



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:18 AM BST

PDB ID : 2KWK
Title : Solution structures of the double PHD fingers of human transcriptional protein DPF3b bound to a H3 peptide wild type
Authors : Zeng, L.; Zhang, Q.; Li, S.; Plotnikov, A.N.; Walsh, M.J.; Zhou, M.
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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

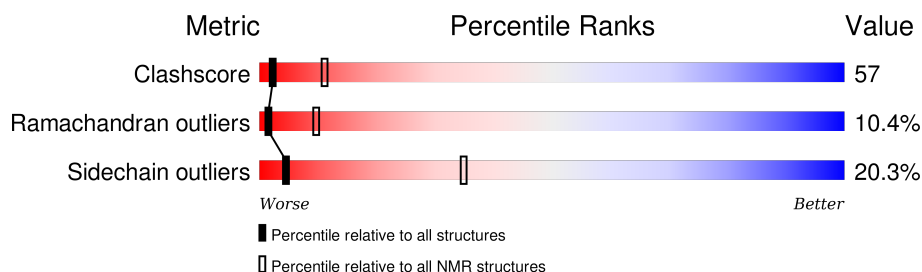
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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

Mol	Chain	Length	Quality of chain
1	B	20	
2	A	114	

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:1-B:4, A:260-A:274, A:278-A:363 (105)	0.26	7

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

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

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

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2021 atoms, of which 984 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
			327	91	174	35	27	

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms	
3	A	4	Total	Zn
			4	4

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

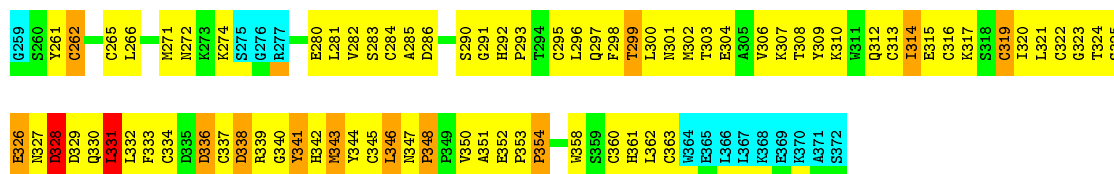
- Molecule 1: Histone peptide

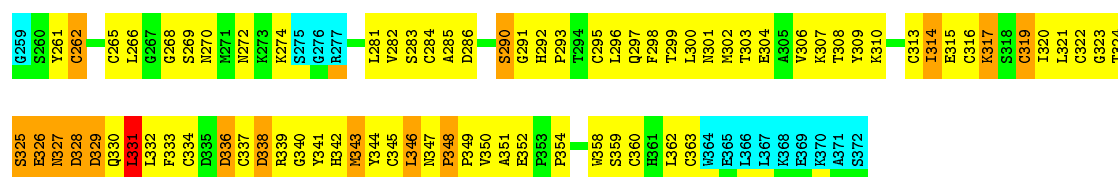
Chain B: 



- Molecule 2: Zinc finger protein DPF3

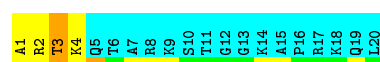
Chain A: 



