.53	2.66	14	1
2:A:314:ILE:HD13	2:A:333:PHE:CZ	0.53	2.39	9	3
2:A:313:CYS:O	2:A:313:CYS:SG	0.53	2.66	16	18
2:A:343:MET:O	2:A:350:VAL:N	0.53	2.41	15	11
2:A:263:ASP:OD1	2:A:264:PHE:CE2	0.53	2.62	5	2
2:A:339:ARG:HB2	2:A:360:CYS:SG	0.53	2.43	10	1
2:A:313:CYS:O	2:A:315:GLU:N	0.53	2.41	10	17
1:B:11:THR:HB	2:A:314:ILE:CD1	0.53	2.33	3	3
2:A:264:PHE:CE1	2:A:296:LEU:HD13	0.53	2.39	17	1
2:A:324:THR:OG1	2:A:326:GLU:HG3	0.52	2.04	1	10
2:A:330:GLN:HA	2:A:343:MET:SD	0.52	2.44	20	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:269:SER:H	2:A:281:LEU:HD21	0.52	1.63	4	2
2:A:314:ILE:O	2:A:317:LYS:N	0.52	2.42	3	11
2:A:330:GLN:OE1	2:A:342:HIS:HB3	0.52	2.05	15	2
2:A:330:GLN:NE2	2:A:330:GLN:C	0.52	2.63	13	1
2:A:266:LEU:HD12	2:A:266:LEU:N	0.52	2.20	19	11
1:B:10:SER:HB3	2:A:297:GLN:NE2	0.52	2.20	11	3
1:B:11:THR:HA	2:A:264:PHE:CE2	0.52	2.40	20	1
2:A:296:LEU:O	2:A:297:GLN:HB2	0.52	2.05	6	10
2:A:317:LYS:HZ1	2:A:333:PHE:HD1	0.52	1.46	10	2
2:A:275:SER:HB3	2:A:277:ARG:NE	0.52	2.20	17	2
1:B:4:LYS:HE2	2:A:314:ILE:CG2	0.52	2.35	11	13
1:B:4:LYS:CB	2:A:328:ASP:O	0.52	2.58	18	9
2:A:330:GLN:NE2	2:A:343:MET:N	0.52	2.53	13	1
2:A:264:PHE:CZ	2:A:296:LEU:HA	0.52	2.39	17	2
1:B:4:LYS:HZ2	2:A:315:GLU:HA	0.52	1.65	1	2
2:A:362:LEU:HD13	2:A:362:LEU:O	0.52	2.05	11	8
1:B:1:ALA:HB2	2:A:358:TRP:CB	0.52	2.35	8	1
1:B:10:SER:HB3	2:A:297:GLN:HE21	0.52	1.65	6	1
1:B:15:ALA:N	2:A:289:ARG:HH21	0.52	2.03	14	1
2:A:303:THR:O	2:A:306:VAL:CG2	0.51	2.58	16	9
2:A:327:ASN:ND2	2:A:344:TYR:OH	0.51	2.43	18	6
2:A:318:SER:HA	2:A:325:SER:HB3	0.51	1.80	8	9
2:A:355:GLU:CD	2:A:355:GLU:N	0.51	2.64	5	3
2:A:320:ILE:HG21	2:A:339:ARG:HB3	0.51	1.82	14	1
1:B:9:LYS:HG3	2:A:314:ILE:HD13	0.51	1.82	8	7
2:A:360:CYS:SG	2:A:362:LEU:HB3	0.51	2.45	13	4
2:A:263:ASP:OD1	2:A:263:ASP:C	0.51	2.49	15	1
1:B:9:LYS:CG	1:B:9:LYS:O	0.51	2.59	11	4
2:A:342:HIS:O	2:A:345:CYS:N	0.51	2.44	8	7
1:B:9:LYS:HA	2:A:314:ILE:CD1	0.51	2.36	4	2
1:B:9:LYS:HB3	2:A:314:ILE:CD1	0.51	2.35	9	2
1:B:15:ALA:H	2:A:263:ASP:HB2	0.51	1.65	19	2
2:A:298:PHE:HE2	2:A:306:VAL:HG11	0.51	1.66	8	8
2:A:298:PHE:CD2	2:A:302:MET:CG	0.51	2.94	14	1
2:A:303:THR:O	2:A:307:LYS:CD	0.50	2.60	10	9
2:A:303:THR:HG22	2:A:307:LYS:CD	0.50	2.36	16	4
2:A:331:LEU:HD11	2:A:340:GLY:CA	0.50	2.37	12	18
2:A:354:PRO:HG2	2:A:358:TRP:CD1	0.50	2.42	10	11
