



Full wwPDB NMR Structure Validation Report ⓘ

Mar 23, 2026 – 02:09 PM UTC

PDB ID : 2CZO / pdb_00002czo
Title : Solution Structure of the PX Domain of Bem1p
Authors : Maeda, A.; Ogura, K.; Horiuchi, M.; Kumeta, H.; Fujioka, Y.; Inagaki, F.
Deposited on : 2005-07-14

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

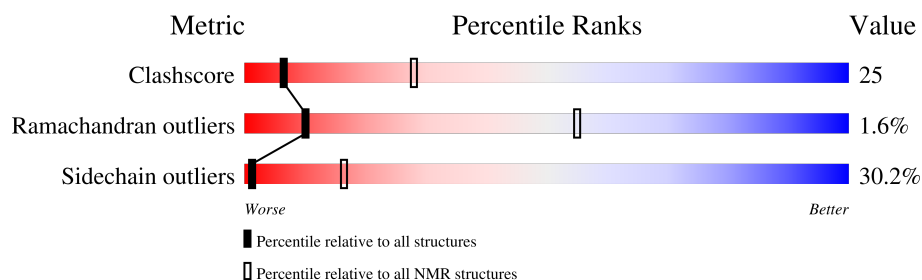
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	A	155	31% 37% • 12% 16%

2 Ensemble composition and analysis

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	A:274-A:339, A:348-A:354, A:362-A:399 (111)	0.72	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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2107 atoms, of which 1056 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bud emergence protein 1.

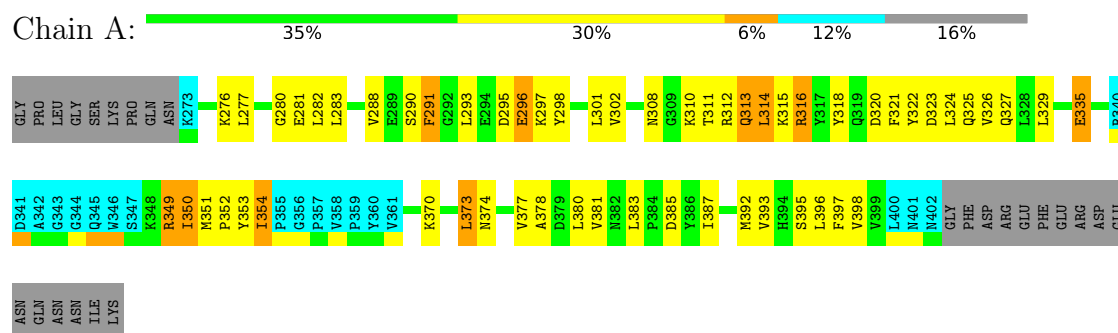
Mol	Chain	Residues	Atoms						Trace
1	A	130	Total	C	H	N	O	S	0
			2107	678	1056	174	195	4	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLY	-	cloning artifact	UNP P29366
A	265	PRO	-	cloning artifact	UNP P29366
A	266	LEU	-	cloning artifact	UNP P29366
A	267	GLY	-	cloning artifact	UNP P29366
A	268	SER	-	cloning artifact	UNP P29366