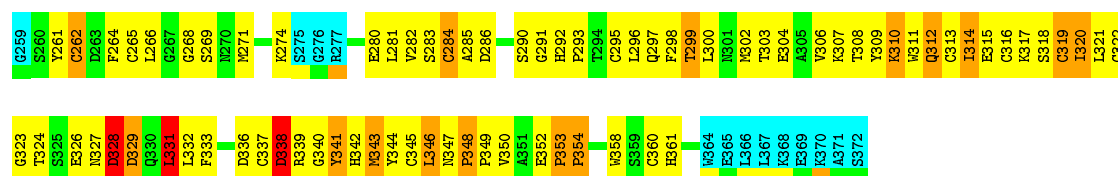


4.2.2 Score per residue for model 2

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3

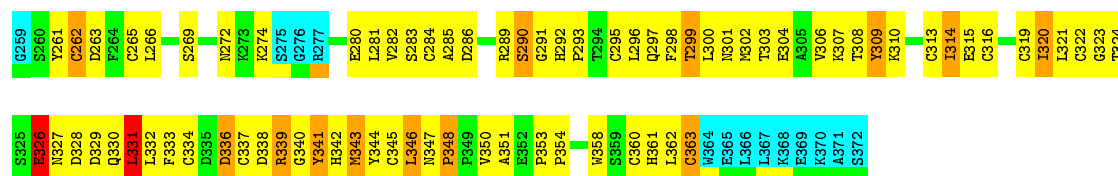


4.2.3 Score per residue for model 3

- Molecule 1: Histone peptide



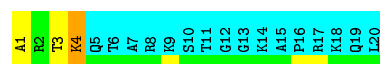
- Molecule 2: Zinc finger protein DPF3




4.2.4 Score per residue for model 4

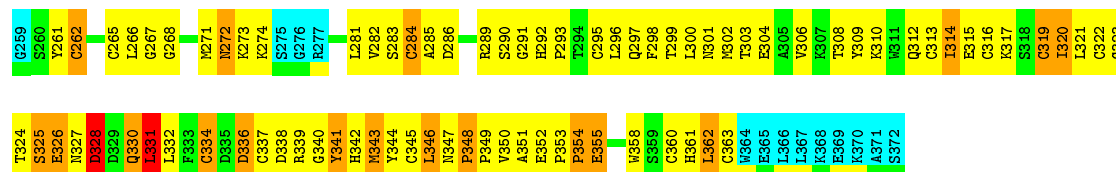
- Molecule 1: Histone peptide

Chain B:  5% 10% 5% 80%



- Molecule 2: Zinc finger protein DPF3

Chain A:  18% 53% 16% 11%



4.2.5 Score per residue for model 5

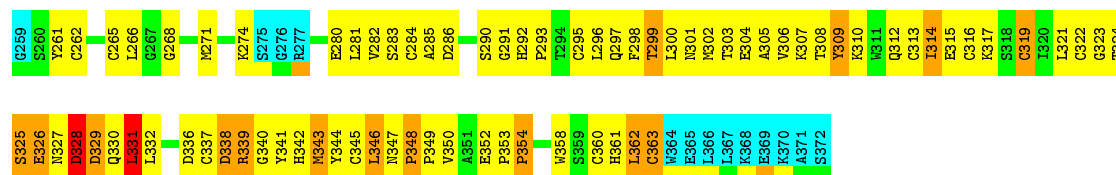
- Molecule 1: Histone peptide

Chain B:  5% 10% 5% 80%



- Molecule 2: Zinc finger protein DPF3

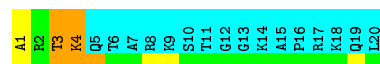
Chain A:  22% 52% 13% 11%



4.2.6 Score per residue for model 6

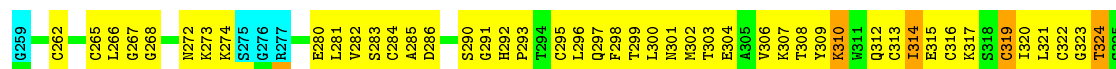
- Molecule 1: Histone peptide

Chain B:  5% 5% 10% 80%



- Molecule 2: Zinc finger protein DPF3

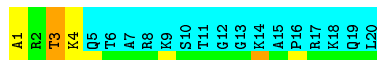
Chain A:  20% 59% 8% 11%





4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Histone peptide

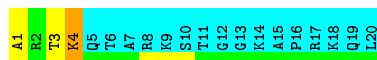


- Molecule 2: Zinc finger protein DPF3



4.2.8 Score per residue for model 8

- Molecule 1: Histone peptide



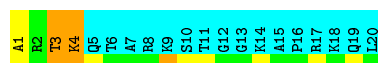
- Molecule 2: Zinc finger protein DPF3



4.2.9 Score per residue for model 9

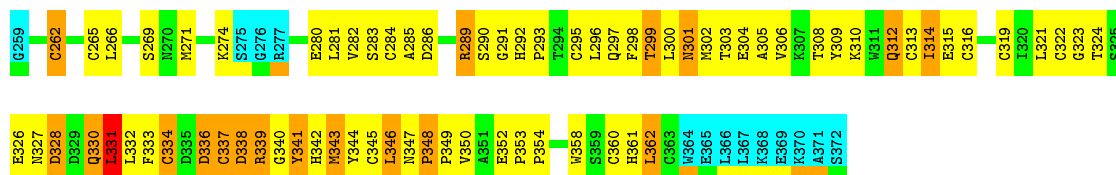
- Molecule 1: Histone peptide





- Molecule 2: Zinc finger protein DPF3

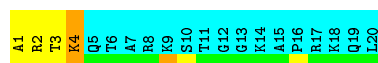
Chain A: 25% 47% 16% 11%



4.2.10 Score per residue for model 10

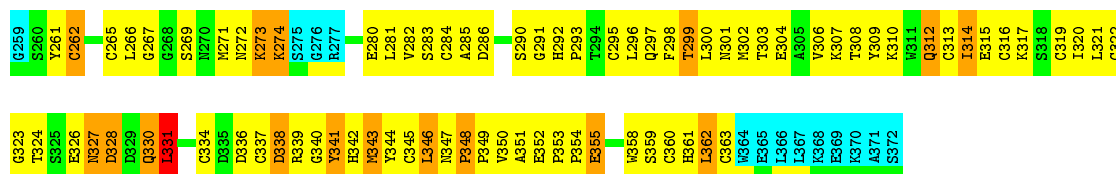
- Molecule 1: Histone peptide

Chain B: 15% 5% 80%



- Molecule 2: Zinc finger protein DPF3

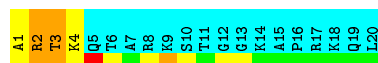
Chain A: 18% 55% 14% 11%



4.2.11 Score per residue for model 11

- Molecule 1: Histone peptide

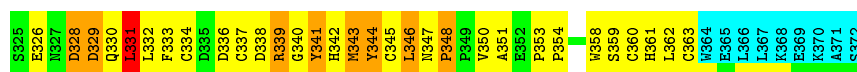
Chain B: 10% 10% 80%



- Molecule 2: Zinc finger protein DPF3

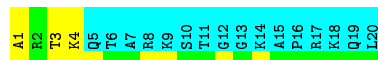
Chain A: 22% 51% 15% 11%



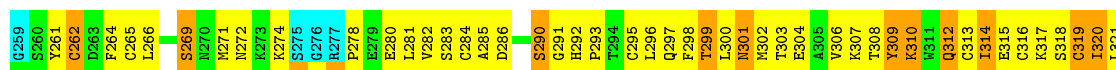


4.2.12 Score per residue for model 12

- Molecule 1: Histone peptide

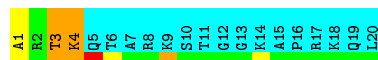


- Molecule 2: Zinc finger protein DPF3

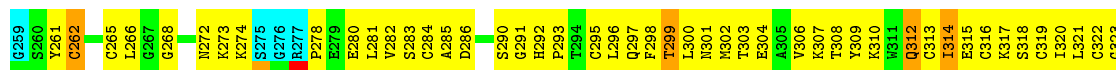


4.2.13 Score per residue for model 13

- Molecule 1: Histone peptide



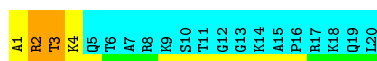
- Molecule 2: Zinc finger protein DPF3



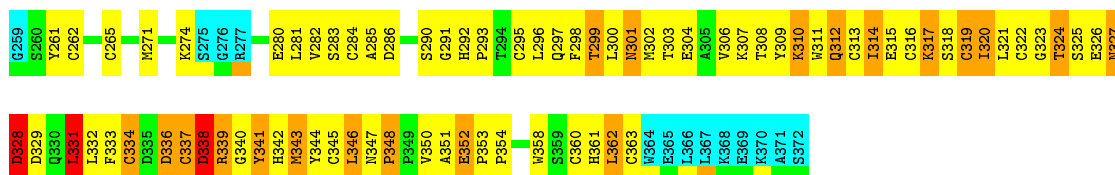
4.2.14 Score per residue for model 14

- Molecule 1: Histone peptide



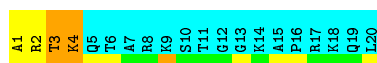


- Molecule 2: Zinc finger protein DPF3

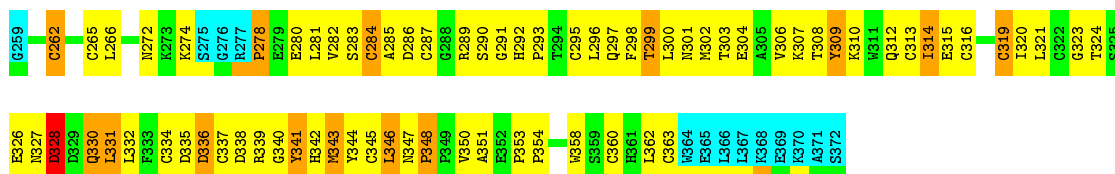


4.2.15 Score per residue for model 15

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3

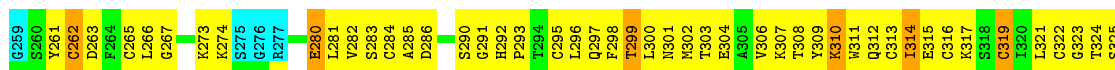
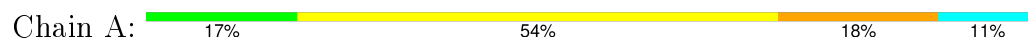