2:A:302:MET:HG2	2:A:336:ASP:C	0.50	2.27	13	3
2:A:260:SER:HB2	2:A:290:SER:OG	0.50	2.07	15	1
2:A:341:TYR:HB2	2:A:346:LEU:HD21	0.50	1.83	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:331:LEU:HA	2:A:342:HIS:HA	0.50	1.83	8	4
1:B:9:LYS:HE2	2:A:315:GLU:HG2	0.50	1.84	7	2
2:A:282:VAL:O	2:A:290:SER:HA	0.50	2.06	4	16
1:B:11:THR:CG2	2:A:296:LEU:HD23	0.50	2.37	13	5
2:A:360:CYS:SG	2:A:362:LEU:N	0.50	2.85	6	4
1:B:9:LYS:HG3	2:A:314:ILE:CD1	0.50	2.36	17	5
2:A:332:LEU:HD22	2:A:343:MET:HG3	0.50	1.83	6	2
1:B:9:LYS:HA	2:A:333:PHE:HE2	0.50	1.66	6	1
2:A:342:HIS:O	2:A:344:TYR:N	0.50	2.45	8	2
1:B:1:ALA:CB	2:A:358:TRP:HB2	0.50	2.37	14	4
2:A:313:CYS:O	2:A:314:ILE:C	0.50	2.49	19	2
1:B:11:THR:HG22	2:A:264:PHE:HZ	0.50	1.67	19	1
2:A:328:ASP:C	2:A:330:GLN:N	0.49	2.65	7	16
2:A:320:ILE:HG21	2:A:339:ARG:HD3	0.49	1.83	13	2
1:B:1:ALA:HB2	2:A:354:PRO:CB	0.49	2.37	9	7
2:A:262:CYS:SG	2:A:265:CYS:N	0.49	2.85	15	1
1:B:4:LYS:HE2	1:B:9:LYS:HZ1	0.49	1.66	17	1
2:A:309:TYR:OH	2:A:337:CYS:HB3	0.49	2.08	15	3
2:A:298:PHE:CE2	2:A:302:MET:SD	0.49	3.06	14	1
2:A:298:PHE:CG	2:A:302:MET:HG2	0.49	2.43	14	1
2:A:289:ARG:HA	2:A:289:ARG:HE	0.49	1.66	20	1
2:A:314:ILE:O	2:A:316:CYS:N	0.49	2.44	16	2
2:A:328:ASP:O	2:A:331:LEU:HB3	0.49	2.08	14	1
2:A:332:LEU:HD11	2:A:350:VAL:HG21	0.49	1.84	17	9
2:A:319:CYS:O	2:A:319:CYS:SG	0.49	2.70	17	7
2:A:341:TYR:HH	2:A:361:HIS:CG	0.49	2.26	20	3
2:A:331:LEU:CD1	2:A:341:TYR:N	0.49	2.76	5	20
2:A:264:PHE:CZ	2:A:296:LEU:CG	0.48	2.96	18	5
2:A:302:MET:SD	2:A:338:ASP:HB3	0.48	2.47	14	1
2:A:322:CYS:HB3	2:A:324:THR:HG22	0.48	1.85	12	3
1:B:15:ALA:HB2	2:A:261:TYR:HE1	0.48	1.68	20	1
2:A:265:CYS:SG	2:A:273:LYS:N	0.48	2.86	12	1
2:A:330:GLN:HB2	2:A:343:MET:SD	0.48	2.48	15	1
2:A:346:LEU:HD23	2:A:346:LEU:H	0.48	1.66	12	10
2:A:313:CYS:SG	2:A:313:CYS:O	0.48	2.71	5	1
2:A:331:LEU:HD11	2:A:340:GLY:HA3	0.48	1.85	12	8
1:B:4:LYS:O	1:B:4:LYS:HG3	0.48	2.08	13	1
1:B:11:THR:HG22	1:B:11:THR:O	0.48	2.09	18	6
2:A:302:MET:SD	2:A:306:VAL:CG1	0.48	3.02	14	1
2:A:347:ASN:N	2:A:348:PRO:CD	0.48	2.76	8	18
2:A:353:PRO:O	2:A:354:PRO:O	0.48	2.31	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:332:LEU:CD1	2:A:346:LEU:HD11	0.48	2.39	9	15
1:B:1:ALA:N	2:A:354:PRO:HB2	0.48	2.24	8	1
1:B:4:LYS:HG3	1:B:9:LYS:HE3	0.48	1.86	20	2