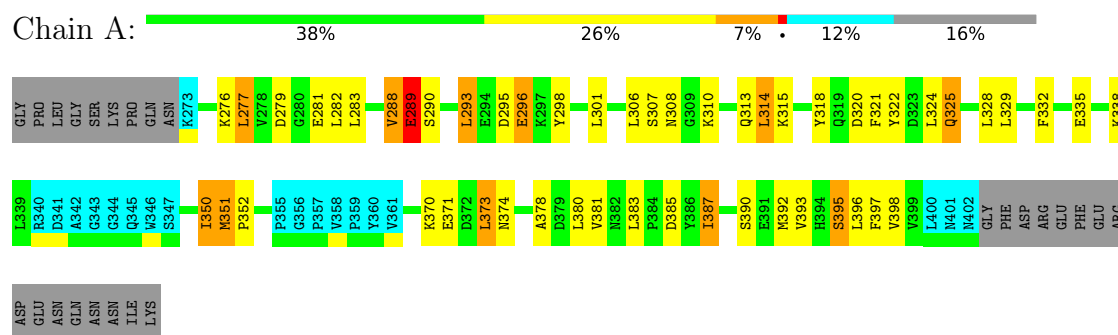
4.2.2 Score per residue for model 2

- Molecule 1: Bud emergence protein 1



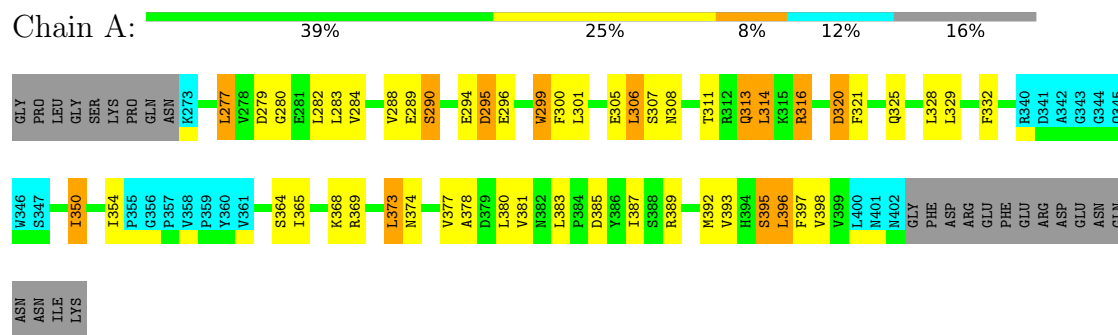
4.2.3 Score per residue for model 3

- Molecule 1: Bud emergence protein 1



4.2.4 Score per residue for model 4

- Molecule 1: Bud emergence protein 1



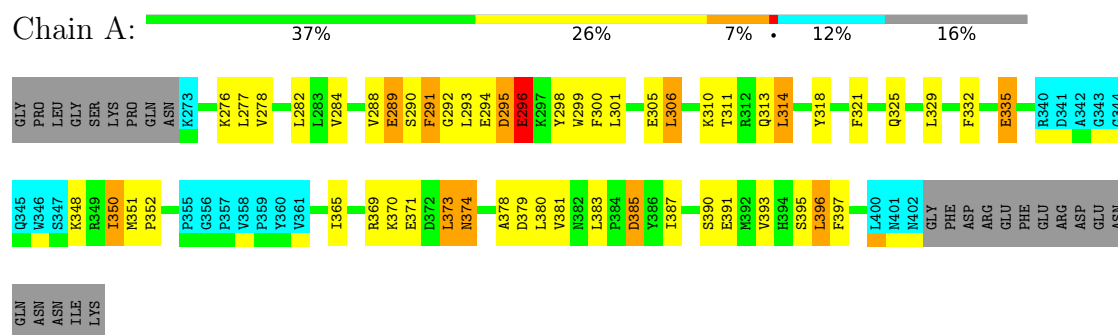
4.2.5 Score per residue for model 5

- Molecule 1: Bud emergence protein 1



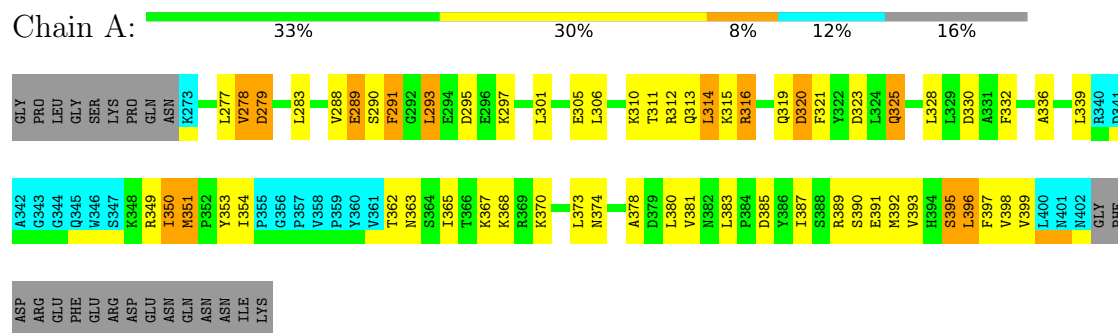
4.2.6 Score per residue for model 6

- Molecule 1: Bud emergence protein 1



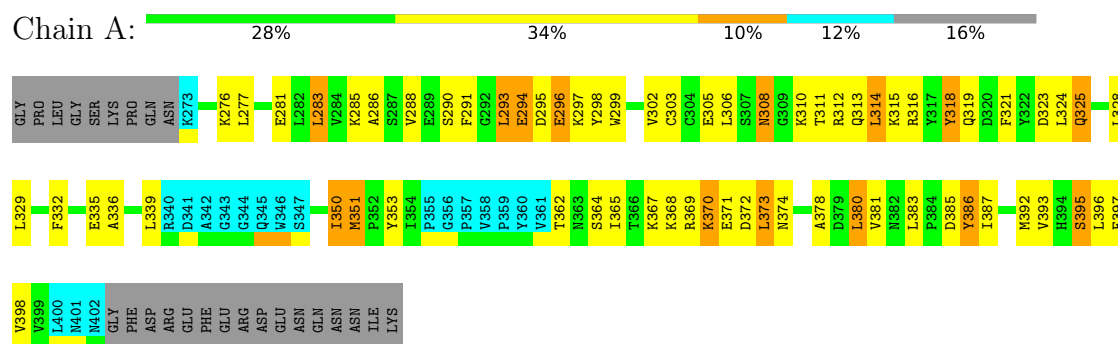
4.2.7 Score per residue for model 7

- Molecule 1: Bud emergence protein 1



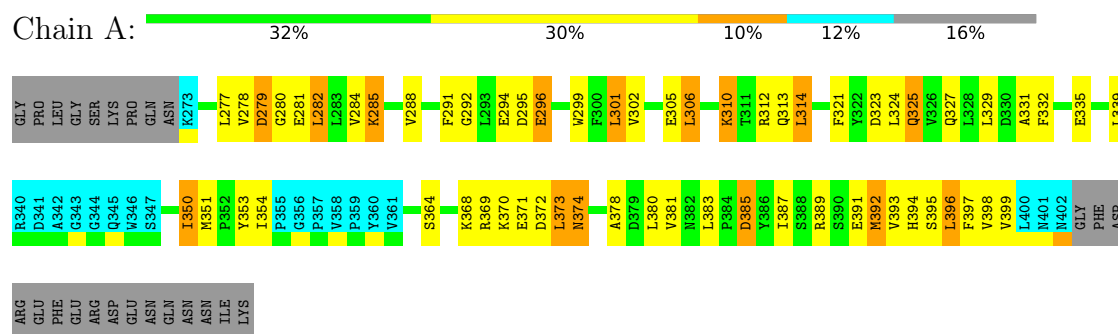
4.2.14 Score per residue for model 14

- Molecule 1: Bud emergence protein 1



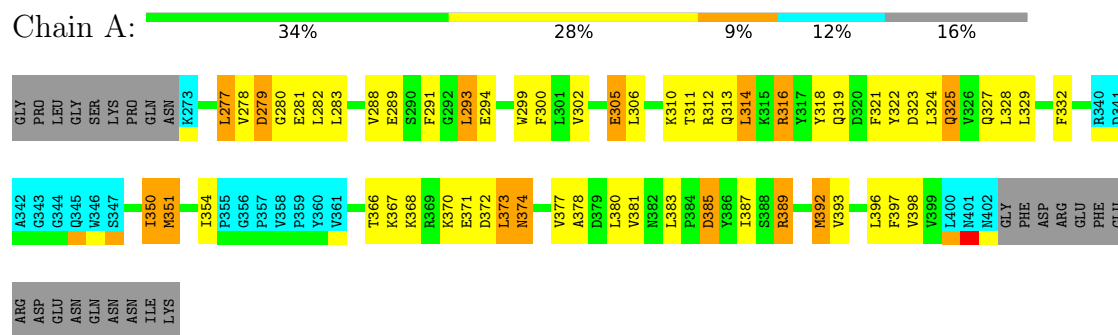
4.2.15 Score per residue for model 15