4.2.16 Score per residue for model 16

- Molecule 1: Histone peptide



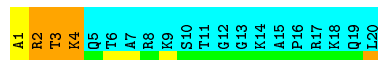
- Molecule 2: Zinc finger protein DPF3



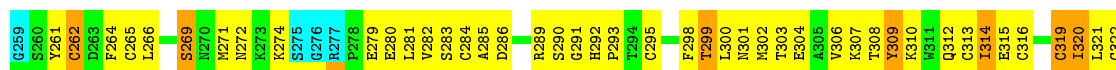


4.2.17 Score per residue for model 17

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3

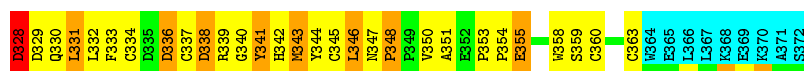
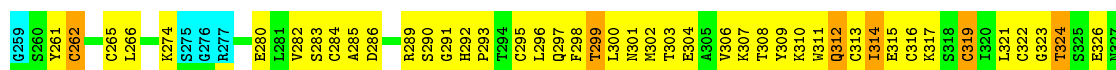


4.2.18 Score per residue for model 18

- Molecule 1: Histone peptide



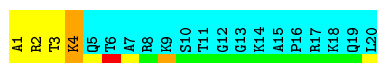
- Molecule 2: Zinc finger protein DPF3



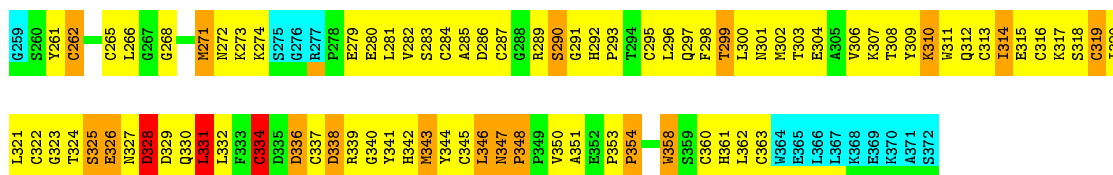
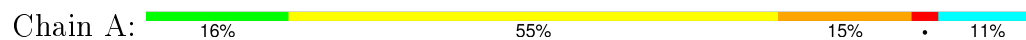
4.2.19 Score per residue for model 19

- Molecule 1: Histone peptide



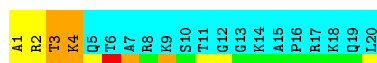


- Molecule 2: Zinc finger protein DPF3

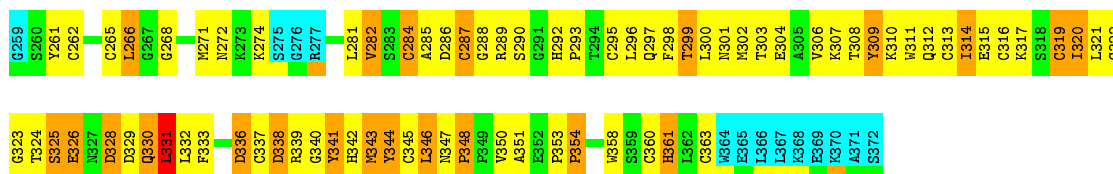
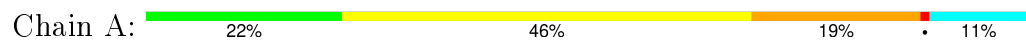


4.2.20 Score per residue for model 20

- Molecule 1: Histone peptide



- Molecule 2: Zinc finger protein DPF3



5 Refinement protocol and experimental data overview ⓘ

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

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

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

Software name	Classification	Version
ARIA	refinement	2.2
CNS	structure solution	1.2

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

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	32	40	40	8±3
2	A	777	704	703	89±8
All	All	16260	14880	14860	1788