1:B:4:LYS:HG3	1:B:9:LYS:HZ1	0.47	1.67	17	1
1:B:4:LYS:O	2:A:329:ASP:HA	0.47	2.10	1	2
2:A:343:MET:O	2:A:346:LEU:HG	0.47	2.09	8	2
2:A:343:MET:HB3	2:A:350:VAL:HB	0.47	1.86	13	14
2:A:337:CYS:SG	2:A:362:LEU:HB3	0.47	2.49	15	2
1:B:4:LYS:CG	2:A:331:LEU:HB3	0.47	2.39	8	1
2:A:306:VAL:HG12	2:A:338:ASP:OD2	0.47	2.09	11	4
2:A:296:LEU:O	2:A:297:GLN:CB	0.47	2.62	14	3
2:A:272:ASN:HB3	2:A:277:ARG:N	0.47	2.24	18	1
2:A:341:TYR:CB	2:A:346:LEU:CD2	0.47	2.93	8	14
2:A:300:LEU:HD13	2:A:300:LEU:O	0.47	2.09	14	9
2:A:311:TRP:CD1	2:A:312:GLN:N	0.47	2.83	11	14
1:B:9:LYS:HG2	2:A:314:ILE:HD13	0.47	1.86	10	2
2:A:286:ASP:HB2	2:A:312:GLN:NE2	0.47	2.25	15	2
1:B:4:LYS:HE2	1:B:9:LYS:HE2	0.47	1.87	8	3
2:A:318:SER:O	2:A:320:ILE:N	0.47	2.47	9	5
1:B:9:LYS:HB3	2:A:314:ILE:HD12	0.47	1.86	9	1
2:A:282:VAL:CG2	2:A:296:LEU:HD21	0.47	2.40	9	1
1:B:13:GLY:O	2:A:289:ARG:HD3	0.47	2.10	16	1
2:A:264:PHE:CE1	2:A:296:LEU:HD23	0.47	2.45	19	1
1:B:11:THR:HA	2:A:264:PHE:CZ	0.47	2.44	20	1
2:A:343:MET:HB3	2:A:350:VAL:HG22	0.47	1.86	12	1
1:B:11:THR:HG23	2:A:296:LEU:CA	0.47	2.40	11	4
1:B:4:LYS:HG2	2:A:331:LEU:HB3	0.47	1.85	8	1
2:A:262:CYS:HA	2:A:291:GLY:HA2	0.47	1.87	11	3
2:A:282:VAL:CG2	2:A:291:GLY:O	0.47	2.63	17	1
2:A:355:GLU:H	2:A:355:GLU:CD	0.47	2.13	12	1
2:A:362:LEU:HD13	2:A:362:LEU:C	0.47	2.30	13	3
1:B:11:THR:HG21	2:A:296:LEU:HD23	0.46	1.86	15	1
2:A:320:ILE:HD12	2:A:339:ARG:HH11	0.46	1.70	16	1
2:A:327:ASN:C	2:A:329:ASP:N	0.46	2.69	13	2
2:A:334:CYS:HB3	2:A:339:ARG:O	0.46	2.10	14	1
2:A:264:PHE:CB	2:A:295:CYS:HB3	0.46	2.40	20	3
2:A:346:LEU:HD13	2:A:358:TRP:HZ2	0.46	1.70	8	1
1:B:4:LYS:CG	2:A:328:ASP:O	0.46	2.64	15	2
2:A:313:CYS:O	2:A:316:CYS:HB2	0.46	2.11	19	1
1:B:9:LYS:O	2:A:314:ILE:HD11	0.46	2.10	6	1
2:A:262:CYS:O	2:A:266:LEU:CA	0.46	2.64	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:2:ARG:HD2	2:A:333:PHE:HD2	0.46	1.71	8	1
2:A:282:VAL:CG2	2:A:296:LEU:CD1	0.46	2.94	8	11
2:A:293:PRO:HA	2:A:296:LEU:HB2	0.46	1.87	17	7
1:B:11:THR:HG22	1:B:12:GLY:N	0.46	2.26	13	1
2:A:319:CYS:SG	2:A:319:CYS:O	0.46	2.73	6	7
2:A:341:TYR:CE1	2:A:360:CYS:HB2	0.46	2.47	10	1
2:A:337:CYS:O	2:A:338:ASP:HB2	0.46	2.10	19	2
2:A:272:ASN:HA	2:A:292:HIS:CE1	0.45	2.45	11	5
1:B:9:LYS:C	1:B:11:THR:H	0.45	2.14	16	1
2:A:332:LEU:HD13	2:A:358:TRP:CE2	0.45	2.46	20	1