- Molecule 1: Bud emergence protein 1



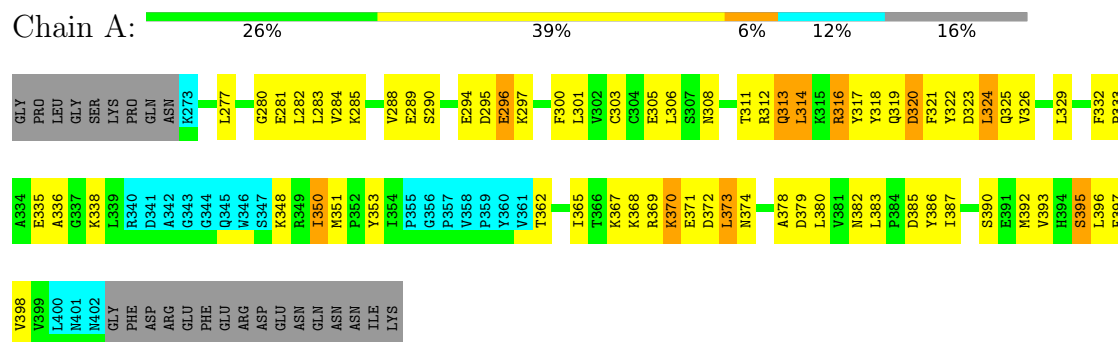
4.2.16 Score per residue for model 16

- Molecule 1: Bud emergence protein 1



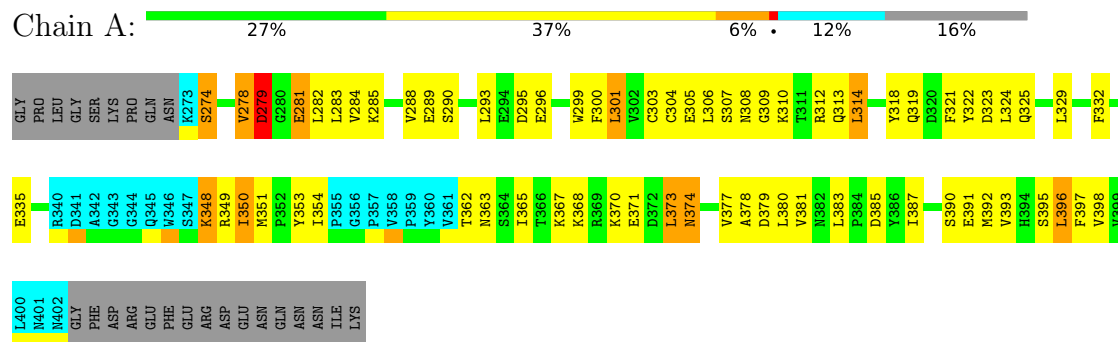
4.2.17 Score per residue for model 17

- Molecule 1: Bud emergence protein 1



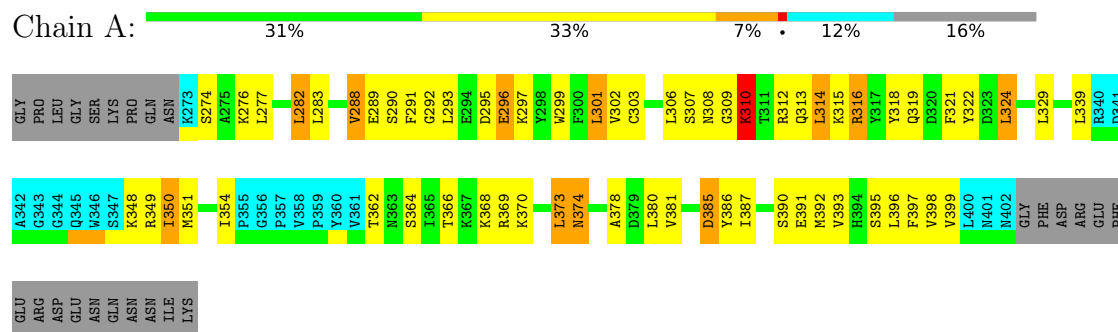
4.2.18 Score per residue for model 18

- Molecule 1: Bud emergence protein 1



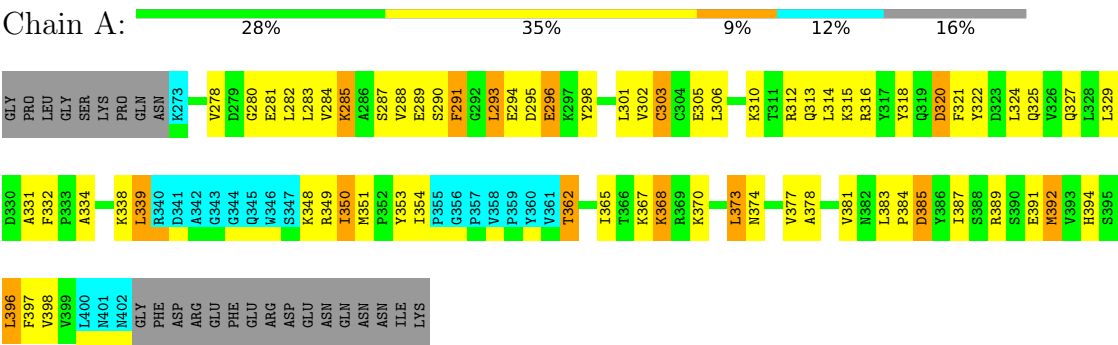
4.2.19 Score per residue for model 19

- Molecule 1: Bud emergence protein 1



4.2.20 Score per residue for model 20

● Molecule 1: Bud emergence protein 1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.0
CYANA	refinement	2.0

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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	A	906	918	918	46±8
All	All	18120	18360	18360	920