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 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:346:LEU:HD12	2:A:350:VAL:HG23	0.82	1.48	2	19
2:A:322:CYS:SG	2:A:324:THR:HG22	0.79	2.18	8	1
2:A:298:PHE:CE2	2:A:306:VAL:HG11	0.78	2.13	14	20
2:A:284:CYS:HB2	2:A:313:CYS:N	0.77	1.94	4	2
2:A:314:ILE:HG22	2:A:315:GLU:N	0.77	1.94	9	18
2:A:346:LEU:HD23	2:A:346:LEU:N	0.74	1.98	5	10
2:A:265:CYS:HB3	2:A:274:LYS:HG3	0.74	1.59	20	10
1:B:4:LYS:HG2	2:A:333:PHE:CZ	0.74	2.17	9	4
2:A:302:MET:HA	2:A:337:CYS:HA	0.71	1.62	12	20
2:A:346:LEU:N	2:A:346:LEU:HD23	0.71	2.01	14	9
2:A:321:LEU:HD11	2:A:341:TYR:CD2	0.70	2.21	17	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:341:TYR:HB3	2:A:346:LEU:HD22	0.70	1.64	5	5
2:A:303:THR:O	2:A:306:VAL:HG22	0.70	1.86	6	20
2:A:342:HIS:HB2	2:A:345:CYS:SG	0.70	2.26	1	20
2:A:292:HIS:HB2	2:A:295:CYS:SG	0.70	2.26	11	2
2:A:317:LYS:HZ1	2:A:340:GLY:HA3	0.69	1.46	12	1
2:A:265:CYS:HB3	2:A:274:LYS:HG2	0.69	1.62	16	7
2:A:284:CYS:HB2	2:A:313:CYS:HB3	0.69	1.63	10	18
2:A:337:CYS:SG	2:A:339:ARG:HG3	0.69	2.27	17	4
2:A:302:MET:O	2:A:306:VAL:HG13	0.68	1.89	8	20
1:B:1:ALA:H3	2:A:355:GLU:N	0.68	1.86	17	1
2:A:341:TYR:HH	2:A:361:HIS:CG	0.67	2.08	14	8
1:B:1:ALA:HB3	2:A:354:PRO:HD2	0.67	1.67	5	17
2:A:350:VAL:HG11	2:A:354:PRO:HD3	0.67	1.65	8	20
2:A:284:CYS:SG	2:A:285:ALA:N	0.66	2.67	13	20
2:A:313:CYS:O	2:A:315:GLU:N	0.66	2.29	20	20
2:A:321:LEU:HD12	2:A:345:CYS:CB	0.66	2.20	17	13
1:B:1:ALA:HB2	2:A:358:TRP:HB3	0.65	1.67	17	8
2:A:336:ASP:HB3	2:A:363:CYS:SG	0.65	2.31	12	4
1:B:4:LYS:HD3	2:A:328:ASP:HB2	0.64	1.69	16	4
2:A:317:LYS:HZ1	2:A:331:LEU:HD11	0.64	1.52	12	1
1:B:1:ALA:HB2	2:A:358:TRP:CB	0.64	2.22	17	17
2:A:319:CYS:HA	2:A:340:GLY:O	0.64	1.92	14	20
2:A:321:LEU:HD12	2:A:345:CYS:HB2	0.64	1.67	2	13
2:A:282:VAL:HG23	2:A:293:PRO:HD3	0.63	1.70	18	18
2:A:346:LEU:CD1	2:A:350:VAL:HG23	0.62	2.24	8	19
2:A:317:LYS:NZ	2:A:340:GLY:HA3	0.62	2.09	12	1
2:A:317:LYS:NZ	2:A:333:PHE:CD2	0.62	2.64	18	2
1:B:4:LYS:HE2	2:A:314:ILE:HG22	0.62	1.71	20	1
2:A:346:LEU:H	2:A:346:LEU:CD1	0.62	2.08	7	1
2:A:314:ILE:HD13	2:A:333:PHE:CE1	0.61	2.31	16	3
2:A:337:CYS:O	2:A:338:ASP:HB3	0.61	1.95	18	3
2:A:319:CYS:SG	2:A:321:LEU:HB2	0.61	2.36	1	20
2:A:347:ASN:HB2	2:A:348:PRO:HD3	0.60	1.73	1	19
2:A:314:ILE:CG2	2:A:315:GLU:N	0.60	2.63	9	13
2:A:341:TYR:HB3	2:A:346:LEU:CD2	0.60	2.26	5	19
2:A:321:LEU:HD21	2:A:341:TYR:CZ	0.60	2.32	6	10
1:B:4:LYS:HB3	2:A:328:ASP:O	0.60	1.95	11	11
2:A:265:CYS:SG	2:A:274:LYS:HG3	0.60	2.36	11	2
2:A:285:ALA:HB2	2:A:310:LYS:HD2	0.59	1.72	5	6
2:A:346:LEU:N	2:A:346:LEU:CD1	0.59	2.65	7	1
2:A:286:ASP:HB3	2:A:316:CYS:SG	0.59	2.37	4	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:346:LEU:H	2:A:346:LEU:HD23	0.59	1.58	14	10
2:A:317:LYS:HD3	2:A:331:LEU:HD11	0.59	1.75	14	1
2:A:282:VAL:O	2:A:290:SER:HA	0.59	1.98	12	17
2:A:320:ILE:HG23	2:A:321:LEU:HD23	0.59	1.75	3	5
2:A:262:CYS:O	2:A:266:LEU:HG	0.58	1.98	11	12
2:A:324:THR:HB	2:A:326:GLU:HG2	0.58	1.75	16	6
2:A:286:ASP:HB2	2:A:316:CYS:SG	0.58	2.39	20	11
2:A:346:LEU:N	2:A:346:LEU:CD2	0.58	2.66	5	7
1:B:1:ALA:HB3	2:A:354:PRO:CD	0.58	2.29	17	2
2:A:304:GLU:O	2:A:308:THR:HG23	0.57	1.99	20	20
2:A:285:ALA:HB2	2:A:310:LYS:HD3	0.57	1.76	3	3
2:A:342:HIS:O	2:A:344:TYR:N	0.57	2.37	7	20
2:A:283:SER:HA	2:A:289:ARG:O	0.57	2.00	9	2
2:A:293:PRO:HG2	2:A:303:THR:HG23	0.57	1.76	11	17
2:A:341:TYR:CZ	2:A:360:CYS:HB2	0.57	2.34	15	18
2:A:346:LEU:CD2	2:A:350:VAL:HG23	0.57	2.29	7	1
1:B:4:LYS:HD3	2:A:328:ASP:CB	0.56	2.30	3	12
2:A:322:CYS:O	2:A:324:THR:HG23	0.56	2.00	3	15
2:A:341:TYR:HH	2:A:361:HIS:CE1	0.56	2.19	4	7
2:A:262:CYS:SG	2:A:264:PHE:HB2	0.56	2.41	17	3
2:A:292:HIS:O	2:A:295:CYS:SG	0.56	2.63	11	1
2:A:298:PHE:HA	2:A:302:MET:SD	0.55	2.42	10	20
2:A:339:ARG:HD2	2:A:362:LEU:HB2	0.55	1.76	9	6
2:A:337:CYS:O	2:A:338:ASP:CB	0.55	2.54	18	7
2:A:319:CYS:O	2:A:323:GLY:N	0.55	2.40	19	20
2:A:303:THR:HG22	2:A:307:LYS:HE3	0.55	1.77	11	12
2:A:343:MET:HA	2:A:346:LEU:HD11	0.55	1.79	19	19
2:A:261:TYR:O	2:A:290:SER:HB2	0.55	2.02	11	10
2:A:286:ASP:HB2	2:A:316:CYS:HB3	0.55	1.79	17	3
2:A:282:VAL:HG12	2:A:293:PRO:HD3	0.55	1.77	8	2
2:A:299:THR:HG23	2:A:302:MET:SD	0.54	2.41	14	14