1:B:4:LYS:CB	2:A:331:LEU:HB3	0.45	2.41	2	2
2:A:312:GLN:NE2	2:A:317:LYS:HA	0.45	2.25	16	2
2:A:319:CYS:HB3	2:A:324:THR:O	0.45	2.12	6	1
2:A:321:LEU:HD12	2:A:345:CYS:CB	0.45	2.41	19	5
1:B:4:LYS:HD2	2:A:333:PHE:CZ	0.45	2.46	19	2
2:A:361:HIS:CD2	2:A:362:LEU:N	0.45	2.84	20	4
2:A:264:PHE:CE2	2:A:291:GLY:CA	0.45	3.00	10	4
2:A:341:TYR:OH	2:A:361:HIS:N	0.45	2.49	10	1
1:B:4:LYS:HA	2:A:333:PHE:CZ	0.45	2.46	13	1
1:B:11:THR:HG22	1:B:12:GLY:H	0.45	1.72	16	1
2:A:266:LEU:N	2:A:266:LEU:HD12	0.45	2.26	7	4
2:A:296:LEU:HB3	2:A:298:PHE:CE1	0.45	2.47	12	3
2:A:305:ALA:HB1	2:A:309:TYR:CZ	0.45	2.46	4	3
2:A:319:CYS:O	2:A:322:CYS:N	0.45	2.50	8	5
2:A:263:ASP:OD1	2:A:263:ASP:O	0.45	2.35	15	1
2:A:265:CYS:O	2:A:266:LEU:HB2	0.45	2.12	15	1
2:A:298:PHE:HB3	2:A:302:MET:HB2	0.45	1.89	9	16
1:B:10:SER:HB3	2:A:297:GLN:HG3	0.45	1.88	6	1
2:A:334:CYS:SG	2:A:339:ARG:HB2	0.45	2.52	16	3
2:A:265:CYS:HB3	2:A:273:LYS:HB2	0.45	1.89	15	2
2:A:261:TYR:O	2:A:290:SER:HB2	0.45	2.12	9	1
1:B:2:ARG:HH11	2:A:333:PHE:HB2	0.45	1.72	11	1
1:B:9:LYS:O	1:B:11:THR:N	0.45	2.50	6	2
2:A:298:PHE:CG	2:A:302:MET:CG	0.45	3.00	14	1
2:A:327:ASN:HB3	2:A:330:GLN:HG2	0.45	1.89	15	1
2:A:282:VAL:HG11	2:A:306:VAL:CG2	0.45	2.42	9	2
2:A:263:ASP:OD2	2:A:289:ARG:HB3	0.44	2.13	12	4
2:A:326:GLU:N	2:A:342:HIS:HE2	0.44	2.09	9	2
2:A:343:MET:CB	2:A:350:VAL:HB	0.44	2.43	13	1
2:A:330:GLN:HG3	2:A:331:LEU:N	0.44	2.25	15	1
2:A:306:VAL:HB	2:A:311:TRP:CB	0.44	2.43	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:347:ASN:O	2:A:349:PRO:HD3	0.44	2.12	12	9
2:A:266:LEU:HD23	2:A:266:LEU:N	0.44	2.26	5	2
1:B:4:LYS:O	1:B:4:LYS:CG	0.44	2.66	1	1
2:A:355:GLU:CD	2:A:355:GLU:H	0.44	2.15	2	1
2:A:264:PHE:CZ	2:A:291:GLY:HA3	0.44	2.47	12	5
2:A:272:ASN:HB3	2:A:276:GLY:N	0.44	2.27	18	1
1:B:10:SER:HB3	2:A:297:GLN:HE22	0.44	1.71	3	1
2:A:305:ALA:HB1	2:A:309:TYR:OH	0.44	2.11	4	3
2:A:347:ASN:OD1	2:A:348:PRO:HD3	0.44	2.12	5	1
1:B:11:THR:HG22	2:A:296:LEU:HD23	0.44	1.90	12	2
2:A:302:MET:N	2:A:336:ASP:O	0.44	2.50	19	3
2:A:314:ILE:O	2:A:317:LYS:CB	0.44	2.65	11	5
2:A:334:CYS:SG	2:A:338:ASP:N	0.44	2.91	5	2
2:A:272:ASN:N	2:A:277:ARG:O	0.44	2.51	4	2
1:B:1:ALA:O	1:B:3:THR:HG23	0.44	2.12	17	2
2:A:263:ASP:OD2	2:A:264:PHE:CE1	0.44	2.71	10	1
2:A:317:LYS:HD2	2:A:338:ASP:O	0.44	2.13	16	3