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:321:PHE:CD2	1:A:373:LEU:HD11	0.91	2.00	14	4
1:A:396:LEU:HD22	1:A:396:LEU:O	0.86	1.70	13	2
1:A:288:VAL:HG12	1:A:302:VAL:HG13	0.85	1.49	12	4
1:A:339:LEU:C	1:A:339:LEU:HD22	0.83	1.99	20	2
1:A:288:VAL:HG22	1:A:302:VAL:HG22	0.81	1.50	2	4
1:A:313:GLN:C	1:A:314:LEU:HD13	0.81	2.01	6	16
1:A:314:LEU:N	1:A:314:LEU:HD13	0.80	1.92	10	8
1:A:314:LEU:HD22	1:A:314:LEU:N	0.79	1.93	8	8
1:A:321:PHE:CZ	1:A:373:LEU:HD21	0.79	2.13	16	2
1:A:354:ILE:HD13	1:A:354:ILE:N	0.77	1.95	12	1
1:A:283:LEU:HD21	1:A:397:PHE:CD2	0.77	2.15	19	2
1:A:306:LEU:HD22	1:A:310:LYS:HD3	0.76	1.58	15	1
1:A:314:LEU:HD13	1:A:314:LEU:N	0.76	1.96	6	6
1:A:306:LEU:HD22	1:A:310:LYS:HB3	0.74	1.57	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:277:LEU:HD22	1:A:389:ARG:HG3	0.74	1.58	7	1
1:A:380:LEU:HD12	1:A:393:VAL:HG23	0.74	1.59	12	11
1:A:380:LEU:CD1	1:A:393:VAL:HG23	0.73	2.14	12	16
1:A:339:LEU:N	1:A:339:LEU:HD13	0.73	1.98	8	1
1:A:314:LEU:HD22	1:A:314:LEU:H	0.72	1.44	5	7
1:A:288:VAL:HG21	1:A:373:LEU:HB3	0.70	1.62	17	5
1:A:328:LEU:HA	1:A:392:MET:HE1	0.70	1.62	8	1
1:A:291:PHE:CE2	1:A:366:THR:HG21	0.70	2.21	16	2
1:A:305:GLU:C	1:A:306:LEU:HD12	0.70	2.12	10	16
1:A:288:VAL:HG21	1:A:373:LEU:HD12	0.70	1.62	9	2
1:A:339:LEU:HD22	1:A:339:LEU:O	0.69	1.86	8	2
1:A:288:VAL:HG13	1:A:301:LEU:O	0.69	1.86	15	8
1:A:313:GLN:O	1:A:314:LEU:HD13	0.68	1.87	16	4
1:A:321:PHE:CE2	1:A:373:LEU:HD11	0.68	2.24	10	3
1:A:306:LEU:N	1:A:306:LEU:HD12	0.68	2.04	13	5
1:A:396:LEU:CD1	1:A:397:PHE:CE1	0.68	2.77	20	3
1:A:321:PHE:CD1	1:A:322:TYR:N	0.68	2.61	18	7
1:A:288:VAL:HG12	1:A:302:VAL:HA	0.68	1.66	20	1
1:A:293:LEU:HD23	1:A:298:TYR:CE1	0.67	2.24	20	6
1:A:396:LEU:HD12	1:A:397:PHE:CE1	0.67	2.25	16	2
1:A:283:LEU:CD1	1:A:397:PHE:CD2	0.67	2.78	4	6
1:A:293:LEU:HD23	1:A:298:TYR:CD2	0.67	2.25	10	2
1:A:293:LEU:HD13	1:A:294:GLU:N	0.66	2.04	13	6
1:A:293:LEU:C	1:A:293:LEU:HD13	0.66	2.16	1	6
1:A:291:PHE:C	1:A:291:PHE:CD1	0.66	2.74	20	6
1:A:328:LEU:HB3	1:A:351:MET:HE1	0.65	1.68	12	5
1:A:306:LEU:HD22	1:A:310:LYS:CB	0.65	2.21	1	2
1:A:321:PHE:CE2	1:A:373:LEU:HD21	0.65	2.27	16	3
1:A:325:GLN:HG2	1:A:354:ILE:HG21	0.65	1.68	4	1
1:A:306:LEU:HD22	1:A:310:LYS:HB2	0.65	1.67	6	3
1:A:306:LEU:HD12	1:A:306:LEU:N	0.65	2.07	9	5
1:A:339:LEU:HD13	1:A:339:LEU:H	0.64	1.52	8	2
1:A:277:LEU:HD13	1:A:389:ARG:NE	0.64	2.07	15	1
1:A:395:SER:O	1:A:398:VAL:HG22	0.64	1.93	17	14
1:A:282:LEU:HD13	1:A:389:ARG:NE	0.64	2.08	5	1
1:A:324:LEU:HD21	1:A:392:MET:O	0.64	1.92	17	1
1:A:350:ILE:H	1:A:350:ILE:HD13	0.64	1.53	2	19
1:A:301:LEU:C	1:A:301:LEU:HD13	0.63	2.17	7	3
1:A:318:TYR:O	1:A:321:PHE:CD2	0.63	2.52	17	7
1:A:282:LEU:N	1:A:282:LEU:HD23	0.63	2.09	15	1
1:A:350:ILE:HD13	1:A:350:ILE:O	0.62	1.94	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:324:LEU:HD23	1:A:376:TYR:OH	0.62	1.94	10	1
1:A:277:LEU:HD11	1:A:386:TYR:HB2	0.62	1.72	17	2
1:A:327:GLN:HB3	1:A:392:MET:HE3	0.62	1.71	15	1
1:A:314:LEU:HD12	1:A:398:VAL:C	0.62	2.20	4	2
1:A:318:TYR:CD1	1:A:318:TYR:C	0.62	2.77	14	4
1:A:329:LEU:HD12	1:A:329:LEU:O	0.61	1.94	17	1
1:A:396:LEU:C	1:A:396:LEU:HD13	0.61	2.21	20	2
1:A:396:LEU:CD1	1:A:397:PHE:CD1	0.61	2.83	20	3
1:A:321:PHE:C	1:A:321:PHE:CD1	0.61	2.79	2	5
1:A:318:TYR:O	1:A:321:PHE:CE2	0.61	2.54	16	7
1:A:324:LEU:HD11	1:A:393:VAL:HA	0.61	1.71	8	2
1:A:396:LEU:O	1:A:396:LEU:HD13	0.61	1.96	16	1
1:A:321:PHE:CD1	1:A:321:PHE:C	0.61	2.79	18	2
1:A:313:GLN:C	1:A:314:LEU:HD22	0.60	2.21	8	3
1:A:321:PHE:CZ	1:A:373:LEU:HD11	0.60	2.32	10	2
1:A:300:PHE:CZ	1:A:316:ARG:O	0.60	2.55	17	2
1:A:288:VAL:HG11	1:A:373:LEU:HB3	0.60	1.71	12	2
1:A:277:LEU:HD22	1:A:277:LEU:N	0.60	2.10	3	7
1:A:314:LEU:N	1:A:314:LEU:CD2	0.60	2.64	8	4
1:A:292:GLY:O	1:A:299:TRP:CD1	0.59	2.55	5	7
1:A:284:VAL:HG22	1:A:305:GLU:O	0.59	1.97	13	8
1:A:321:PHE:CD2	1:A:373:LEU:HD21	0.59	2.32	2	6
1:A:374:ASN:C	1:A:374:ASN:ND2	0.59	2.60	18	3
1:A:396:LEU:HD13	1:A:396:LEU:C	0.59	2.22	16	1
1:A:329:LEU:HD13	1:A:336:ALA:CB	0.59	2.28	17	1
1:A:293:LEU:HD21	1:A:296:GLU:O	0.59	1.98	6	1
1:A:282:LEU:HD23	1:A:282:LEU:H	0.59	1.58	15	1
1:A:331:ALA:HB2	1:A:392:MET:HE1	0.59	1.73	15	1
1:A:325:GLN:CD	1:A:325:GLN:C	0.59	2.70	10	13
1:A:293:LEU:HD22	1:A:297:LYS:O	0.59	1.98	13	1
1:A:380:LEU:HD13	1:A:393:VAL:CG2	0.58	2.28	17	5
1:A:292:GLY:C	1:A:299:TRP:CD1	0.58	2.82	15	5
1:A:277:LEU:HD21	1:A:386:TYR:CE2	0.58	2.34	14	1
1:A:283:LEU:HD23	1:A:306:LEU:HD11	0.57	1.76	20	2