1:B:4:LYS:NZ	2:A:315:GLU:HA	0.54	2.17	18	3
2:A:265:CYS:HB2	2:A:273:LYS:HB2	0.54	1.78	19	1
1:B:3:THR:HG21	2:A:343:MET:SD	0.54	2.42	17	2
2:A:354:PRO:HG2	2:A:358:TRP:CD1	0.54	2.37	9	4
2:A:311:TRP:NE1	2:A:338:ASP:OD2	0.54	2.40	14	2
2:A:261:TYR:CD1	2:A:266:LEU:HB3	0.54	2.38	20	1
2:A:334:CYS:HB2	2:A:360:CYS:HB3	0.54	1.80	3	14
2:A:322:CYS:SG	2:A:324:THR:HG23	0.54	2.43	18	4
2:A:346:LEU:HD23	2:A:346:LEU:H	0.53	1.63	9	8
1:B:4:LYS:HG3	2:A:331:LEU:HB3	0.53	1.80	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:267:GLY:HA2	2:A:273:LYS:HE3	0.53	1.81	10	2
1:B:3:THR:HG22	2:A:332:LEU:CD2	0.53	2.34	20	14
2:A:317:LYS:O	2:A:317:LYS:NZ	0.53	2.41	14	1
2:A:282:VAL:HG12	2:A:283:SER:H	0.53	1.62	9	18
1:B:1:ALA:CB	2:A:332:LEU:HD22	0.53	2.34	3	6
2:A:355:GLU:CD	2:A:355:GLU:N	0.53	2.62	16	2
2:A:313:CYS:O	2:A:313:CYS:SG	0.53	2.67	20	10
2:A:292:HIS:C	2:A:296:LEU:HD12	0.53	2.25	3	17
1:B:1:ALA:HB2	2:A:354:PRO:CD	0.53	2.33	14	1
2:A:339:ARG:HD2	2:A:360:CYS:SG	0.52	2.44	7	5
2:A:341:TYR:CB	2:A:346:LEU:HD22	0.52	2.34	2	14
2:A:328:ASP:HA	2:A:331:LEU:CB	0.52	2.34	14	12
2:A:284:CYS:HB3	2:A:289:ARG:N	0.52	2.19	18	2
1:B:1:ALA:HB3	2:A:332:LEU:HD22	0.52	1.80	3	4
2:A:346:LEU:H	2:A:346:LEU:CD2	0.52	2.18	10	10
1:B:1:ALA:HB2	2:A:358:TRP:HB2	0.52	1.81	18	10
2:A:299:THR:HG23	2:A:302:MET:HG3	0.52	1.82	18	10
1:B:1:ALA:CB	2:A:354:PRO:HD2	0.51	2.35	14	3
2:A:336:ASP:CB	2:A:363:CYS:SG	0.51	2.98	19	2
2:A:346:LEU:CD2	2:A:346:LEU:H	0.51	2.17	12	6
1:B:2:ARG:O	2:A:332:LEU:HA	0.51	2.05	14	1
2:A:309:TYR:OH	2:A:337:CYS:HB2	0.51	2.05	20	4
2:A:300:LEU:HD13	2:A:300:LEU:O	0.51	2.06	4	10
2:A:293:PRO:CG	2:A:307:LYS:HZ1	0.51	2.18	2	5
2:A:321:LEU:HD21	2:A:341:TYR:CE2	0.51	2.41	15	12
2:A:333:PHE:HA	2:A:339:ARG:O	0.51	2.05	13	3
1:B:4:LYS:HE3	2:A:314:ILE:O	0.51	2.04	2	6
1:B:4:LYS:HB3	1:B:4:LYS:NZ	0.51	2.21	3	1
2:A:282:VAL:HG12	2:A:283:SER:N	0.51	2.20	9	18
2:A:347:ASN:N	2:A:348:PRO:CD	0.51	2.74	17	17
2:A:314:ILE:HG23	2:A:333:PHE:CE2	0.51	2.41	20	2
2:A:341:TYR:CB	2:A:346:LEU:CD2	0.51	2.89	17	14
2:A:340:GLY:C	2:A:341:TYR:HD1	0.50	2.09	9	15
2:A:285:ALA:HB3	2:A:312:GLN:HG2	0.50	1.83	16	12
2:A:346:LEU:CD2	2:A:346:LEU:N	0.50	2.73	20	3
2:A:342:HIS:O	2:A:345:CYS:N	0.50	2.45	15	19
2:A:350:VAL:CG1	2:A:354:PRO:HD3	0.50	2.37	12	11
2:A:331:LEU:C	2:A:331:LEU:HD12	0.50	2.26	14	5
2:A:262:CYS:O	2:A:266:LEU:N	0.50	2.44	17	1
2:A:284:CYS:SG	2:A:288:GLY:N	0.50	2.83	20	1
2:A:281:LEU:HD22	2:A:290:SER:OG	0.50	2.07	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:300:LEU:O	2:A:300:LEU:HD13	0.50	2.07	7	10
2:A:296:LEU:O	2:A:297:GLN:HB2	0.50	2.07	15	18
2:A:320:ILE:HG22	2:A:340:GLY:O	0.50	2.07	2	8
1:B:4:LYS:HE3	2:A:315:GLU:HA	0.50	1.84	9	1
2:A:341:TYR:HB3	2:A:346:LEU:HD12	0.50	1.83	7	1
2:A:298:PHE:CD1	2:A:302:MET:HE2	0.50	2.42	18	10
2:A:331:LEU:HD12	2:A:331:LEU:C	0.49	2.28	1	11
2:A:261:TYR:C	2:A:290:SER:HG	0.49	2.10	1	3
2:A:336:ASP:HB2	2:A:363:CYS:SG	0.49	2.47	19	2
2:A:313:CYS:SG	2:A:313:CYS:O	0.49	2.70	2	9
2:A:354:PRO:HG2	2:A:358:TRP:HB2	0.49	1.85	20	17
2:A:284:CYS:CB	2:A:313:CYS:HB3	0.49	2.37	20	2
1:B:1:ALA:HA	1:B:2:ARG:HH21	0.49	1.67	17	1
2:A:267:GLY:HA2	2:A:273:LYS:CE	0.49	2.38	4	1
1:B:1:ALA:HB3	2:A:354:PRO:CG	0.49	2.38	17	1
1:B:1:ALA:N	2:A:356:GLY:N	0.49	2.61	17	1
2:A:285:ALA:HB2	2:A:310:LYS:CD	0.49	2.37	4	8
2:A:355:GLU:N	2:A:355:GLU:CD	0.49	2.66	10	2
2:A:324:THR:O	2:A:325:SER:CB	0.49	2.61	4	7
2:A:330:GLN:HA	2:A:330:GLN:HE21	0.49	1.68	10	5
2:A:317:LYS:CD	2:A:331:LEU:HD11	0.49	2.38	14	1
2:A:346:LEU:HD13	2:A:358:TRP:CZ2	0.49	2.43	17	4
2:A:262:CYS:HA	2:A:290:SER:HG	0.49	1.68	12	2
2:A:353:PRO:O	2:A:355:GLU:N	0.49	2.46	17	1
2:A:314:ILE:C	2:A:316:CYS:H	0.48	2.11	10	7
2:A:285:ALA:HB2	2:A:310:LYS:HB3	0.48	1.84	18	1
2:A:341:TYR:CE1	2:A:360:CYS:HB2	0.48	2.43	7	1
2:A:306:VAL:HG12	2:A:338:ASP:OD2	0.48	2.08	2	1
2:A:282:VAL:HG23	2:A:291:GLY:O	0.48	2.08	5	18
2:A:273:LYS:HD3	2:A:273:LYS:N	0.48	2.22	10	1
1:B:4:LYS:HE2	2:A:314:ILE:O	0.48	2.08	18	3
2:A:314:ILE:HG23	2:A:333:PHE:CZ	0.48	2.43	18	2
2:A:281:LEU:HB3	2:A:290:SER:HB3	0.48	1.86	8	9
1:B:1:ALA:HB1	2:A:354:PRO:HD2	0.48	1.84	12	1
2:A:317:LYS:O	2:A:331:LEU:HD21	0.48	2.09	7	5