2:A:337:CYS:SG	2:A:338:ASP:N	0.44	2.91	19	2
2:A:360:CYS:O	2:A:363:CYS:HB2	0.44	2.13	18	4
1:B:15:ALA:HB2	2:A:261:TYR:CE1	0.44	2.47	14	1
2:A:339:ARG:NH1	2:A:362:LEU:HD22	0.44	2.28	14	1
1:B:4:LYS:CE	2:A:315:GLU:H	0.44	2.26	19	1
1:B:2:ARG:HG3	2:A:333:PHE:HB2	0.43	1.89	2	1
2:A:277:ARG:N	2:A:277:ARG:HD3	0.43	2.27	17	2
2:A:265:CYS:C	2:A:266:LEU:HD12	0.43	2.33	12	1
2:A:264:PHE:CZ	2:A:296:LEU:HD13	0.43	2.48	17	1
2:A:311:TRP:NE1	2:A:338:ASP:OD2	0.43	2.52	12	3
1:B:1:ALA:HB2	2:A:354:PRO:CG	0.43	2.43	7	1
2:A:343:MET:HG2	2:A:350:VAL:HB	0.43	1.89	8	1
2:A:269:SER:OG	2:A:280:GLU:HG2	0.43	2.13	19	3
2:A:330:GLN:OE1	2:A:344:TYR:CD1	0.43	2.71	13	1
2:A:317:LYS:HD2	2:A:338:ASP:OD2	0.43	2.13	16	2
2:A:267:GLY:HA3	2:A:271:MET:O	0.43	2.13	12	3
2:A:261:TYR:HD1	2:A:262:CYS:O	0.43	1.96	20	2
2:A:332:LEU:CD1	2:A:343:MET:HG3	0.43	2.43	13	1
2:A:262:CYS:SG	2:A:264:PHE:HB2	0.43	2.54	19	2
2:A:287:CYS:SG	2:A:289:ARG:HG3	0.43	2.53	1	2
1:B:1:ALA:H1	2:A:354:PRO:HB2	0.43	1.72	8	1
2:A:342:HIS:O	2:A:343:MET:C	0.43	2.56	8	4
1:B:4:LYS:HG2	2:A:328:ASP:CB	0.43	2.43	1	2
1:B:4:LYS:CE	2:A:314:ILE:HG23	0.43	2.44	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:318:SER:HA	2:A:325:SER:HB2	0.43	1.90	7	1
2:A:302:MET:HG3	2:A:303:THR:N	0.43	2.28	14	1
2:A:324:THR:CG2	2:A:326:GLU:HG3	0.43	2.43	16	1
1:B:11:THR:OG1	2:A:297:GLN:NE2	0.43	2.52	19	1
2:A:312:GLN:HB3	2:A:316:CYS:C	0.43	2.34	4	2
2:A:264:PHE:CE2	2:A:291:GLY:HA3	0.43	2.49	13	4
2:A:262:CYS:SG	2:A:264:PHE:N	0.43	2.89	11	1
2:A:296:LEU:HD13	2:A:298:PHE:CE2	0.43	2.49	15	2
1:B:2:ARG:HD3	2:A:297:GLN:NE2	0.43	2.29	18	1
1:B:9:LYS:HD3	1:B:9:LYS:O	0.43	2.14	7	1
2:A:330:GLN:OE1	2:A:342:HIS:CB	0.43	2.67	15	1
2:A:330:GLN:NE2	2:A:344:TYR:HD1	0.42	2.11	15	1
2:A:346:LEU:N	2:A:346:LEU:CD2	0.42	2.80	12	10
2:A:319:CYS:O	2:A:321:LEU:N	0.42	2.52	8	3
1:B:3:THR:HA	2:A:332:LEU:HA	0.42	1.91	15	1
1:B:11:THR:CG2	2:A:296:LEU:O	0.42	2.67	18	1
1:B:9:LYS:HD2	2:A:314:ILE:CG2	0.42	2.43	4	1
2:A:314:ILE:CG2	2:A:315:GLU:OE1	0.42	2.66	4	1
1:B:1:ALA:CB	2:A:354:PRO:CD	0.42	2.97	9	5
2:A:346:LEU:O	2:A:349:PRO:HD3	0.42	2.15	8	7
2:A:317:LYS:O	2:A:318:SER:C	0.42	2.58	5	1
1:B:9:LYS:HG2	2:A:314:ILE:CG2	0.42	2.43	10	1
1:B:4:LYS:HB3	2:A:328:ASP:C	0.42	2.34	11	2
2:A:261:TYR:HB2	2:A:266:LEU:CA	0.42	2.45	11	2
2:A:357:SER:O	2:A:358:TRP:HB3	0.42	2.14	14	1