1:A:378:ALA:O	1:A:381:VAL:HG22	0.57	1.98	2	18
1:A:306:LEU:N	1:A:306:LEU:CD1	0.57	2.66	13	7
1:A:306:LEU:CD1	1:A:306:LEU:N	0.57	2.67	4	6
1:A:339:LEU:C	1:A:339:LEU:CD2	0.57	2.76	10	3
1:A:291:PHE:CD1	1:A:299:TRP:O	0.57	2.57	6	1
1:A:339:LEU:N	1:A:339:LEU:CD1	0.57	2.68	8	2
1:A:321:PHE:CE1	1:A:373:LEU:HD11	0.57	2.35	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:353:TYR:C	1:A:354:ILE:HD13	0.57	2.23	12	1
1:A:293:LEU:CD1	1:A:293:LEU:C	0.57	2.76	16	3
1:A:292:GLY:C	1:A:299:TRP:NE1	0.57	2.63	13	6
1:A:293:LEU:HD22	1:A:297:LYS:C	0.57	2.25	13	1
1:A:376:TYR:C	1:A:376:TYR:CD1	0.56	2.83	1	2
1:A:383:LEU:CD1	1:A:387:ILE:CG2	0.56	2.84	14	3
1:A:301:LEU:HD11	1:A:313:GLN:HG2	0.56	1.77	8	1
1:A:324:LEU:HD12	1:A:396:LEU:HB2	0.56	1.77	8	1
1:A:383:LEU:HD12	1:A:387:ILE:CG2	0.56	2.30	4	14
1:A:301:LEU:C	1:A:301:LEU:CD1	0.56	2.79	15	3
1:A:283:LEU:CD2	1:A:397:PHE:CD2	0.56	2.89	14	2
1:A:324:LEU:CD2	1:A:328:LEU:HD11	0.55	2.31	3	1
1:A:398:VAL:HG23	1:A:398:VAL:O	0.55	2.01	14	3
1:A:284:VAL:HG23	1:A:285:LYS:HG2	0.55	1.78	10	2
1:A:293:LEU:HD13	1:A:293:LEU:C	0.55	2.26	13	1
1:A:299:TRP:CD1	1:A:299:TRP:N	0.55	2.75	4	2
1:A:380:LEU:CD1	1:A:393:VAL:CG2	0.55	2.85	17	15
1:A:282:LEU:HD13	1:A:389:ARG:CZ	0.55	2.31	5	1
1:A:321:PHE:CE1	1:A:396:LEU:HD11	0.54	2.37	4	2
1:A:354:ILE:HG23	1:A:354:ILE:O	0.54	2.02	4	1
1:A:335:GLU:OE2	1:A:387:ILE:HD11	0.54	2.02	18	2
1:A:327:GLN:C	1:A:392:MET:HE1	0.54	2.26	20	3
1:A:293:LEU:C	1:A:293:LEU:CD1	0.54	2.81	13	5
1:A:385:ASP:HB2	1:A:387:ILE:HD12	0.54	1.78	17	4
1:A:383:LEU:HD13	1:A:387:ILE:HD13	0.54	1.79	12	10
1:A:332:PHE:CE2	1:A:387:ILE:HG13	0.54	2.38	8	3
1:A:385:ASP:CB	1:A:387:ILE:HD12	0.54	2.33	1	8
1:A:331:ALA:CB	1:A:392:MET:HE1	0.54	2.33	15	1
1:A:380:LEU:HD12	1:A:393:VAL:CG2	0.54	2.32	11	11
1:A:306:LEU:HD12	1:A:310:LYS:O	0.54	2.03	19	1
1:A:394:HIS:O	1:A:398:VAL:HG22	0.54	2.03	20	1
1:A:325:GLN:HA	1:A:328:LEU:HD12	0.53	1.81	8	2
1:A:339:LEU:HD13	1:A:339:LEU:N	0.53	2.17	10	1
1:A:396:LEU:HD23	1:A:397:PHE:CE1	0.53	2.38	18	6
1:A:291:PHE:CZ	1:A:300:PHE:CD2	0.53	2.96	5	1
1:A:382:ASN:OD1	1:A:382:ASN:C	0.53	2.51	9	1
1:A:351:MET:HE2	1:A:352:PRO:HD2	0.53	1.80	3	1
1:A:362:THR:HG23	1:A:365:ILE:HD12	0.53	1.80	14	1
1:A:279:ASP:OD1	1:A:279:ASP:C	0.53	2.51	16	1
1:A:332:PHE:CE2	1:A:387:ILE:HG12	0.52	2.40	7	6
1:A:328:LEU:HD23	1:A:332:PHE:CE1	0.52	2.40	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:321:PHE:CG	1:A:373:LEU:HD11	0.52	2.39	8	1
1:A:325:GLN:CG	1:A:354:ILE:HG21	0.52	2.34	4	1
1:A:332:PHE:CZ	1:A:387:ILE:HG13	0.52	2.40	17	2
1:A:295:ASP:C	1:A:296:GLU:CG	0.52	2.83	12	8
1:A:314:LEU:N	1:A:314:LEU:HD22	0.52	2.20	19	4
1:A:283:LEU:CD2	1:A:397:PHE:CE2	0.52	2.92	19	1
1:A:339:LEU:HD22	1:A:339:LEU:C	0.51	2.30	8	1
1:A:284:VAL:HG23	1:A:285:LYS:HG3	0.51	1.82	15	3
1:A:314:LEU:N	1:A:314:LEU:CD1	0.51	2.67	18	12
1:A:293:LEU:CD2	1:A:298:TYR:CD2	0.51	2.93	10	1
1:A:332:PHE:CE1	1:A:387:ILE:HG12	0.51	2.40	17	1
1:A:380:LEU:HD13	1:A:393:VAL:HG23	0.51	1.81	5	4
1:A:373:LEU:O	1:A:377:VAL:HG22	0.51	2.05	20	2
1:A:291:PHE:CE1	1:A:300:PHE:CD2	0.51	2.99	5	1
1:A:332:PHE:CE2	1:A:387:ILE:CG1	0.51	2.93	8	3
1:A:395:SER:O	1:A:398:VAL:HG13	0.51	2.06	13	3
1:A:325:GLN:OE1	1:A:325:GLN:C	0.51	2.54	13	2
1:A:362:THR:O	1:A:363:ASN:C	0.51	2.54	7	4
1:A:327:GLN:HB3	1:A:392:MET:HE1	0.51	1.81	20	1
1:A:332:PHE:CZ	1:A:387:ILE:CG1	0.50	2.94	10	2
1:A:299:TRP:CZ3	1:A:301:LEU:HD23	0.50	2.41	18	1
1:A:301:LEU:HD13	1:A:302:VAL:N	0.50	2.21	15	1
1:A:295:ASP:N	1:A:295:ASP:OD1	0.50	2.43	11	2
1:A:396:LEU:HD13	1:A:397:PHE:CD1	0.50	2.42	20	2
1:A:371:GLU:O	1:A:374:ASN:ND2	0.50	2.45	6	1
1:A:389:ARG:O	1:A:390:SER:C	0.50	2.55	10	1
1:A:293:LEU:HD23	1:A:298:TYR:CE2	0.50	2.41	3	1
1:A:283:LEU:HD21	1:A:397:PHE:CD1	0.50	2.42	7	1
1:A:390:SER:HB3	1:A:393:VAL:HG12	0.50	1.84	6	2
1:A:335:GLU:O	1:A:349:ARG:C	0.50	2.55	18	3
1:A:324:LEU:HD11	1:A:392:MET:O	0.50	2.06	12	1
1:A:396:LEU:HD22	1:A:396:LEU:C	0.50	2.32	13	1
1:A:294:GLU:C	1:A:295:ASP:OD1	0.50	2.54	20	1
1:A:386:TYR:C	1:A:386:TYR:CD1	0.50	2.86	14	1
1:A:295:ASP:O	1:A:296:GLU:CG	0.50	2.60	4	4
1:A:335:GLU:C	1:A:351:MET:SD	0.50	2.95	6	1
1:A:278:VAL:O	1:A:279:ASP:C	0.50	2.55	18	3
1:A:332:PHE:CD2	1:A:387:ILE:HG12	0.49	2.42	11	4
1:A:326:VAL:HG13	1:A:327:GLN:N	0.49	2.21	5	3
1:A:289:GLU:HB2	1:A:301:LEU:HD23	0.49	1.85	3	1
1:A:333:PRO:O	1:A:338:LYS:CG	0.49	2.61	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:291:PHE:CD1	1:A:291:PHE:O	0.49	2.66	2	1