1:B:3:THR:HG22	2:A:332:LEU:HD21	0.48	1.86	20	4
2:A:280:GLU:HG3	2:A:281:LEU:N	0.48	2.24	10	3
2:A:317:LYS:HZ3	2:A:333:PHE:HD2	0.48	1.45	2	1
2:A:347:ASN:O	2:A:349:PRO:HD3	0.48	2.09	2	10
2:A:330:GLN:HE21	2:A:330:GLN:HA	0.48	1.68	9	1
2:A:350:VAL:O	2:A:351:ALA:HB3	0.47	2.09	12	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:296:LEU:HD13	2:A:298:PHE:CE2	0.47	2.44	3	4
2:A:322:CYS:SG	2:A:324:THR:CG2	0.47	2.98	8	1
2:A:330:GLN:HA	2:A:343:MET:SD	0.47	2.50	15	5
2:A:327:ASN:ND2	2:A:344:TYR:OH	0.47	2.47	15	8
2:A:268:GLY:O	2:A:292:HIS:NE2	0.47	2.47	2	6
2:A:341:TYR:HB3	2:A:346:LEU:CD1	0.47	2.39	7	1
2:A:343:MET:O	2:A:346:LEU:HG	0.47	2.10	12	17
2:A:287:CYS:HB2	2:A:289:ARG:HG3	0.47	1.87	20	3
2:A:314:ILE:HG22	2:A:315:GLU:CD	0.47	2.29	16	2
2:A:334:CYS:SG	2:A:337:CYS:N	0.47	2.87	9	2
1:B:1:ALA:N	2:A:354:PRO:HB2	0.47	2.24	8	3
2:A:312:GLN:NE2	2:A:317:LYS:HA	0.47	2.25	16	1
2:A:346:LEU:N	2:A:346:LEU:HD12	0.47	2.24	7	1
1:B:4:LYS:HB3	2:A:328:ASP:HB2	0.47	1.87	12	4
2:A:292:HIS:HB2	2:A:295:CYS:HB2	0.47	1.87	15	18
2:A:328:ASP:O	2:A:330:GLN:N	0.47	2.48	11	2
2:A:324:THR:OG1	2:A:326:GLU:HG3	0.47	2.10	3	2
2:A:303:THR:O	2:A:307:LYS:HD2	0.46	2.10	14	1
2:A:346:LEU:HD13	2:A:346:LEU:H	0.46	1.70	7	1
2:A:317:LYS:HD3	2:A:338:ASP:O	0.46	2.10	11	9
2:A:265:CYS:SG	2:A:273:LYS:HB2	0.46	2.50	4	1
2:A:293:PRO:CG	2:A:303:THR:HG23	0.46	2.41	14	11
2:A:328:ASP:HA	2:A:331:LEU:HB2	0.46	1.87	8	5
2:A:334:CYS:SG	2:A:338:ASP:N	0.46	2.89	9	1
2:A:311:TRP:HE1	2:A:317:LYS:NZ	0.46	2.09	19	1
1:B:4:LYS:HB2	2:A:328:ASP:O	0.46	2.11	16	3
2:A:317:LYS:HZ1	2:A:340:GLY:HA2	0.46	1.71	2	2
2:A:303:THR:CG2	2:A:307:LYS:HE3	0.45	2.42	18	11
2:A:322:CYS:SG	2:A:324:THR:OG1	0.45	2.68	16	2
2:A:271:MET:HG2	2:A:273:LYS:NZ	0.45	2.26	19	1
2:A:306:VAL:HG12	2:A:338:ASP:CG	0.45	2.32	19	2
2:A:311:TRP:O	2:A:317:LYS:NZ	0.45	2.50	16	1
2:A:301:ASN:HB3	2:A:336:ASP:O	0.45	2.12	20	1
2:A:334:CYS:SG	2:A:336:ASP:N	0.45	2.89	3	6
2:A:267:GLY:CA	2:A:273:LYS:HG3	0.45	2.42	4	3
2:A:302:MET:HG2	2:A:336:ASP:C	0.45	2.32	17	3
2:A:305:ALA:CB	2:A:337:CYS:HB3	0.45	2.42	9	1
2:A:320:ILE:N	2:A:340:GLY:O	0.45	2.49	19	4
2:A:347:ASN:CG	2:A:348:PRO:HD3	0.45	2.32	19	1
2:A:266:LEU:N	2:A:266:LEU:HD12	0.45	2.27	10	5
2:A:327:ASN:O	2:A:329:ASP:N	0.45	2.49	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:328:ASP:C	2:A:330:GLN:N	0.45	2.70	11	11
2:A:268:GLY:HA2	2:A:281:LEU:HD11	0.45	1.89	19	2
2:A:272:ASN:OD1	2:A:279:GLU:HB3	0.45	2.12	17	2
2:A:281:LEU:HD23	2:A:292:HIS:CD2	0.45	2.46	15	9
2:A:350:VAL:HG13	2:A:352:GLU:O	0.45	2.12	14	1
2:A:305:ALA:HB1	2:A:309:TYR:OH	0.45	2.12	5	1
2:A:324:THR:OG1	2:A:326:GLU:HG2	0.45	2.12	8	1
2:A:330:GLN:HB3	2:A:343:MET:SD	0.45	2.51	11	3
2:A:360:CYS:O	2:A:363:CYS:SG	0.44	2.75	7	4
2:A:354:PRO:O	2:A:356:GLY:N	0.44	2.50	17	1
2:A:317:LYS:HE3	2:A:340:GLY:HA3	0.44	1.89	18	1
2:A:267:GLY:HA2	2:A:273:LYS:HG3	0.44	1.88	4	1
2:A:266:LEU:HD12	2:A:266:LEU:N	0.44	2.27	11	2
2:A:293:PRO:O	2:A:298:PHE:N	0.44	2.50	11	4
1:B:1:ALA:HB1	2:A:332:LEU:HD22	0.44	1.88	9	1
2:A:324:THR:OG1	2:A:325:SER:N	0.44	2.50	16	3
2:A:293:PRO:HG3	2:A:307:LYS:HZ1	0.44	1.71	2	3
2:A:306:VAL:HB	2:A:311:TRP:HB2	0.44	1.89	2	3
2:A:344:TYR:N	2:A:344:TYR:CD1	0.44	2.86	20	2
2:A:339:ARG:HE	2:A:362:LEU:HB2	0.44	1.73	15	1
2:A:262:CYS:O	2:A:266:LEU:HA	0.44	2.13	4	4
2:A:328:ASP:HA	2:A:331:LEU:HB3	0.44	1.89	14	1
2:A:261:TYR:HD1	2:A:262:CYS:O	0.44	1.96	11	1
2:A:332:LEU:HG	2:A:343:MET:HG3	0.43	1.88	7	6
1:B:4:LYS:NZ	2:A:315:GLU:HG3	0.43	2.28	9	2
2:A:292:HIS:N	2:A:295:CYS:SG	0.43	2.91	11	1
2:A:334:CYS:SG	2:A:335:ASP:N	0.43	2.91	16	2
2:A:302:MET:HA	2:A:337:CYS:CA	0.43	2.43	2	3
2:A:261:TYR:CE1	2:A:266:LEU:HD23	0.43	2.49	3	9
2:A:274:LYS:HD3	2:A:295:CYS:SG	0.43	2.53	4	1
2:A:318:SER:HB2	2:A:324:THR:C	0.43	2.33	2	3
2:A:327:ASN:C	2:A:329:ASP:N	0.43	2.72	8	2
2:A:319:CYS:HB3	2:A:324:THR:O	0.43	2.13	15	1
1:B:4:LYS:HG3	2:A:331:LEU:HG	0.43	1.91	3	1
2:A:314:ILE:HD13	2:A:333:PHE:CE2	0.43	2.48	2	1
1:B:1:ALA:N	2:A:355:GLU:N	0.43	2.65	17	1
2:A:265:CYS:O	2:A:273:LYS:NZ	0.43	2.46	13	1
2:A:328:ASP:N	2:A:328:ASP:OD1	0.43	2.51	16	1
2:A:344:TYR:CD1	2:A:344:TYR:N	0.43	2.86	16	1
2:A:320:ILE:HD13	2:A:339:ARG:HE	0.43	1.73	17	1