1:B:2:ARG:HB3	2:A:333:PHE:HD2	0.42	1.74	3	1
2:A:346:LEU:HD13	2:A:358:TRP:CZ2	0.42	2.50	8	1
2:A:264:PHE:CZ	2:A:296:LEU:CD2	0.42	3.02	18	2
2:A:268:GLY:O	2:A:270:ASN:N	0.42	2.53	12	1
2:A:271:MET:HA	2:A:271:MET:CE	0.42	2.45	12	1
1:B:1:ALA:CB	2:A:332:LEU:HD22	0.42	2.41	19	1
1:B:11:THR:HB	2:A:314:ILE:CG1	0.42	2.43	6	1
2:A:361:HIS:CD2	2:A:361:HIS:C	0.42	2.93	12	4
2:A:293:PRO:O	2:A:298:PHE:HB2	0.42	2.15	19	1
2:A:320:ILE:HD13	2:A:339:ARG:HD3	0.42	1.91	20	2
1:B:9:LYS:HA	2:A:314:ILE:HD13	0.42	1.92	12	2
2:A:342:HIS:HB3	2:A:344:TYR:CE1	0.42	2.49	12	1
1:B:4:LYS:HG2	2:A:328:ASP:O	0.42	2.15	15	1
2:A:343:MET:HA	2:A:350:VAL:CG1	0.42	2.43	16	2
2:A:274:LYS:O	2:A:275:SER:HB2	0.42	2.15	18	1
1:B:9:LYS:HA	2:A:333:PHE:CE2	0.42	2.48	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:269:SER:H	2:A:281:LEU:CG	0.42	2.27	12	2
2:A:311:TRP:CD1	2:A:338:ASP:OD2	0.42	2.72	3	1
1:B:11:THR:O	1:B:11:THR:HG22	0.42	2.15	8	1
1:B:4:LYS:O	1:B:9:LYS:HE3	0.42	2.14	15	1
2:A:292:HIS:O	2:A:295:CYS:N	0.42	2.53	17	1
2:A:301:ASN:HB3	2:A:336:ASP:O	0.42	2.15	19	1
2:A:261:TYR:HB2	2:A:266:LEU:C	0.42	2.35	15	1
2:A:326:GLU:H	2:A:342:HIS:CE1	0.41	2.33	3	1
2:A:330:GLN:HA	2:A:330:GLN:HE21	0.41	1.75	3	2
1:B:1:ALA:CB	2:A:354:PRO:HD2	0.41	2.45	4	1
1:B:4:LYS:NZ	1:B:4:LYS:HB3	0.41	2.30	8	1
2:A:271:MET:HE1	2:A:276:GLY:O	0.41	2.15	6	6
2:A:314:ILE:C	2:A:316:CYS:H	0.41	2.18	5	1
2:A:341:TYR:OH	2:A:361:HIS:HB2	0.41	2.14	10	1
2:A:327:ASN:O	2:A:329:ASP:N	0.41	2.52	13	1
2:A:263:ASP:HB3	2:A:289:ARG:HD2	0.41	1.92	18	1
2:A:314:ILE:C	2:A:316:CYS:N	0.41	2.74	3	1
2:A:302:MET:HA	2:A:337:CYS:O	0.41	2.15	5	1
2:A:332:LEU:HD21	2:A:350:VAL:HG21	0.41	1.91	6	2
1:B:11:THR:C	2:A:314:ILE:HD12	0.41	2.35	8	1
1:B:4:LYS:HD2	2:A:333:PHE:HE1	0.41	1.73	9	1
1:B:2:ARG:O	2:A:333:PHE:N	0.41	2.53	7	1
2:A:262:CYS:HA	2:A:290:SER:O	0.41	2.14	18	3
2:A:267:GLY:CA	2:A:273:LYS:HG2	0.41	2.45	8	1
1:B:15:ALA:HB1	2:A:266:LEU:HD21	0.41	1.92	9	1
2:A:264:PHE:HE2	2:A:292:HIS:N	0.41	2.12	13	2
2:A:296:LEU:HB3	2:A:298:PHE:CD1	0.41	2.50	12	1
2:A:302:MET:SD	2:A:306:VAL:HG13	0.41	2.55	14	1
2:A:311:TRP:CG	2:A:312:GLN:N	0.41	2.88	1	2
2:A:322:CYS:CB	2:A:324:THR:HG22	0.41	2.46	9	2
1:B:11:THR:O	1:B:12:GLY:C	0.41	2.58	19	1
2:A:296:LEU:O	2:A:297:GLN:HG2	0.41	2.15	19	1