1:A:294:GLU:O	1:A:295:ASP:CB	0.49	2.60	9	4
1:A:335:GLU:N	1:A:335:GLU:OE1	0.49	2.46	6	1
1:A:288:VAL:CG1	1:A:302:VAL:HG13	0.49	2.37	20	1
1:A:295:ASP:O	1:A:296:GLU:CB	0.49	2.60	1	7
1:A:288:VAL:N	1:A:374:ASN:OD1	0.49	2.45	17	2
1:A:377:VAL:HG23	1:A:378:ALA:N	0.49	2.22	16	7
1:A:274:SER:HB2	1:A:332:PHE:CE1	0.49	2.43	18	1
1:A:308:ASN:OD1	1:A:308:ASN:N	0.49	2.45	1	1
1:A:291:PHE:CD1	1:A:370:LYS:HE2	0.49	2.43	7	1
1:A:300:PHE:CD1	1:A:300:PHE:N	0.49	2.80	5	3
1:A:288:VAL:HG22	1:A:302:VAL:HG13	0.49	1.85	11	1
1:A:283:LEU:HD21	1:A:397:PHE:CE2	0.49	2.43	19	1
1:A:378:ALA:O	1:A:381:VAL:CG2	0.48	2.61	9	19
1:A:318:TYR:CE2	1:A:319:GLN:HG2	0.48	2.43	19	1
1:A:283:LEU:HD13	1:A:397:PHE:CD2	0.48	2.42	4	2
1:A:277:LEU:CD2	1:A:277:LEU:N	0.48	2.76	10	2
1:A:322:TYR:O	1:A:326:VAL:HG23	0.48	2.08	1	1
1:A:291:PHE:CE1	1:A:300:PHE:HB3	0.48	2.43	10	1
1:A:383:LEU:HD12	1:A:387:ILE:HG21	0.48	1.85	4	2
1:A:328:LEU:HB3	1:A:351:MET:HE2	0.48	1.86	13	1
1:A:277:LEU:N	1:A:277:LEU:HD22	0.48	2.23	10	1
1:A:304:CYS:HB3	1:A:397:PHE:CD2	0.48	2.44	11	3
1:A:320:ASP:CG	1:A:321:PHE:N	0.48	2.71	20	1
1:A:352:PRO:HB2	1:A:376:TYR:CE2	0.47	2.43	1	1
1:A:291:PHE:CE2	1:A:366:THR:CG2	0.47	2.97	16	1
1:A:294:GLU:CG	1:A:295:ASP:OD1	0.47	2.62	11	1
1:A:277:LEU:N	1:A:277:LEU:CD2	0.47	2.77	2	6
1:A:283:LEU:HD11	1:A:397:PHE:CD2	0.47	2.44	17	1
1:A:350:ILE:HD11	1:A:384:PRO:CD	0.47	2.39	20	1
1:A:292:GLY:HA3	1:A:299:TRP:CZ2	0.47	2.45	8	1
1:A:354:ILE:N	1:A:354:ILE:CD1	0.47	2.67	12	1
1:A:326:VAL:CG1	1:A:327:GLN:N	0.47	2.78	9	2
1:A:353:TYR:CD1	1:A:353:TYR:O	0.47	2.67	12	1
1:A:354:ILE:HG23	1:A:369:ARG:NH2	0.47	2.25	13	1
1:A:295:ASP:O	1:A:297:LYS:N	0.47	2.48	19	1
1:A:331:ALA:HB2	1:A:392:MET:HE2	0.47	1.86	20	1
1:A:291:PHE:CE1	1:A:300:PHE:CE2	0.47	3.03	5	1
1:A:308:ASN:O	1:A:308:ASN:CG	0.47	2.57	9	1
1:A:394:HIS:ND1	1:A:394:HIS:C	0.47	2.73	10	1
1:A:399:VAL:O	1:A:399:VAL:HG13	0.47	2.08	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:332:PHE:N	1:A:332:PHE:CD1	0.47	2.83	13	2
1:A:374:ASN:OD1	1:A:374:ASN:C	0.47	2.57	15	6
1:A:293:LEU:HD11	1:A:296:GLU:HA	0.47	1.85	10	1
1:A:281:GLU:CG	1:A:281:GLU:O	0.47	2.62	15	2
1:A:352:PRO:HB2	1:A:376:TYR:CD1	0.47	2.44	5	2
1:A:373:LEU:O	1:A:377:VAL:HG13	0.46	2.10	1	1
1:A:387:ILE:O	1:A:390:SER:CB	0.46	2.63	19	5
1:A:318:TYR:HA	1:A:321:PHE:CE2	0.46	2.46	11	7
1:A:395:SER:O	1:A:398:VAL:CG2	0.46	2.62	17	1
1:A:288:VAL:HG11	1:A:373:LEU:HD12	0.46	1.85	20	2
1:A:362:THR:O	1:A:365:ILE:N	0.46	2.47	18	3
1:A:350:ILE:O	1:A:350:ILE:CD1	0.46	2.63	6	1
1:A:329:LEU:CD1	1:A:336:ALA:CB	0.46	2.93	17	1
1:A:306:LEU:CD1	1:A:310:LYS:O	0.46	2.64	19	1
1:A:294:GLU:O	1:A:295:ASP:C	0.46	2.58	17	2
1:A:352:PRO:HB2	1:A:376:TYR:CE1	0.46	2.45	5	1
1:A:321:PHE:CD1	1:A:373:LEU:HD11	0.46	2.45	4	1
1:A:335:GLU:CB	1:A:351:MET:SD	0.46	3.04	6	2
1:A:329:LEU:HD12	1:A:329:LEU:C	0.46	2.35	17	1
1:A:325:GLN:CD	1:A:354:ILE:CG2	0.46	2.89	4	1
1:A:312:ARG:HG2	1:A:399:VAL:HG13	0.46	1.88	7	1
1:A:348:LYS:O	1:A:350:ILE:HD13	0.46	2.11	19	1
1:A:309:GLY:O	1:A:310:LYS:C	0.45	2.57	19	1
1:A:283:LEU:HD23	1:A:306:LEU:CD1	0.45	2.40	16	3
1:A:353:TYR:O	1:A:354:ILE:CG2	0.45	2.64	2	1
1:A:294:GLU:CG	1:A:299:TRP:CD1	0.45	2.99	14	1
1:A:289:GLU:CB	1:A:301:LEU:HD23	0.45	2.41	3	1
1:A:318:TYR:HA	1:A:321:PHE:CD2	0.45	2.46	8	2
1:A:278:VAL:O	1:A:280:GLY:N	0.45	2.49	15	1
1:A:288:VAL:CG2	1:A:302:VAL:HG22	0.45	2.35	15	1
1:A:291:PHE:CZ	1:A:300:PHE:HB3	0.45	2.46	10	1
1:A:316:ARG:NH1	1:A:398:VAL:O	0.45	2.50	16	1
1:A:279:ASP:OD1	1:A:280:GLY:N	0.45	2.50	16	1
1:A:318:TYR:CA	1:A:321:PHE:CE2	0.45	3.00	20	2
1:A:279:ASP:O	1:A:280:GLY:C	0.45	2.58	5	1
1:A:278:VAL:O	1:A:389:ARG:NH1	0.45	2.50	20	1
1:A:353:TYR:O	1:A:353:TYR:CG	0.45	2.69	7	1
1:A:325:GLN:NE2	1:A:352:PRO:O	0.45	2.50	6	2
1:A:295:ASP:C	1:A:297:LYS:N	0.45	2.74	19	3
1:A:324:LEU:HD22	1:A:396:LEU:HB2	0.45	1.89	20	2
1:A:353:TYR:C	1:A:353:TYR:CD1	0.45	2.95	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:299:TRP:CD1	1:A:299:TRP:H	0.44	2.31	6	2
1:A:294:GLU:HG2	1:A:299:TRP:CD1	0.44	2.47	16	2
1:A:279:ASP:CG	1:A:280:GLY:N	0.44	2.74	15	1
1:A:283:LEU:CD1	1:A:397:PHE:CD1	0.44	3.00	18	1
1:A:295:ASP:O	1:A:296:GLU:C	0.44	2.58	19	2
1:A:294:GLU:O	1:A:297:LYS:N	0.44	2.50	1	2
1:A:316:ARG:CZ	1:A:320:ASP:OD1	0.44	2.65	7	1
1:A:328:LEU:CB	1:A:351:MET:HE1	0.44	2.43	3	1
1:A:304:CYS:SG	1:A:397:PHE:CD2	0.44	3.10	5	1
1:A:306:LEU:HD13	1:A:310:LYS:HE2	0.44	1.89	15	1