2:A:293:PRO:N	2:A:296:LEU:HD12	0.43	2.29	11	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:339:ARG:HH11	2:A:362:LEU:HG	0.43	1.72	5	1
2:A:303:THR:CG2	2:A:307:LYS:NZ	0.43	2.82	14	1
2:A:355:GLU:H	2:A:355:GLU:CD	0.43	2.18	4	2
2:A:337:CYS:O	2:A:338:ASP:OD1	0.43	2.36	19	1
1:B:1:ALA:CB	2:A:354:PRO:CD	0.43	2.96	9	1
2:A:301:ASN:ND2	2:A:336:ASP:O	0.42	2.52	9	6
2:A:337:CYS:O	2:A:338:ASP:HB2	0.42	2.14	14	1
1:B:1:ALA:HB2	2:A:354:PRO:CB	0.42	2.44	14	1
2:A:289:ARG:HD2	2:A:313:CYS:SG	0.42	2.54	17	2
2:A:262:CYS:SG	2:A:265:CYS:N	0.42	2.90	11	1
2:A:318:SER:HA	2:A:325:SER:HB3	0.42	1.91	19	1
2:A:317:LYS:HE3	2:A:333:PHE:CE2	0.42	2.49	12	1
2:A:314:ILE:HA	2:A:317:LYS:HE3	0.42	1.91	19	1
2:A:314:ILE:H	2:A:317:LYS:HZ1	0.42	1.57	6	1
2:A:314:ILE:HG22	2:A:315:GLU:HG2	0.42	1.89	1	3
1:B:4:LYS:HD2	2:A:331:LEU:HD23	0.42	1.92	17	1
2:A:312:GLN:NE2	2:A:316:CYS:O	0.42	2.52	8	1
2:A:262:CYS:SG	2:A:264:PHE:N	0.42	2.91	11	1
2:A:337:CYS:O	2:A:338:ASP:OD2	0.42	2.37	2	1
2:A:314:ILE:HG12	2:A:317:LYS:HZ2	0.42	1.74	1	1
2:A:265:CYS:HB3	2:A:274:LYS:CG	0.42	2.42	1	2
2:A:298:PHE:HB3	2:A:302:MET:HB2	0.42	1.91	8	2
2:A:360:CYS:O	2:A:363:CYS:HB2	0.42	2.14	19	2
2:A:320:ILE:HG13	2:A:339:ARG:NH2	0.42	2.29	14	1
2:A:352:GLU:O	2:A:353:PRO:C	0.42	2.57	8	3
2:A:328:ASP:C	2:A:330:GLN:H	0.42	2.18	20	1
1:B:1:ALA:HB2	2:A:354:PRO:CG	0.42	2.45	14	1
2:A:269:SER:HA	2:A:281:LEU:HG	0.42	1.91	10	2
2:A:274:LYS:NZ	2:A:274:LYS:HB3	0.42	2.30	1	1
2:A:292:HIS:CB	2:A:295:CYS:SG	0.42	3.04	11	1
2:A:334:CYS:O	2:A:338:ASP:HA	0.42	2.14	6	2
2:A:302:MET:CE	2:A:338:ASP:OD1	0.42	2.68	14	1
2:A:362:LEU:O	2:A:362:LEU:HD13	0.42	2.15	9	3
2:A:267:GLY:HA3	2:A:273:LYS:HG2	0.42	1.92	6	1
2:A:320:ILE:CG2	2:A:341:TYR:CE1	0.42	3.03	14	2
1:B:4:LYS:HD2	2:A:331:LEU:CD2	0.42	2.44	3	1
2:A:314:ILE:O	2:A:317:LYS:N	0.41	2.52	20	1
2:A:269:SER:HB2	2:A:281:LEU:H	0.41	1.74	12	1
2:A:317:LYS:HG2	2:A:318:SER:N	0.41	2.30	14	1
2:A:300:LEU:O	2:A:304:GLU:HB2	0.41	2.15	11	2
2:A:262:CYS:SG	2:A:263:ASP:N	0.41	2.93	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:314:ILE:C	2:A:316:CYS:N	0.41	2.73	11	2
1:B:2:ARG:HD3	1:B:2:ARG:H	0.41	1.75	11	1
2:A:347:ASN:OD1	2:A:348:PRO:HD3	0.41	2.16	19	1
2:A:317:LYS:NZ	2:A:331:LEU:HD11	0.41	2.27	12	1
2:A:272:ASN:OD1	2:A:295:CYS:SG	0.41	2.78	10	1
2:A:353:PRO:C	2:A:355:GLU:H	0.41	2.19	17	1
2:A:330:GLN:HB3	2:A:343:MET:HB2	0.41	1.91	18	1
2:A:320:ILE:HD13	2:A:339:ARG:CZ	0.41	2.46	6	1
2:A:265:CYS:C	2:A:266:LEU:HD12	0.41	2.35	17	1
1:B:4:LYS:CE	2:A:315:GLU:HA	0.41	2.46	16	1
2:A:271:MET:HB3	2:A:273:LYS:HE2	0.41	1.93	10	1
2:A:266:LEU:N	2:A:266:LEU:HD23	0.41	2.31	20	1
2:A:327:ASN:OD1	2:A:327:ASN:N	0.41	2.54	10	1
2:A:354:PRO:C	2:A:356:GLY:H	0.41	2.19	17	1
2:A:361:HIS:C	2:A:361:HIS:CD2	0.41	2.94	20	2
2:A:341:TYR:OH	2:A:361:HIS:CG	0.41	2.74	16	1
2:A:319:CYS:HA	2:A:340:GLY:C	0.41	2.36	19	1
2:A:353:PRO:C	2:A:355:GLU:N	0.41	2.74	17	1
2:A:269:SER:OG	2:A:281:LEU:N	0.41	2.52	17	1
2:A:330:GLN:HG3	2:A:344:TYR:CZ	0.41	2.51	11	1
2:A:347:ASN:ND2	2:A:347:ASN:H	0.41	2.14	19	1
2:A:268:GLY:C	2:A:281:LEU:HD11	0.40	2.36	6	1
2:A:331:LEU:HD11	2:A:340:GLY:CA	0.40	2.46	6	1
2:A:286:ASP:HB2	2:A:316:CYS:CB	0.40	2.44	17	1
2:A:346:LEU:HD13	2:A:358:TRP:NE1	0.40	2.32	9	1
2:A:262:CYS:O	2:A:266:LEU:CA	0.40	2.70	10	1
2:A:346:LEU:HD23	2:A:358:TRP:HE1	0.40	1.77	7	1
1:B:4:LYS:HD3	2:A:328:ASP:HB3	0.40	1.94	7	1
2:A:341:TYR:HB2	2:A:358:TRP:CH2	0.40	2.50	6	1
2:A:269:SER:N	2:A:281:LEU:CD1	0.40	2.85	1	1
2:A:332:LEU:O	2:A:340:GLY:HA2	0.40	2.16	16	1
2:A:342:HIS:O	2:A:343:MET:C	0.40	2.60	7	1
2:A:284:CYS:SG	2:A:286:ASP:N	0.40	2.94	19	1
2:A:265:CYS:SG	2:A:274:LYS:CG	0.40	3.08	11	1
2:A:354:PRO:HG2	2:A:358:TRP:CG	0.40	2.52	6	1
2:A:309:TYR:OH	2:A:337:CYS:HB3	0.40	2.16	5	1
2:A:269:SER:N	2:A:281:LEU:HD11	0.40	2.32	1	1
2:A:361:HIS:CD2	2:A:361:HIS:C	0.40	2.95	13	1
2:A:309:TYR:HB2	2:A:310:LYS:H	0.40	1.57	3	1
2:A:285:ALA:CB	2:A:310:LYS:HD2	0.40	2.47	16	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	3/20 (15%)	2±0 (72±16%)	0±1 (10±19%)	1±0 (18±17%)	0	3
2	A	101/114 (89%)	69±2 (69±2%)	22±3 (21±3%)	10±1 (10±1%)	1	10
All	All	2080/2680 (78%)	1428 (69%)	436 (21%)	216 (10%)	1	10