1:B:1:ALA:HB2	2:A:354:PRO:HG2	0.41	1.92	6	1
2:A:330:GLN:NE2	2:A:343:MET:CB	0.41	2.80	13	1
2:A:262:CYS:O	2:A:266:LEU:HD22	0.41	2.16	5	1
2:A:328:ASP:O	2:A:329:ASP:C	0.41	2.57	14	1
1:B:9:LYS:C	1:B:11:THR:N	0.41	2.74	15	1
2:A:341:TYR:OH	2:A:361:HIS:ND1	0.41	2.54	14	1
2:A:360:CYS:O	2:A:363:CYS:SG	0.41	2.79	2	1
2:A:321:LEU:HD12	2:A:345:CYS:HB3	0.41	1.93	8	1
2:A:350:VAL:HG12	2:A:351:ALA:N	0.41	2.31	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:296:LEU:HD23	2:A:298:PHE:CE2	0.41	2.50	9	1
1:B:4:LYS:HB2	2:A:331:LEU:HB3	0.41	1.92	15	2
1:B:13:GLY:O	2:A:263:ASP:O	0.41	2.39	19	1
2:A:337:CYS:HB2	2:A:339:ARG:HG3	0.41	1.93	3	1
2:A:281:LEU:HB3	2:A:290:SER:HB3	0.41	1.90	5	1
1:B:15:ALA:N	2:A:263:ASP:HB2	0.41	2.31	19	1
2:A:294:THR:CG2	2:A:295:CYS:N	0.40	2.83	2	1
2:A:293:PRO:O	2:A:298:PHE:N	0.40	2.53	3	1
2:A:265:CYS:SG	2:A:273:LYS:HB2	0.40	2.56	7	1
2:A:325:SER:O	2:A:325:SER:OG	0.40	2.38	9	1
2:A:330:GLN:NE2	2:A:344:TYR:CD1	0.40	2.89	15	1
2:A:337:CYS:O	2:A:338:ASP:OD2	0.40	2.39	17	1
2:A:264:PHE:CD2	2:A:295:CYS:HB3	0.40	2.51	18	1
1:B:11:THR:C	2:A:264:PHE:CZ	0.40	2.95	19	1
2:A:265:CYS:O	2:A:273:LYS:HG3	0.40	2.15	19	1
2:A:303:THR:HG22	2:A:307:LYS:HD3	0.40	1.93	20	1
2:A:341:TYR:CE2	2:A:360:CYS:HB2	0.40	2.51	6	1
1:B:11:THR:HG21	2:A:298:PHE:HE1	0.40	1.76	16	1
2:A:334:CYS:HB3	2:A:339:ARG:N	0.40	2.31	1	1
2:A:346:LEU:CD1	2:A:350:VAL:CG1	0.40	2.99	12	1
2:A:318:SER:CB	2:A:325:SER:HB3	0.40	2.45	4	1
2:A:300:LEU:O	2:A:300:LEU:HD13	0.40	2.17	5	1
1:B:3:THR:HA	2:A:331:LEU:O	0.40	2.16	8	1
2:A:341:TYR:HB2	2:A:346:LEU:CD2	0.40	2.46	9	1
2:A:271:MET:CE	2:A:271:MET:HA	0.40	2.47	10	1
2:A:320:ILE:HD12	2:A:339:ARG:NH1	0.40	2.30	17	1
2:A:286:ASP:HB2	2:A:312:GLN:HE22	0.40	1.76	1	1
2:A:285:ALA:HB1	2:A:310:LYS:HD2	0.40	1.93	12	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	10/20 (50%)	4±1 (43±13%)	4±1 (36±12%)	2±1 (20±9%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	104/114 (91%)	74±3 (71±3%)	20±3 (20±3%)	10±2 (9±2%)	1 11
All	All	2280/2680 (85%)	1564 (69%)	481 (21%)	235 (10%)	1 9

All 39 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	15	ALA	20
2	A	314	ILE	20
2	A	331	LEU	20
2	A	348	PRO	20
2	A	310	LYS	17
2	A	329	ASP	17
2	A	354	PRO	15
2	A	338	ASP	13
2	A	346	LEU	10
1	B	2	ARG	8
2	A	317	LYS	7
2	A	319	CYS	7
2	A	326	GLU	6