1:A:362:THR:H	1:A:365:ILE:HD12	0.44	1.72	17	2
1:A:387:ILE:O	1:A:393:VAL:HG11	0.44	2.13	13	1
1:A:324:LEU:CD2	1:A:328:LEU:CD1	0.44	2.96	3	1
1:A:291:PHE:CZ	1:A:300:PHE:CE2	0.44	3.05	5	1
1:A:383:LEU:CD1	1:A:387:ILE:HG21	0.44	2.43	14	1
1:A:383:LEU:HD12	1:A:387:ILE:HB	0.43	1.90	1	4
1:A:354:ILE:CG1	1:A:354:ILE:O	0.43	2.65	2	1
1:A:299:TRP:CE3	1:A:299:TRP:C	0.43	2.96	8	1
1:A:325:GLN:CD	1:A:325:GLN:O	0.43	2.61	17	1
1:A:367:LYS:HG2	1:A:368:LYS:N	0.43	2.29	20	1
1:A:292:GLY:HA3	1:A:299:TRP:CE2	0.43	2.48	8	1
1:A:286:ALA:HB1	1:A:397:PHE:CZ	0.43	2.48	14	1
1:A:288:VAL:HG12	1:A:302:VAL:CA	0.43	2.41	20	1
1:A:324:LEU:HD22	1:A:328:LEU:HD11	0.43	1.89	3	1
1:A:289:GLU:HB2	1:A:301:LEU:HD12	0.43	1.90	7	1
1:A:325:GLN:CG	1:A:326:VAL:N	0.43	2.82	10	1
1:A:283:LEU:CD2	1:A:306:LEU:HD11	0.43	2.42	20	1
1:A:379:ASP:O	1:A:382:ASN:OD1	0.43	2.37	9	1
1:A:328:LEU:HD22	1:A:351:MET:HE1	0.43	1.90	14	1
1:A:336:ALA:HB2	1:A:351:MET:HG3	0.43	1.91	14	2
1:A:374:ASN:O	1:A:378:ALA:CB	0.43	2.66	7	2
1:A:398:VAL:O	1:A:398:VAL:CG2	0.43	2.67	14	1
1:A:362:THR:H	1:A:365:ILE:HD13	0.43	1.74	7	1
1:A:335:GLU:OE2	1:A:387:ILE:CD1	0.43	2.67	14	1
1:A:287:SER:O	1:A:303:CYS:CB	0.43	2.66	20	1
1:A:389:ARG:CZ	1:A:389:ARG:HB2	0.42	2.44	4	1
1:A:291:PHE:HB3	1:A:300:PHE:CE1	0.42	2.49	13	1
1:A:353:TYR:C	1:A:354:ILE:HG23	0.42	2.39	2	1
1:A:314:LEU:HD12	1:A:398:VAL:O	0.42	2.14	4	1
1:A:316:ARG:HG2	1:A:320:ASP:CG	0.42	2.39	17	2
1:A:396:LEU:HD23	1:A:397:PHE:CZ	0.42	2.49	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:366:THR:O	1:A:370:LYS:CG	0.42	2.66	11	1
1:A:370:LYS:HG2	1:A:371:GLU:N	0.42	2.29	8	6
1:A:332:PHE:CE1	1:A:387:ILE:CG1	0.42	3.02	17	1
1:A:287:SER:O	1:A:303:CYS:N	0.42	2.52	20	1
1:A:328:LEU:HD23	1:A:332:PHE:HE1	0.42	1.73	1	1
1:A:322:TYR:CD1	1:A:322:TYR:C	0.42	2.98	3	1
1:A:325:GLN:HG3	1:A:326:VAL:N	0.42	2.29	13	1
1:A:396:LEU:C	1:A:396:LEU:CD1	0.42	2.90	13	2
1:A:396:LEU:HD12	1:A:397:PHE:CZ	0.42	2.49	16	1
1:A:277:LEU:HD12	1:A:389:ARG:HG3	0.42	1.91	10	1
1:A:321:PHE:CD1	1:A:321:PHE:N	0.42	2.87	7	1
1:A:293:LEU:HD11	1:A:296:GLU:CA	0.42	2.44	10	1
1:A:387:ILE:O	1:A:390:SER:N	0.42	2.53	10	1
1:A:380:LEU:HD23	1:A:380:LEU:N	0.42	2.29	12	1
1:A:277:LEU:HD21	1:A:386:TYR:CD1	0.42	2.48	17	1
1:A:390:SER:O	1:A:393:VAL:HG12	0.42	2.14	18	1
1:A:338:LYS:HB2	1:A:339:LEU:HD13	0.42	1.91	8	1
1:A:293:LEU:HD23	1:A:298:TYR:CD1	0.42	2.49	13	2
1:A:282:LEU:N	1:A:282:LEU:CD2	0.42	2.80	15	1
1:A:377:VAL:CG2	1:A:378:ALA:N	0.42	2.83	1	3
1:A:291:PHE:CD1	1:A:291:PHE:C	0.42	2.98	2	1
1:A:374:ASN:O	1:A:378:ALA:HB2	0.42	2.15	17	1
1:A:312:ARG:CZ	1:A:312:ARG:HB2	0.41	2.45	5	1
1:A:286:ALA:O	1:A:378:ALA:HB2	0.41	2.14	8	1
1:A:288:VAL:HG12	1:A:302:VAL:CG1	0.41	2.45	20	1
1:A:300:PHE:CZ	1:A:316:ARG:C	0.41	2.98	10	1
1:A:325:GLN:NE2	1:A:326:VAL:HA	0.41	2.30	10	1
1:A:315:LYS:O	1:A:315:LYS:CG	0.41	2.68	13	1
1:A:334:ALA:HA	1:A:339:LEU:HD13	0.41	1.92	20	1
1:A:339:LEU:HD13	1:A:339:LEU:O	0.41	2.15	20	1
1:A:332:PHE:CD2	1:A:387:ILE:HD11	0.41	2.51	10	1
1:A:335:GLU:CD	1:A:387:ILE:CD1	0.41	2.94	14	1
1:A:293:LEU:HD23	1:A:298:TYR:CZ	0.41	2.50	6	1
1:A:293:LEU:CD2	1:A:296:GLU:O	0.41	2.69	6	1
1:A:383:LEU:CD1	1:A:387:ILE:HB	0.41	2.46	6	3
1:A:370:LYS:CG	1:A:371:GLU:N	0.41	2.84	13	1
1:A:301:LEU:HD11	1:A:313:GLN:NE2	0.41	2.31	2	1
1:A:328:LEU:CA	1:A:392:MET:HE1	0.41	2.39	8	1
1:A:288:VAL:CG2	1:A:373:LEU:HD12	0.41	2.45	1	1
1:A:302:VAL:HG12	1:A:397:PHE:CE2	0.41	2.50	5	1
1:A:324:LEU:CD2	1:A:376:TYR:OH	0.41	2.69	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:282:LEU:HD11	1:A:307:SER:HB2	0.41	1.92	19	1
1:A:306:LEU:HD13	1:A:310:LYS:HB2	0.41	1.93	5	1
1:A:370:LYS:CE	1:A:371:GLU:N	0.41	2.84	11	1
1:A:396:LEU:O	1:A:396:LEU:HD22	0.41	2.16	16	1
1:A:382:ASN:O	1:A:382:ASN:CG	0.41	2.63	17	1
1:A:316:ARG:HB3	1:A:316:ARG:CZ	0.41	2.46	19	1
1:A:277:LEU:CD1	1:A:389:ARG:HG3	0.41	2.46	16	1
1:A:385:ASP:HB3	1:A:387:ILE:HD12	0.40	1.92	1	1
1:A:370:LYS:HE3	1:A:370:LYS:C	0.40	2.42	11	1
1:A:302:VAL:O	1:A:314:LEU:HD22	0.40	2.16	14	1
1:A:335:GLU:C	1:A:351:MET:HG2	0.40	2.42	18	1
1:A:350:ILE:HD11	1:A:383:LEU:HD22	0.40	1.93	8	1
1:A:354:ILE:O	1:A:354:ILE:HG22	0.40	2.16	13	1
1:A:306:LEU:CB	1:A:308:ASN:OD1	0.40	2.69	14	1
1:A:329:LEU:HD13	1:A:336:ALA:HB2	0.40	1.92	17	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	A	111/155 (72%)	101±2 (91±2%)	9±2 (8±2%)	2±1 (2±1%)	10	55
All	All	2220/3100 (72%)	2012 (91%)	172 (8%)	36 (2%)	10	55