All 23 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	348	PRO	20
2	A	331	LEU	20
2	A	314	ILE	20
2	A	343	MET	20
2	A	326	GLU	20
2	A	353	PRO	18
2	A	338	ASP	17
2	A	328	ASP	16
2	A	312	GLN	14
1	B	4	LYS	11
2	A	354	PRO	10
2	A	325	SER	6
2	A	339	ARG	6
2	A	334	CYS	4
2	A	319	CYS	4
2	A	358	TRP	2
2	A	317	LYS	2
2	A	356	GLY	1
2	A	278	PRO	1
2	A	346	LEU	1
2	A	271	MET	1
2	A	289	ARG	1
2	A	263	ASP	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	3/15 (20%)	1±1 (45±24%)	2±1 (55±24%)	0	1
2	A	91/101 (90%)	74±3 (81±3%)	17±3 (19±3%)	5	37
All	All	1880/2320 (81%)	1498 (80%)	382 (20%)	4	35

All 52 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	262	CYS	20
2	A	336	ASP	20
2	A	299	THR	20
2	A	346	LEU	20
2	A	309	TYR	20
2	A	331	LEU	19
1	B	3	THR	19
2	A	328	ASP	16
2	A	301	ASN	16
2	A	280	GLU	15
2	A	341	TYR	13
2	A	352	GLU	12
2	A	362	LEU	11
2	A	320	ILE	11
1	B	2	ARG	11
2	A	271	MET	11
2	A	319	CYS	11
2	A	363	CYS	10
2	A	310	LYS	9
2	A	359	SER	9
2	A	327	ASN	7
2	A	330	GLN	7
2	A	329	ASP	6
2	A	324	THR	5
2	A	339	ARG	5
2	A	361	HIS	4
2	A	290	SER	4
2	A	284	CYS	4

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Mol	Chain	Res	Type	Models (Total)
2	A	355	GLU	4
2	A	269	SER	4
2	A	338	ASP	4
2	A	334	CYS	3
2	A	317	LYS	3
2	A	344	TYR	3
1	B	4	LYS	3
2	A	335	ASP	3
2	A	360	CYS	2
2	A	337	CYS	2
2	A	282	VAL	2
2	A	274	LYS	2
2	A	295	CYS	1
2	A	325	SER	1
2	A	270	ASN	1
2	A	272	ASN	1
2	A	287	CYS	1
2	A	266	LEU	1
2	A	289	ARG	1
2	A	265	CYS	1
2	A	347	ASN	1
2	A	273	LYS	1
2	A	326	GLU	1
2	A	263	ASP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

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