2	A	270	ASN	5
2	A	360	CYS	5
2	A	320	ILE	5
2	A	343	MET	5
2	A	268	GLY	4
1	B	16	PRO	3
1	B	11	THR	3
2	A	297	GLN	3
1	B	10	SER	3
2	A	328	ASP	2
1	B	12	GLY	2
1	B	9	LYS	1
1	B	4	LYS	1
2	A	356	GLY	1
2	A	353	PRO	1
2	A	325	SER	1
2	A	298	PHE	1
2	A	267	GLY	1
2	A	269	SER	1
2	A	272	ASN	1
2	A	260	SER	1
2	A	316	CYS	1

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Mol	Chain	Res	Type	Models (Total)
2	A	275	SER	1
2	A	277	ARG	1
2	A	315	GLU	1
2	A	265	CYS	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	7/14 (50%)	6±1 (89±12%)	1±1 (11±12%)	9 52
2	A	93/101 (92%)	76±3 (82±3%)	17±3 (18±3%)	4 38
All	All	2000/2300 (87%)	1652 (83%)	348 (17%)	4 39

All 53 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	309	TYR	20
2	A	320	ILE	20
2	A	331	LEU	20
2	A	341	TYR	20
2	A	262	CYS	19
2	A	271	MET	19
2	A	319	CYS	19
2	A	281	LEU	18
2	A	337	CYS	15
2	A	330	GLN	14
2	A	294	THR	13
2	A	336	ASP	12
2	A	317	LYS	9
2	A	359	SER	8
2	A	308	THR	8
2	A	324	THR	8
2	A	363	CYS	7
2	A	334	CYS	6
2	A	263	ASP	6
2	A	328	ASP	6

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Mol	Chain	Res	Type	Models (Total)
2	A	264	PHE	6
2	A	277	ARG	6
2	A	300	LEU	5
2	A	329	ASP	5
2	A	338	ASP	4
1	B	9	LYS	4
2	A	280	GLU	4
2	A	350	VAL	4
1	B	4	LYS	3
2	A	347	ASN	3
2	A	360	CYS	3
1	B	11	THR	3
2	A	269	SER	3
1	B	2	ARG	3
2	A	335	ASP	2
2	A	332	LEU	2
1	B	3	THR	2
2	A	286	ASP	2
2	A	304	GLU	2
2	A	289	ARG	2
1	B	10	SER	1
2	A	266	LEU	1
2	A	290	SER	1
2	A	315	GLU	1
2	A	343	MET	1
2	A	296	LEU	1
2	A	361	HIS	1
2	A	362	LEU	1
2	A	310	LYS	1
2	A	312	GLN	1
2	A	355	GLU	1
2	A	302	MET	1
2	A	282	VAL	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	ALY	B	14	1	10,11,12	0.67±0.08	0±0 (1±3%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	ALY	B	14	1	7,12,14	0.99±0.11	0±0 (2±6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ALY	B	14	1	-	0±0,9,10,12	-

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	14	ALY	CH3-CH	2.14	1.55	1.50	10	2

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	14	ALY	OH-CH-CH3	2.51	117.39	122.06	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	14	ALY	CH3-CH-NZ	2.27	120.11	116.09	16	2

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)

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 (i)

No chemical shift data were provided