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	280	GLY	8
1	A	296	GLU	8
1	A	289	GLU	4
1	A	279	ASP	4
1	A	274	SER	4
1	A	290	SER	3
1	A	390	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	354	ILE	1
1	A	385	ASP	1
1	A	309	GLY	1
1	A	310	LYS	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	101/138 (73%)	70±4 (70±4%)	30±4 (30±4%)	1	16
All	All	2020/2760 (73%)	1410 (70%)	610 (30%)	1	16

All 75 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)
1	A	350	ILE	20
1	A	373	LEU	20
1	A	314	LEU	19
1	A	385	ASP	19
1	A	396	LEU	19
1	A	329	LEU	18
1	A	282	LEU	17
1	A	310	LYS	16
1	A	351	MET	14
1	A	368	LYS	14
1	A	370	LYS	14
1	A	374	ASN	14
1	A	392	MET	14
1	A	289	GLU	13
1	A	296	GLU	13
1	A	391	GLU	13
1	A	312	ARG	13
1	A	323	ASP	12
1	A	369	ARG	12
1	A	290	SER	12
1	A	311	THR	11

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Mol	Chain	Res	Type	Models (Total)
1	A	316	ARG	11
1	A	395	SER	11
1	A	293	LEU	11
1	A	315	LYS	10
1	A	281	GLU	10
1	A	372	ASP	10
1	A	308	ASN	9
1	A	335	GLU	9
1	A	339	LEU	9
1	A	324	LEU	9
1	A	354	ILE	9
1	A	303	CYS	9
1	A	294	GLU	8
1	A	320	ASP	8
1	A	306	LEU	8
1	A	379	ASP	8
1	A	285	LYS	8
1	A	349	ARG	7
1	A	367	LYS	7
1	A	371	GLU	7
1	A	276	LYS	7
1	A	325	GLN	7
1	A	319	GLN	6
1	A	279	ASP	6
1	A	364	SER	6
1	A	348	LYS	6
1	A	278	VAL	5
1	A	313	GLN	5
1	A	295	ASP	5
1	A	301	LEU	5
1	A	297	LYS	4
1	A	291	PHE	4
1	A	288	VAL	4
1	A	389	ARG	4
1	A	326	VAL	4
1	A	277	LEU	3
1	A	307	SER	3
1	A	382	ASN	3
1	A	330	ASP	3
1	A	353	TYR	3
1	A	338	LYS	2
1	A	300	PHE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	318	TYR	2
1	A	305	GLU	2
1	A	394	HIS	2
1	A	380	LEU	2
1	A	390	SER	2
1	A	386	TYR	2
1	A	387	ILE	1
1	A	299	TRP	1
1	A	283	LEU	1
1	A	399	VAL	1
1	A	317	TYR	1
1	A	362	THR	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 oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided