



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 10:12 pm GMT

PDB ID : 2J8L
Title : FXI APPLE 4 DOMAIN LOOP-OUT CONFORMATION
Authors : Samuel, D.; Cheng, H.; Riley, P.W.; Canutescu, A.A.; Bu, Z.; Walsh, P.N.;
Roder, H.
Deposited on : 2006-10-25

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

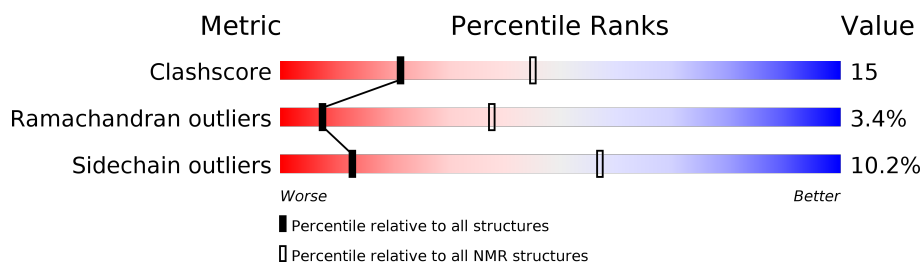
1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	90	 64% 34% .
1	B	90	 69% 31%

2 Ensemble composition and analysis

This entry contains 14 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:273-A:361, B:272-B:361 (179)	1.12	5

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

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

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

Cluster number	Models
1	2, 3, 4, 5, 7, 8, 10, 12, 13
2	9, 11
3	1, 14
Single-model clusters	6

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2484 atoms, of which 1098 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called COAGULATION FACTOR XI.

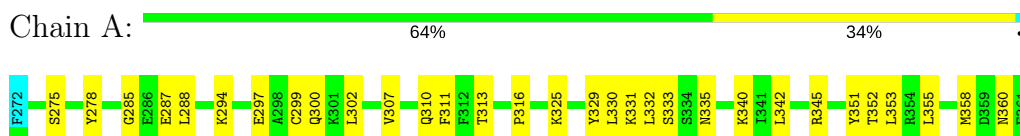
Mol	Chain	Residues	Atoms						Trace
1	A	90	Total	C	H	N	O	S	0
			1242	431	549	121	133	8	
1	B	90	Total	C	H	N	O	S	0
			1242	431	549	121	133	8	

4 Residue-property plots [i](#)

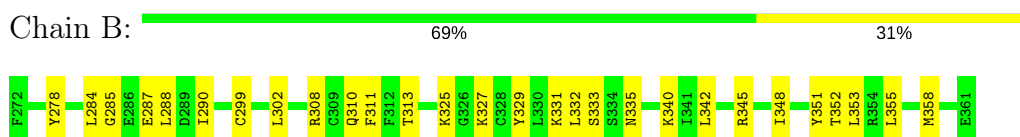
4.1 Average score per residue in the NMR ensemble

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: COAGULATION FACTOR XI



• Molecule 1: COAGULATION FACTOR XI

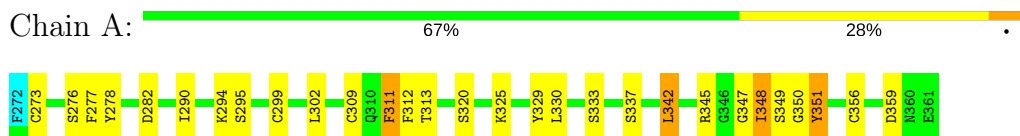


4.2 Scores per residue for each member of the ensemble

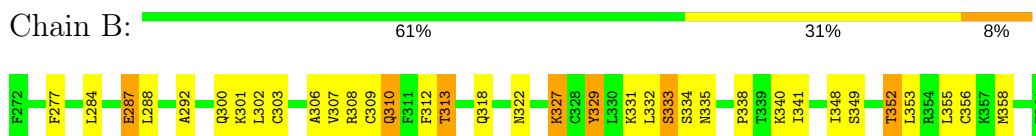
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: COAGULATION FACTOR XI

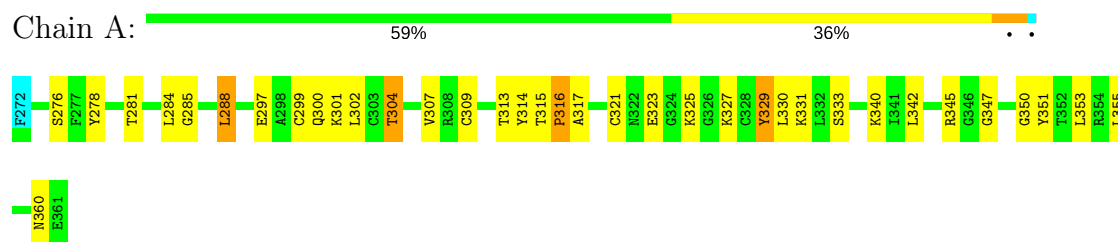


• Molecule 1: COAGULATION FACTOR XI

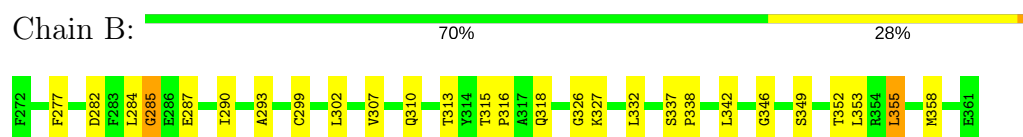


4.2.2 Score per residue for model 2

- Molecule 1: COAGULATION FACTOR XI

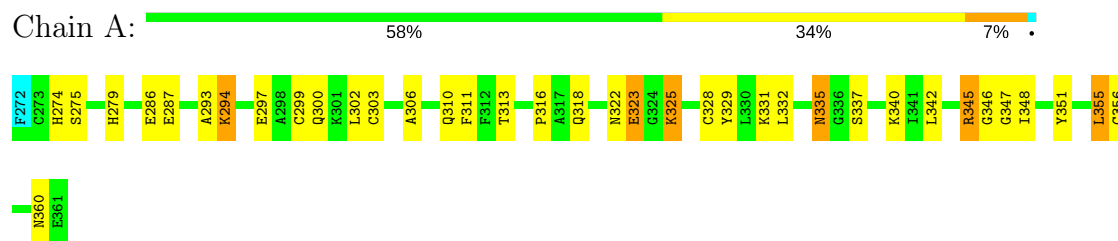


- Molecule 1: COAGULATION FACTOR XI

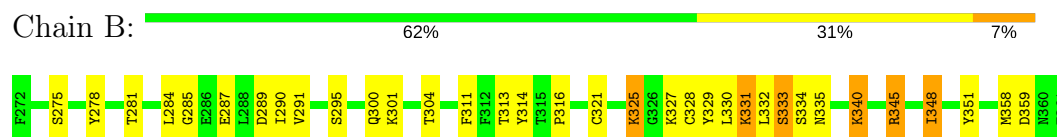


4.2.3 Score per residue for model 3

- Molecule 1: COAGULATION FACTOR XI

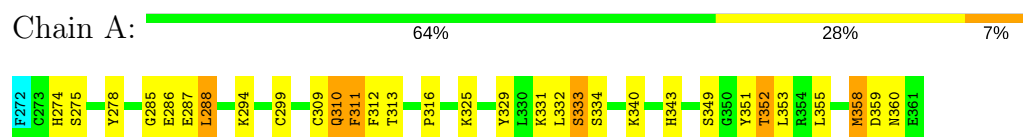


- Molecule 1: COAGULATION FACTOR XI

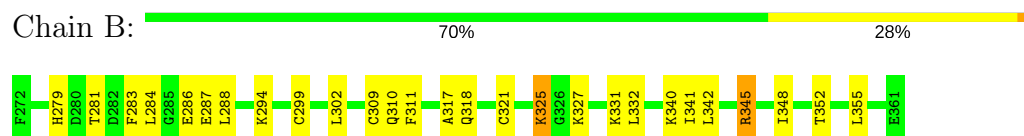


4.2.4 Score per residue for model 4

- Molecule 1: COAGULATION FACTOR XI

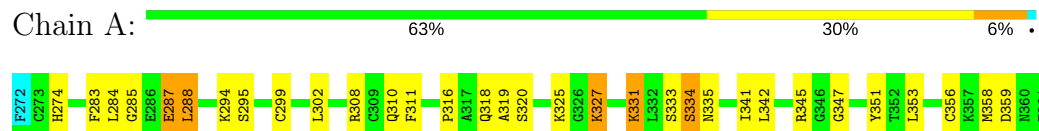


- Molecule 1: COAGULATION FACTOR XI

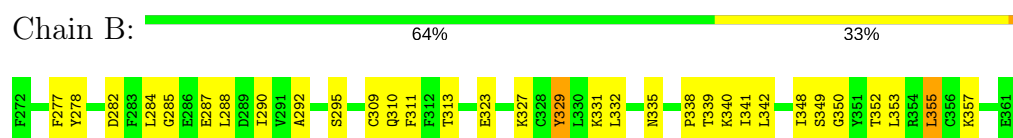


4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: COAGULATION FACTOR XI

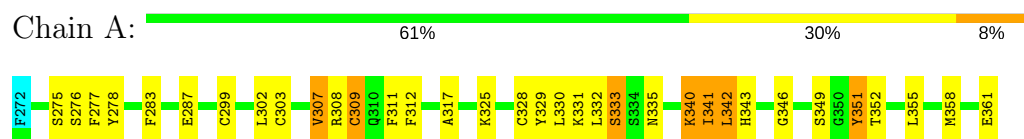


- Molecule 1: COAGULATION FACTOR XI

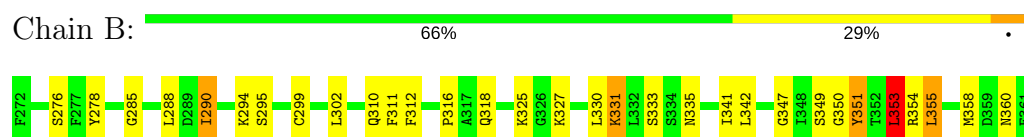


4.2.6 Score per residue for model 6

- Molecule 1: COAGULATION FACTOR XI

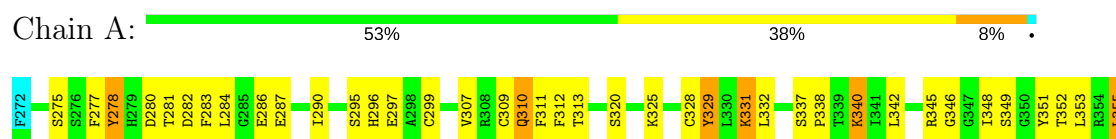


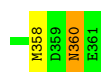
- Molecule 1: COAGULATION FACTOR XI



4.2.7 Score per residue for model 7

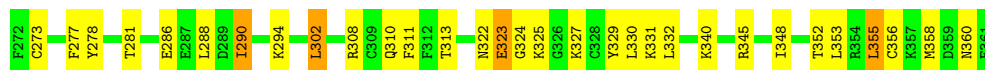
- Molecule 1: COAGULATION FACTOR XI





• Molecule 1: COAGULATION FACTOR XI

Chain B: 66% 30% .



4.2.8 Score per residue for model 8

• Molecule 1: COAGULATION FACTOR XI

Chain A: 69% 26% . .



• Molecule 1: COAGULATION FACTOR XI

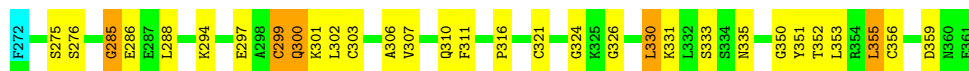
Chain B: 74% 24% .



4.2.9 Score per residue for model 9

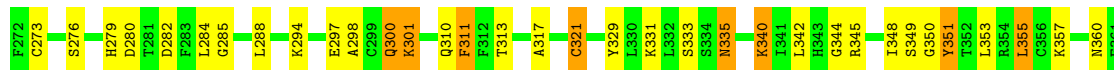
• Molecule 1: COAGULATION FACTOR XI

Chain A: 64% 29% 6% .



• Molecule 1: COAGULATION FACTOR XI

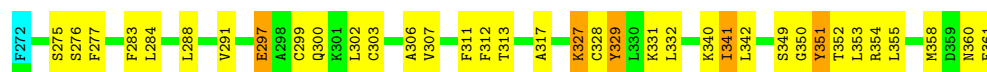
Chain B: 62% 29% 9%



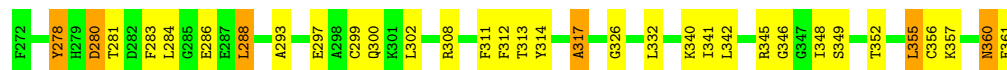
4.2.10 Score per residue for model 10

• Molecule 1: COAGULATION FACTOR XI

Chain A: 59% 34% 6% .



- Molecule 1: COAGULATION FACTOR XI

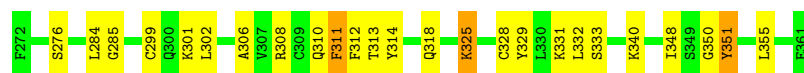


4.2.11 Score per residue for model 11

- Molecule 1: COAGULATION FACTOR XI



- Molecule 1: COAGULATION FACTOR XI



4.2.12 Score per residue for model 12

- Molecule 1: COAGULATION FACTOR XI



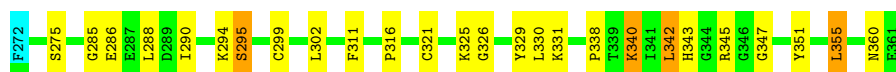
- Molecule 1: COAGULATION FACTOR XI



4.2.13 Score per residue for model 13

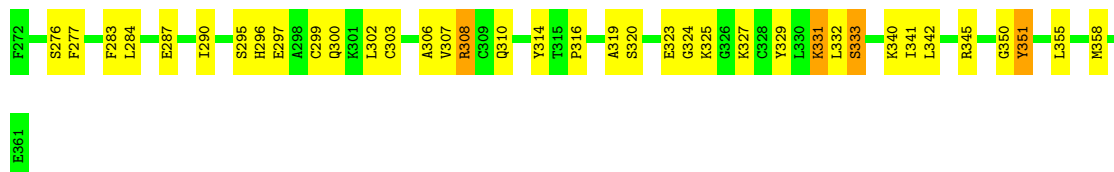
- Molecule 1: COAGULATION FACTOR XI





• Molecule 1: COAGULATION FACTOR XI

Chain B: 59% 37% .



4.2.14 Score per residue for model 14

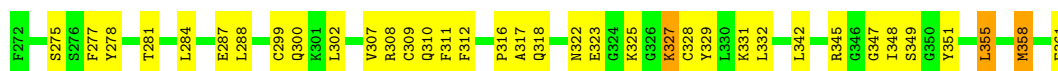
• Molecule 1: COAGULATION FACTOR XI

Chain A: 57% 37% 6% .



• Molecule 1: COAGULATION FACTOR XI

Chain B: 60% 37% .



5 Refinement protocol and experimental data overview

The models were refined using the following method: *CNS*.

Of the 1 calculated structures, 14 were deposited, based on the following criterion: *NO RESTRAINT VIOLATION AND LOWEST ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
CNS	structure solution	

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

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	682	538	650	21±5
1	B	693	549	658	21±5
All	All	19250	15218	18312	555

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:334:SER:HB3	1:B:359:ASP:HA	1.02	1.21	3	1
1:A:342:LEU:HG	1:B:288:LEU:HD21	1.00	1.33	10	1
1:B:313:THR:HG23	1:B:329:TYR:HB3	0.98	1.35	1	1
1:B:310:GLN:HA	1:B:355:LEU:HB2	0.97	1.36	6	1
1:A:311:PHE:HA	1:A:351:TYR:HB2	0.96	1.37	1	3
1:B:313:THR:HB	1:B:329:TYR:HB2	0.95	1.38	12	2
1:A:352:THR:HB	1:A:355:LEU:HD11	0.94	1.37	7	1
1:B:303:CYS:HA	1:B:307:VAL:HB	0.94	1.40	13	1
1:B:285:GLY:HA3	1:B:333:SER:HB3	0.91	1.43	9	3
1:B:336:GLY:HA2	1:B:361:GLU:HA	0.88	1.42	8	1
1:A:308:ARG:HD3	1:A:358:MET:HB2	0.86	1.47	14	1
1:A:277:PHE:HB3	1:A:348:ILE:HD11	0.85	1.45	7	2
1:A:310:GLN:HE21	1:A:359:ASP:HB3	0.85	1.31	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:313:THR:HB	1:B:329:TYR:HB3	0.83	1.48	9	2
1:A:302:LEU:HD11	1:A:330:LEU:HD21	0.80	1.52	12	1
1:A:288:LEU:HB2	1:B:342:LEU:HG	0.80	1.51	13	1
1:B:355:LEU:HD13	1:B:355:LEU:H	0.79	1.37	7	3
1:A:313:THR:HB	1:A:329:TYR:HB2	0.79	1.52	3	3
1:B:352:THR:HB	1:B:355:LEU:HD11	0.78	1.54	12	1
1:B:310:GLN:HB2	1:B:332:LEU:HD12	0.78	1.54	13	6
1:A:303:CYS:HA	1:A:307:VAL:HB	0.77	1.55	9	1
1:A:320:SER:HA	1:B:322:ASN:HB3	0.77	1.57	7	1
1:B:283:PHE:HB2	1:B:341:ILE:HA	0.76	1.57	12	1
1:B:284:LEU:HB2	1:B:288:LEU:HD11	0.75	1.57	9	1
1:B:301:LYS:HA	1:B:304:THR:HG22	0.75	1.59	3	1
1:B:355:LEU:H	1:B:355:LEU:HD13	0.75	1.41	9	2
1:A:355:LEU:HD13	1:A:355:LEU:H	0.75	1.42	7	2
1:B:291:VAL:HA	1:B:328:CYS:O	0.74	1.83	3	1
1:B:325:LYS:HE3	1:B:325:LYS:HA	0.73	1.60	4	1
1:B:290:ILE:HG12	1:B:291:VAL:H	0.73	1.43	3	1
1:A:299:CYS:O	1:A:302:LEU:HG	0.73	1.84	11	8
1:B:299:CYS:O	1:B:302:LEU:HG	0.72	1.85	8	6
1:B:308:ARG:O	1:B:308:ARG:HD2	0.72	1.84	13	1
1:B:316:PRO:HB2	1:B:318:GLN:HG3	0.71	1.60	2	1
1:B:351:TYR:HB3	1:B:355:LEU:HD11	0.71	1.61	11	1
1:B:313:THR:HG22	1:B:349:SER:HA	0.70	1.61	2	2
1:A:300:GLN:HE21	1:A:300:GLN:HA	0.70	1.46	12	1
1:A:352:THR:HB	1:A:355:LEU:HD13	0.70	1.62	4	1
1:B:307:VAL:HG12	1:B:355:LEU:HB3	0.70	1.64	14	1
1:B:310:GLN:HA	1:B:355:LEU:CB	0.69	2.17	6	2
1:B:277:PHE:HB3	1:B:348:ILE:HD11	0.69	1.65	7	4
1:A:288:LEU:HG	1:B:342:LEU:HD21	0.69	1.64	10	1
1:A:299:CYS:HB3	1:A:312:PHE:HZ	0.69	1.47	4	1
1:A:310:GLN:HA	1:A:355:LEU:HB2	0.69	1.63	9	2
1:B:314:TYR:HB2	1:B:348:ILE:HB	0.68	1.64	11	1
1:B:329:TYR:HE1	1:B:331:LYS:HE3	0.68	1.48	14	1
1:A:275:SER:HB3	1:A:351:TYR:HB2	0.67	1.66	6	1
1:A:355:LEU:H	1:A:355:LEU:HD13	0.67	1.49	13	1
1:A:313:THR:HG22	1:A:349:SER:HB3	0.67	1.67	10	1
1:B:311:PHE:HB2	1:B:331:LYS:HG2	0.67	1.66	3	1
1:A:294:LYS:HA	1:A:325:LYS:HG2	0.66	1.66	13	1
1:B:273:CYS:SG	1:B:353:LEU:HA	0.66	2.30	7	1
1:B:355:LEU:H	1:B:355:LEU:HD23	0.66	1.51	14	1
1:B:308:ARG:HB3	1:B:332:LEU:HD12	0.65	1.68	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:284:LEU:HD22	1:A:288:LEU:HG	0.65	1.69	5	1
1:A:303:CYS:HA	1:A:307:VAL:HA	0.65	1.68	11	1
1:A:311:PHE:HB2	1:A:349:SER:HB3	0.65	1.67	6	1
1:A:316:PRO:HD3	1:A:347:GLY:HA3	0.65	1.68	13	2
1:A:279:HIS:HB3	1:A:347:GLY:O	0.64	1.93	12	1
1:B:281:THR:HA	1:B:342:LEU:O	0.64	1.93	12	1
1:A:311:PHE:HB2	1:A:331:LYS:HB2	0.63	1.69	13	2
1:A:288:LEU:HB2	1:A:331:LYS:HA	0.63	1.70	14	1
1:B:283:PHE:HB2	1:B:341:ILE:CA	0.63	2.24	12	1
1:B:278:TYR:HD2	1:B:281:THR:HB	0.62	1.53	3	1
1:A:288:LEU:HD11	1:B:342:LEU:HA	0.62	1.70	9	1
1:B:276:SER:O	1:B:350:GLY:HA2	0.62	1.95	9	4
1:B:323:GLU:HG3	1:B:324:GLY:H	0.62	1.52	7	1
1:B:288:LEU:HG	1:B:331:LYS:HB3	0.62	1.71	6	2
1:B:313:THR:HB	1:B:329:TYR:CB	0.62	2.25	3	1
1:A:342:LEU:HD21	1:B:288:LEU:HB2	0.62	1.70	14	1
1:B:310:GLN:HG2	1:B:332:LEU:HA	0.61	1.72	5	1
1:B:316:PRO:HD3	1:B:347:GLY:HA3	0.61	1.71	14	1
1:B:279:HIS:HB3	1:B:348:ILE:HG12	0.61	1.71	4	1
1:A:297:GLU:HA	1:A:300:GLN:HE21	0.61	1.54	2	1
1:B:284:LEU:HB2	1:B:340:LYS:HG3	0.60	1.70	10	1
1:A:275:SER:HA	1:A:351:TYR:O	0.60	1.95	11	7
1:B:308:ARG:HD3	1:B:358:MET:HG3	0.60	1.73	13	1
1:A:287:GLU:HG3	1:A:331:LYS:CB	0.60	2.26	14	1
1:A:310:GLN:HG2	1:A:311:PHE:CD2	0.60	2.31	7	1
1:B:327:LYS:HD2	1:B:329:TYR:CE1	0.60	2.32	12	1
1:B:355:LEU:HD13	1:B:356:CYS:N	0.60	2.11	10	1
1:B:332:LEU:HG	1:B:333:SER:N	0.59	2.12	13	2
1:B:313:THR:OG1	1:B:331:LYS:HE2	0.59	1.97	11	1
1:A:294:LYS:HA	1:A:325:LYS:HG3	0.59	1.71	1	1
1:A:302:LEU:HD12	1:A:330:LEU:HD12	0.59	1.73	2	2
1:B:297:GLU:O	1:B:300:GLN:HG3	0.59	1.98	9	2
1:A:352:THR:O	1:A:355:LEU:HD12	0.59	1.96	9	1
1:A:330:LEU:H	1:A:330:LEU:HD13	0.59	1.58	9	1
1:B:290:ILE:HG12	1:B:291:VAL:N	0.59	2.11	3	1
1:B:352:THR:O	1:B:355:LEU:HD12	0.58	1.97	10	1
1:A:311:PHE:HA	1:A:351:TYR:CB	0.58	2.22	1	1
1:B:283:PHE:HB3	1:B:340:LYS:O	0.58	1.98	12	1
1:A:286:GLU:HB3	1:B:340:LYS:HE3	0.58	1.73	13	1
1:A:284:LEU:HB3	1:A:340:LYS:HB2	0.58	1.74	14	1
1:A:279:HIS:HE1	1:A:313:THR:HG23	0.58	1.57	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:285:GLY:HA3	1:B:333:SER:OG	0.58	1.98	3	1
1:A:276:SER:O	1:A:350:GLY:HA2	0.58	1.98	10	4
1:A:275:SER:CB	1:A:351:TYR:HB2	0.58	2.28	6	1
1:A:288:LEU:HB2	1:A:330:LEU:O	0.58	1.98	14	1
1:B:329:TYR:HB3	1:B:331:LYS:HE3	0.58	1.73	3	1
1:A:284:LEU:HA	1:A:331:LYS:HE3	0.58	1.76	7	1
1:A:297:GLU:HA	1:A:300:GLN:NE2	0.57	2.13	2	1
1:A:293:ALA:HB2	1:A:328:CYS:HB2	0.57	1.74	3	1
1:A:299:CYS:O	1:A:302:LEU:HB3	0.57	1.99	9	1
1:A:297:GLU:O	1:A:300:GLN:HG3	0.57	1.98	14	3
1:B:284:LEU:HG	1:B:288:LEU:HD13	0.57	1.75	12	1
1:B:313:THR:HB	1:B:349:SER:HA	0.57	1.76	1	1
1:B:291:VAL:CA	1:B:328:CYS:H	0.57	2.12	3	1
1:B:287:GLU:O	1:B:331:LYS:HA	0.57	1.99	13	2
1:B:273:CYS:O	1:B:353:LEU:HA	0.57	1.99	9	1
1:A:315:THR:HB	1:A:316:PRO:HD3	0.57	1.76	8	1
1:A:313:THR:HB	1:A:329:TYR:HB3	0.57	1.74	2	2
1:B:290:ILE:HD11	1:B:327:LYS:HD2	0.56	1.77	7	2
1:B:355:LEU:H	1:B:355:LEU:CD1	0.56	2.12	12	2
1:A:313:THR:HG22	1:A:347:GLY:H	0.56	1.61	14	1
1:B:285:GLY:HA3	1:B:333:SER:CB	0.56	2.30	3	2
1:A:288:LEU:HD12	1:A:331:LYS:HE2	0.56	1.78	11	1
1:A:286:GLU:HA	1:B:340:LYS:HE2	0.56	1.75	4	1
1:B:357:LYS:HE2	1:B:357:LYS:HA	0.56	1.78	10	1
1:A:310:GLN:HA	1:A:355:LEU:HD23	0.56	1.76	11	1
1:B:283:PHE:CD1	1:B:342:LEU:HB2	0.56	2.36	12	1
1:A:287:GLU:O	1:A:331:LYS:HA	0.56	2.00	6	4
1:A:352:THR:HG22	1:A:355:LEU:HD23	0.56	1.78	14	1
1:A:276:SER:HB2	1:A:278:TYR:CE2	0.56	2.36	6	1
1:B:311:PHE:HA	1:B:351:TYR:HB2	0.56	1.76	11	2
1:B:284:LEU:HB2	1:B:342:LEU:HD11	0.56	1.77	13	1
1:A:285:GLY:HA3	1:A:337:SER:HB3	0.55	1.78	14	1
1:A:279:HIS:HB2	1:A:348:ILE:HA	0.55	1.76	3	1
1:B:316:PRO:HB2	1:B:319:ALA:HB3	0.55	1.79	13	1
1:A:299:CYS:HB3	1:A:312:PHE:CE2	0.55	2.35	7	1
1:B:355:LEU:HD12	1:B:356:CYS:N	0.55	2.17	1	1
1:A:352:THR:HB	1:A:355:LEU:CD1	0.55	2.32	4	1
1:A:340:LYS:HE2	1:B:286:GLU:HG3	0.55	1.78	12	1
1:A:332:LEU:HD11	1:A:358:MET:SD	0.55	2.41	10	1
1:A:284:LEU:HD21	1:B:284:LEU:HD21	0.55	1.77	14	1
1:B:283:PHE:CD2	1:B:341:ILE:HG22	0.55	2.37	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:279:HIS:CD2	1:B:348:ILE:HG12	0.55	2.37	9	1
1:A:332:LEU:HD11	1:A:358:MET:HG2	0.55	1.79	12	1
1:B:280:ASP:O	1:B:344:GLY:HA2	0.55	2.02	9	1
1:A:290:ILE:HD11	1:B:345:ARG:HB2	0.55	1.79	13	1
1:A:345:ARG:HA	1:A:345:ARG:NE	0.55	2.17	8	1
1:B:355:LEU:O	1:B:358:MET:HG2	0.54	2.02	7	2
1:B:310:GLN:OE1	1:B:310:GLN:HA	0.54	2.02	2	1
1:A:309:CYS:HB3	1:A:330:LEU:HD23	0.54	1.79	12	1
1:A:276:SER:O	1:A:351:TYR:HA	0.54	2.02	6	1
1:A:288:LEU:HD12	1:A:331:LYS:HG2	0.54	1.78	4	1
1:B:292:ALA:HB3	1:B:327:LYS:HA	0.54	1.78	1	2
1:B:310:GLN:O	1:B:351:TYR:HB2	0.54	2.02	6	3
1:A:303:CYS:CA	1:A:307:VAL:HB	0.54	2.31	9	1
1:A:353:LEU:HB3	1:A:355:LEU:HG	0.53	1.80	8	1
1:A:310:GLN:HB2	1:A:332:LEU:HA	0.53	1.80	4	1
1:B:308:ARG:HG2	1:B:358:MET:HB2	0.53	1.80	1	1
1:B:332:LEU:HD11	1:B:358:MET:SD	0.53	2.43	3	1
1:B:306:ALA:HB1	1:B:308:ARG:HH11	0.53	1.63	11	1
1:A:286:GLU:HB3	1:A:332:LEU:O	0.53	2.04	7	1
1:B:352:THR:HB	1:B:355:LEU:CD1	0.53	2.32	12	2
1:B:325:LYS:CE	1:B:325:LYS:HA	0.53	2.27	4	1
1:B:320:SER:HB2	1:B:324:GLY:HA3	0.53	1.79	13	1
1:A:355:LEU:HD13	1:A:356:CYS:N	0.53	2.19	9	2
1:B:302:LEU:HD11	1:B:330:LEU:HD22	0.52	1.82	7	1
1:B:310:GLN:HA	1:B:355:LEU:HD23	0.52	1.81	12	1
1:A:288:LEU:HB2	1:B:342:LEU:HD23	0.52	1.81	5	1
1:A:290:ILE:HA	1:A:329:TYR:HB2	0.52	1.80	7	1
1:A:352:THR:HG21	1:A:355:LEU:HD11	0.52	1.80	6	1
1:A:352:THR:H	1:A:355:LEU:HD22	0.52	1.64	4	1
1:B:310:GLN:OE1	1:B:332:LEU:HA	0.52	2.04	4	1
1:B:291:VAL:CA	1:B:328:CYS:O	0.52	2.56	3	1
1:B:332:LEU:HD11	1:B:358:MET:HG2	0.52	1.82	8	1
1:A:312:PHE:HD1	1:A:328:CYS:HB2	0.52	1.64	10	1
1:B:291:VAL:HA	1:B:328:CYS:H	0.52	1.63	3	1
1:A:345:ARG:HA	1:A:345:ARG:HE	0.52	1.65	13	1
1:A:307:VAL:O	1:A:308:ARG:HD2	0.52	2.05	6	1
1:A:309:CYS:O	1:A:355:LEU:HB2	0.52	2.04	2	1
1:A:302:LEU:HD13	1:A:330:LEU:HG	0.51	1.82	11	1
1:A:340:LYS:HD2	1:B:287:GLU:HB2	0.51	1.82	2	1
1:B:314:TYR:HB3	1:B:348:ILE:HG12	0.51	1.80	3	1
1:B:284:LEU:HD13	1:B:285:GLY:N	0.51	2.21	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:352:THR:HG23	1:A:353:LEU:HG	0.51	1.80	10	1
1:A:295:SER:N	1:A:325:LYS:HE3	0.51	2.20	13	1
1:B:283:PHE:CE2	1:B:341:ILE:HG12	0.51	2.41	13	1
1:A:287:GLU:HG3	1:A:331:LYS:HB2	0.51	1.81	14	1
1:A:288:LEU:HB2	1:B:342:LEU:HD21	0.51	1.81	4	1
1:A:355:LEU:HD13	1:A:356:CYS:H	0.51	1.65	9	1
1:A:279:HIS:NE2	1:A:346:GLY:HA3	0.51	2.20	3	1
1:B:329:TYR:CE1	1:B:331:LYS:HE3	0.51	2.37	14	1
1:B:352:THR:H	1:B:355:LEU:HD11	0.51	1.64	4	1
1:B:283:PHE:CZ	1:B:342:LEU:HD13	0.51	2.41	12	1
1:A:300:GLN:HA	1:A:351:TYR:OH	0.51	2.05	14	1
1:A:329:TYR:OH	1:A:331:LYS:HD2	0.50	2.05	11	1
1:A:310:GLN:HA	1:A:355:LEU:CB	0.50	2.34	9	1
1:A:311:PHE:CZ	1:A:331:LYS:HG3	0.50	2.41	5	1
1:B:345:ARG:NE	1:B:345:ARG:HA	0.50	2.21	10	2
1:A:329:TYR:CE2	1:A:331:LYS:HE3	0.50	2.41	6	1
1:B:303:CYS:CA	1:B:307:VAL:HB	0.50	2.26	13	1
1:A:312:PHE:CZ	1:A:328:CYS:HB2	0.50	2.41	12	2
1:B:311:PHE:HB2	1:B:331:LYS:HG3	0.50	1.81	12	1
1:A:311:PHE:HA	1:A:351:TYR:CD1	0.50	2.42	14	1
1:B:315:THR:O	1:B:327:LYS:HB2	0.50	2.07	2	1
1:A:311:PHE:HA	1:A:351:TYR:HD1	0.50	1.67	14	1
1:B:287:GLU:HB2	1:B:332:LEU:CD2	0.50	2.37	14	1
1:A:337:SER:HB3	1:A:338:PRO:HD2	0.50	1.82	7	1
1:B:284:LEU:HD23	1:B:285:GLY:N	0.49	2.21	11	1
1:B:278:TYR:CD2	1:B:281:THR:HB	0.49	2.43	14	2
1:B:309:CYS:H	1:B:355:LEU:HD12	0.49	1.66	14	1
1:A:282:ASP:HB3	1:A:342:LEU:HD22	0.49	1.83	1	1
1:B:345:ARG:HE	1:B:345:ARG:HA	0.49	1.66	4	1
1:A:310:GLN:HG2	1:A:332:LEU:HB2	0.49	1.84	14	1
1:A:311:PHE:CA	1:A:351:TYR:HD1	0.49	2.21	14	1
1:B:313:THR:CG2	1:B:329:TYR:HB2	0.49	2.36	7	1
1:B:277:PHE:CD1	1:B:350:GLY:HA3	0.49	2.42	5	1
1:B:345:ARG:O	1:B:345:ARG:HD2	0.49	2.07	3	1
1:B:311:PHE:CD2	1:B:331:LYS:HE3	0.49	2.43	5	1
1:B:275:SER:HA	1:B:351:TYR:O	0.49	2.07	3	2
1:A:334:SER:HB3	1:A:359:ASP:HA	0.49	1.83	8	2
1:B:333:SER:HB3	1:B:337:SER:HB2	0.49	1.84	8	1
1:B:280:ASP:HA	1:B:346:GLY:O	0.49	2.07	10	1
1:B:291:VAL:HA	1:B:328:CYS:N	0.49	2.22	3	1
1:A:312:PHE:CD1	1:A:328:CYS:HB2	0.49	2.42	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:282:ASP:HB3	1:A:342:LEU:CD2	0.49	2.37	1	1
1:A:283:PHE:CE2	1:A:341:ILE:HG22	0.49	2.42	5	1
1:A:340:LYS:HB3	1:A:340:LYS:NZ	0.49	2.23	6	1
1:A:284:LEU:HG	1:A:331:LYS:HD2	0.49	1.84	7	1
1:A:290:ILE:HG13	1:A:329:TYR:HB3	0.49	1.83	8	1
1:B:303:CYS:O	1:B:307:VAL:HB	0.49	2.08	1	1
1:A:318:GLN:HE22	1:A:323:GLU:HA	0.49	1.68	3	1
1:B:311:PHE:O	1:B:331:LYS:HG2	0.49	2.07	7	1
1:A:302:LEU:HD13	1:A:330:LEU:HD12	0.49	1.85	1	1
1:A:310:GLN:HG2	1:A:311:PHE:CE2	0.48	2.43	7	1
1:A:342:LEU:HG	1:B:288:LEU:HD23	0.48	1.85	1	1
1:A:287:GLU:HB3	1:A:332:LEU:CD2	0.48	2.38	3	1
1:A:283:PHE:HB2	1:A:311:PHE:HZ	0.48	1.67	5	1
1:A:345:ARG:NE	1:A:345:ARG:HA	0.48	2.22	12	1
1:A:333:SER:HB2	1:A:337:SER:HB3	0.48	1.84	1	1
1:A:353:LEU:HG	1:A:354:ARG:N	0.48	2.23	14	1
1:A:279:HIS:CE1	1:A:313:THR:HG23	0.48	2.42	3	1
1:B:291:VAL:HB	1:B:327:LYS:CA	0.48	2.38	3	1
1:B:288:LEU:HB3	1:B:329:TYR:CE1	0.48	2.43	5	1
1:B:323:GLU:HG3	1:B:324:GLY:N	0.48	2.23	7	1
1:B:313:THR:HG22	1:B:329:TYR:HB2	0.48	1.84	7	1
1:B:284:LEU:HG	1:B:342:LEU:HD11	0.48	1.84	9	1
1:B:334:SER:CB	1:B:359:ASP:HA	0.48	2.15	3	1
1:B:312:PHE:CE1	1:B:328:CYS:HB3	0.48	2.43	11	1
1:A:286:GLU:HG3	1:B:340:LYS:HE2	0.48	1.85	7	1
1:A:318:GLN:HB2	1:A:322:ASN:O	0.48	2.08	14	1
1:A:332:LEU:HD11	1:A:358:MET:HG3	0.48	1.85	4	1
1:A:345:ARG:H	1:A:345:ARG:HD3	0.48	1.68	3	1
1:A:287:GLU:HG3	1:B:340:LYS:HD3	0.48	1.85	5	1
1:A:279:HIS:CB	1:A:348:ILE:HA	0.48	2.37	3	2
1:A:355:LEU:O	1:A:358:MET:HG3	0.48	2.08	10	1
1:A:360:ASN:O	1:A:361:GLU:HB2	0.48	2.08	10	1
1:A:315:THR:HG23	1:A:327:LYS:CG	0.48	2.39	2	1
1:A:342:LEU:HD13	1:A:342:LEU:N	0.48	2.24	12	2
1:B:345:ARG:HA	1:B:345:ARG:HE	0.48	1.68	12	1
1:B:287:GLU:C	1:B:288:LEU:HD12	0.48	2.29	5	1
1:B:312:PHE:CZ	1:B:328:CYS:HB2	0.48	2.43	14	1
1:A:299:CYS:HB3	1:A:312:PHE:CZ	0.48	2.37	4	1
1:B:355:LEU:N	1:B:355:LEU:HD13	0.48	2.19	9	1
1:B:293:ALA:HB1	1:B:314:TYR:CE1	0.47	2.42	10	1
1:A:299:CYS:O	1:A:302:LEU:HD22	0.47	2.09	2	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:334:SER:HA	1:A:359:ASP:HA	0.47	1.85	5	1
1:A:288:LEU:CB	1:B:342:LEU:HG	0.47	2.31	13	1
1:A:320:SER:HB2	1:A:324:GLY:HA3	0.47	1.84	11	1
1:B:284:LEU:HB3	1:B:340:LYS:HG3	0.47	1.86	11	1
1:A:283:PHE:O	1:A:331:LYS:HE3	0.47	2.08	7	1
1:A:330:LEU:CD1	1:A:330:LEU:H	0.47	2.22	9	1
1:B:310:GLN:HA	1:B:355:LEU:HB3	0.47	1.85	13	1
1:B:332:LEU:HG	1:B:333:SER:O	0.47	2.09	8	1
1:B:292:ALA:CB	1:B:327:LYS:HA	0.47	2.39	5	1
1:A:313:THR:HB	1:A:329:TYR:CE1	0.47	2.44	7	2
1:A:311:PHE:CE1	1:A:331:LYS:HG3	0.47	2.45	5	1
1:A:276:SER:O	1:A:351:TYR:CA	0.47	2.62	6	1
1:B:312:PHE:HB2	1:B:351:TYR:CE2	0.47	2.44	11	1
1:A:284:LEU:HA	1:A:331:LYS:CE	0.47	2.38	7	1
1:A:277:PHE:CD1	1:A:350:GLY:HA3	0.47	2.45	10	1
1:A:303:CYS:HA	1:A:306:ALA:O	0.47	2.10	3	2
1:B:313:THR:CB	1:B:349:SER:HA	0.47	2.39	1	1
1:B:335:ASN:ND2	1:B:360:ASN:HA	0.47	2.25	9	1
1:A:285:GLY:HA3	1:A:333:SER:HB3	0.47	1.87	5	1
1:A:308:ARG:O	1:A:309:CYS:SG	0.47	2.73	6	1
1:A:286:GLU:O	1:A:332:LEU:HB3	0.47	2.09	14	1
1:A:354:ARG:N	1:A:354:ARG:HD2	0.47	2.25	10	1
1:A:287:GLU:HB3	1:A:332:LEU:HD21	0.47	1.86	3	1
1:B:311:PHE:HB2	1:B:331:LYS:CG	0.47	2.39	3	1
1:A:342:LEU:HB3	1:A:345:ARG:CG	0.47	2.40	5	1
1:A:284:LEU:O	1:A:340:LYS:HG2	0.47	2.09	7	1
1:B:335:ASN:ND2	1:B:336:GLY:H	0.47	2.07	8	1
1:B:293:ALA:O	1:B:326:GLY:HA3	0.46	2.10	2	1
1:A:331:LYS:N	1:A:331:LYS:HD3	0.46	2.26	8	1
1:B:342:LEU:HD12	1:B:342:LEU:N	0.46	2.26	2	1
1:A:333:SER:HB2	1:A:359:ASP:HB3	0.46	1.85	12	1
1:B:333:SER:O	1:B:335:ASN:N	0.46	2.48	1	1
1:A:355:LEU:O	1:A:358:MET:HG2	0.46	2.10	7	1
1:A:286:GLU:HA	1:B:340:LYS:HD3	0.46	1.87	8	1
1:B:278:TYR:HB2	1:B:281:THR:CG2	0.46	2.41	10	1
1:B:309:CYS:O	1:B:355:LEU:HB2	0.46	2.09	4	1
1:B:278:TYR:CE2	1:B:349:SER:HB3	0.46	2.46	6	2
1:A:327:LYS:HD3	1:A:329:TYR:CD2	0.46	2.46	10	1
1:A:310:GLN:HB2	1:A:332:LEU:HD12	0.46	1.86	8	1
1:B:303:CYS:O	1:B:307:VAL:HA	0.46	2.09	8	1
1:B:299:CYS:O	1:B:302:LEU:HD22	0.46	2.11	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:283:PHE:CE1	1:B:342:LEU:HD22	0.46	2.46	12	1
1:B:342:LEU:HD13	1:B:345:ARG:NH2	0.46	2.26	14	1
1:A:340:LYS:HG3	1:B:286:GLU:O	0.46	2.11	10	1
1:A:333:SER:HA	1:A:359:ASP:OD1	0.46	2.11	1	1
1:A:311:PHE:CE1	1:A:331:LYS:HG2	0.46	2.46	8	1
1:A:352:THR:O	1:A:353:LEU:HB2	0.46	2.11	8	1
1:B:277:PHE:HA	1:B:349:SER:O	0.46	2.10	2	1
1:B:288:LEU:HA	1:B:330:LEU:O	0.46	2.11	6	1
1:A:284:LEU:HG	1:B:284:LEU:HD13	0.45	1.88	8	1
1:A:283:PHE:HB2	1:A:311:PHE:CZ	0.45	2.45	5	1
1:A:274:HIS:HD2	1:A:351:TYR:HB3	0.45	1.71	4	1
1:B:299:CYS:HB3	1:B:312:PHE:CZ	0.45	2.46	14	1
1:A:277:PHE:HA	1:A:349:SER:O	0.45	2.10	1	1
1:A:351:TYR:CD2	1:A:351:TYR:N	0.45	2.83	6	1
1:A:294:LYS:HG2	1:A:324:GLY:O	0.45	2.12	9	1
1:B:311:PHE:HD2	1:B:331:LYS:HE3	0.45	1.71	5	1
1:A:283:PHE:O	1:A:331:LYS:HD2	0.45	2.11	6	2
1:A:287:GLU:HG3	1:B:340:LYS:CD	0.45	2.41	5	1
1:A:355:LEU:H	1:A:355:LEU:CD1	0.45	2.23	13	1
1:B:353:LEU:HD12	1:B:354:ARG:N	0.45	2.26	6	1
1:A:354:ARG:HD2	1:A:354:ARG:H	0.45	1.71	11	1
1:A:296:HIS:HA	1:A:328:CYS:SG	0.45	2.51	7	1
1:A:309:CYS:SG	1:A:355:LEU:HD22	0.45	2.52	2	1
1:A:312:PHE:HA	1:A:329:TYR:O	0.45	2.11	1	2
1:B:282:ASP:HB2	1:B:346:GLY:HA3	0.45	1.88	2	1
1:B:311:PHE:CD1	1:B:331:LYS:HG3	0.45	2.47	11	1
1:B:311:PHE:HD1	1:B:331:LYS:HG3	0.45	1.72	11	1
1:B:278:TYR:CE2	1:B:281:THR:HB	0.45	2.47	14	1
1:A:330:LEU:N	1:A:330:LEU:HD13	0.45	2.27	8	1
1:B:297:GLU:H	1:B:297:GLU:CD	0.45	2.15	10	1
1:A:310:GLN:HB3	1:A:332:LEU:HA	0.45	1.88	3	1
1:B:352:THR:HG22	1:B:353:LEU:HG	0.45	1.87	5	1
1:A:283:PHE:CD1	1:A:341:ILE:HB	0.45	2.47	6	1
1:A:280:ASP:HA	1:A:346:GLY:O	0.45	2.12	7	1
1:A:355:LEU:CD1	1:A:355:LEU:H	0.45	2.19	7	1
1:B:353:LEU:HD23	1:B:353:LEU:H	0.45	1.71	8	1
1:A:314:TYR:O	1:A:347:GLY:HA3	0.45	2.12	2	1
1:A:297:GLU:O	1:A:300:GLN:HB3	0.45	2.11	10	1
1:B:291:VAL:CA	1:B:328:CYS:N	0.45	2.79	3	1
1:A:327:LYS:HA	1:A:327:LYS:HE3	0.45	1.88	5	1
1:B:284:LEU:O	1:B:339:THR:HA	0.45	2.11	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:290:ILE:HD11	1:B:327:LYS:HE3	0.45	1.87	6	1
1:A:278:TYR:CD1	1:A:281:THR:HG23	0.44	2.47	7	1
1:B:311:PHE:CE2	1:B:331:LYS:HB2	0.44	2.47	14	1
1:A:345:ARG:HE	1:A:345:ARG:HA	0.44	1.71	2	1
1:B:284:LEU:CB	1:B:288:LEU:HD21	0.44	2.43	4	1
1:A:342:LEU:N	1:A:342:LEU:HD13	0.44	2.27	6	1
1:B:316:PRO:HD3	1:B:347:GLY:CA	0.44	2.41	6	1
1:A:355:LEU:HD12	1:A:356:CYS:N	0.44	2.27	14	1
1:B:299:CYS:HB3	1:B:312:PHE:HZ	0.44	1.73	14	1
1:B:313:THR:HG22	1:B:349:SER:HB3	0.44	1.89	10	1
1:A:311:PHE:CD1	1:A:351:TYR:HE2	0.44	2.31	4	1
1:A:342:LEU:HB3	1:A:345:ARG:HG3	0.44	1.88	5	1
1:A:291:VAL:HB	1:A:328:CYS:SG	0.44	2.53	10	1
1:B:312:PHE:O	1:B:349:SER:HA	0.44	2.13	6	1
1:A:278:TYR:HD1	1:A:281:THR:HB	0.44	1.73	8	1
1:B:317:ALA:HB3	1:B:326:GLY:CA	0.44	2.43	10	1
1:A:284:LEU:HD11	1:B:340:LYS:HD2	0.44	1.89	10	1
1:B:296:HIS:HB3	1:B:314:TYR:CE2	0.44	2.48	13	1
1:A:284:LEU:HD11	1:B:340:LYS:CD	0.44	2.42	10	1
1:A:287:GLU:HA	1:B:340:LYS:HG2	0.43	1.89	7	1
1:A:341:ILE:HD13	1:A:341:ILE:H	0.43	1.73	10	1
1:B:332:LEU:HD21	1:B:358:MET:SD	0.43	2.53	1	1
1:A:310:GLN:OE1	1:A:356:CYS:HA	0.43	2.13	3	1
1:B:316:PRO:CB	1:B:319:ALA:HB3	0.43	2.43	13	1
1:B:290:ILE:HB	1:B:329:TYR:CD1	0.43	2.48	5	1
1:B:335:ASN:CB	1:B:360:ASN:HA	0.43	2.44	6	1
1:A:334:SER:CB	1:A:359:ASP:HA	0.43	2.44	4	1
1:A:342:LEU:HD21	1:B:288:LEU:HB3	0.43	1.89	7	1
1:B:324:GLY:O	1:B:325:LYS:HG3	0.43	2.13	12	1
1:B:308:ARG:HG2	1:B:358:MET:SD	0.43	2.53	14	1
1:B:318:GLN:HB3	1:B:325:LYS:HD3	0.43	1.91	8	1
1:A:345:ARG:HD3	1:A:345:ARG:N	0.43	2.27	3	1
1:B:278:TYR:CZ	1:B:349:SER:HB3	0.43	2.48	5	1
1:B:303:CYS:HA	1:B:307:VAL:CB	0.43	2.27	13	1
1:A:320:SER:HA	1:B:322:ASN:CB	0.43	2.38	7	1
1:A:335:ASN:HD22	1:A:336:GLY:N	0.43	2.11	12	1
1:B:317:ALA:HB3	1:B:327:LYS:HE2	0.43	1.90	14	1
1:B:311:PHE:CD2	1:B:331:LYS:HG3	0.43	2.49	12	1
1:B:289:ASP:HB3	1:B:330:LEU:HB3	0.43	1.90	3	1
1:B:340:LYS:HB3	1:B:340:LYS:NZ	0.43	2.29	9	1
1:A:278:TYR:CZ	1:A:349:SER:HB3	0.43	2.49	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:286:GLU:HA	1:B:340:LYS:CE	0.43	2.43	4	1
1:B:278:TYR:CE1	1:B:349:SER:HB3	0.43	2.49	5	1
1:B:355:LEU:HD22	1:B:356:CYS:N	0.42	2.29	7	1
1:A:288:LEU:HD21	1:B:284:LEU:HD22	0.42	1.91	13	1
1:A:335:ASN:HB3	1:A:358:MET:O	0.42	2.14	6	1
1:A:294:LYS:HA	1:A:326:GLY:HA3	0.42	1.90	9	1
1:A:276:SER:C	1:A:351:TYR:HA	0.42	2.35	6	1
1:A:342:LEU:HB3	1:A:345:ARG:HB2	0.42	1.91	7	1
1:A:285:GLY:HA3	1:A:333:SER:OG	0.42	2.15	2	2
1:A:342:LEU:HD23	1:A:342:LEU:N	0.42	2.28	13	1
1:B:360:ASN:C	1:B:360:ASN:HD22	0.42	2.18	10	1
1:B:282:ASP:HB2	1:B:349:SER:HB2	0.42	1.92	9	1
1:A:302:LEU:HD11	1:A:330:LEU:CD2	0.42	2.37	12	1
1:B:277:PHE:CD2	1:B:350:GLY:HA3	0.42	2.50	13	1
1:A:313:THR:HB	1:A:329:TYR:CG	0.42	2.49	11	1
1:B:285:GLY:HA2	1:B:338:PRO:HA	0.42	1.91	2	1
1:B:352:THR:N	1:B:355:LEU:HD11	0.42	2.30	4	1
1:B:357:LYS:O	1:B:357:LYS:HG2	0.42	2.14	9	1
1:A:345:ARG:H	1:A:345:ARG:CD	0.42	2.28	3	1
1:A:313:THR:HG22	1:A:349:SER:CB	0.42	2.42	10	1
1:A:294:LYS:HG3	1:A:325:LYS:HG3	0.42	1.91	3	1
1:A:335:ASN:HD22	1:A:335:ASN:C	0.42	2.18	3	1
1:A:325:LYS:HD2	1:A:326:GLY:N	0.42	2.30	13	1
1:A:338:PRO:HB2	1:A:340:LYS:HE3	0.42	1.90	13	1
1:A:315:THR:HB	1:A:316:PRO:CD	0.42	2.45	8	1
1:A:288:LEU:HD21	1:B:284:LEU:HD23	0.42	1.92	2	1
1:A:336:GLY:H	1:A:361:GLU:C	0.42	2.18	12	1
1:A:311:PHE:HB3	1:A:351:TYR:HB3	0.42	1.91	5	1
1:A:278:TYR:CE2	1:A:349:SER:HB3	0.41	2.50	7	1
1:B:331:LYS:N	1:B:331:LYS:HD2	0.41	2.29	3	1
1:B:278:TYR:HE1	1:B:282:ASP:HA	0.41	1.74	5	1
1:B:294:LYS:HG2	1:B:325:LYS:HG3	0.41	1.92	7	1
1:B:316:PRO:O	1:B:325:LYS:HA	0.41	2.15	3	1
1:A:301:LYS:HA	1:A:304:THR:OG1	0.41	2.16	2	1
1:A:284:LEU:HB2	1:A:342:LEU:CD1	0.41	2.45	2	1
1:A:285:GLY:H	1:A:288:LEU:HD11	0.41	1.74	4	1
1:B:286:GLU:HG3	1:B:287:GLU:HG3	0.41	1.93	4	1
1:A:345:ARG:O	1:A:345:ARG:HG2	0.41	2.15	3	1
1:B:301:LYS:HA	1:B:304:THR:CG2	0.41	2.40	3	1
1:A:303:CYS:SG	1:A:330:LEU:HD11	0.41	2.55	6	1
1:A:279:HIS:C	1:A:281:THR:N	0.41	2.74	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:342:LEU:CD2	1:B:345:ARG:HB2	0.41	2.45	12	1
1:B:284:LEU:O	1:B:340:LYS:HG2	0.41	2.15	3	1
1:A:294:LYS:HB2	1:A:294:LYS:NZ	0.41	2.30	5	1
1:B:288:LEU:HG	1:B:331:LYS:CB	0.41	2.43	6	1
1:B:292:ALA:HB3	1:B:327:LYS:HG2	0.41	1.92	5	1
1:A:309:CYS:O	1:A:355:LEU:HG	0.41	2.15	7	2
1:B:342:LEU:HD13	1:B:345:ARG:HH21	0.41	1.74	14	1
1:A:342:LEU:HD13	1:A:342:LEU:H	0.41	1.75	1	1
1:A:352:THR:CG2	1:A:355:LEU:HD11	0.41	2.44	6	1
1:B:278:TYR:HD2	1:B:281:THR:HG23	0.41	1.75	7	1
1:B:286:GLU:HB3	1:B:332:LEU:O	0.41	2.16	7	1
1:A:310:GLN:O	1:A:355:LEU:HD13	0.41	2.15	12	1
1:B:357:LYS:O	1:B:361:GLU:HG2	0.41	2.16	10	1
1:A:278:TYR:O	1:A:348:ILE:HA	0.41	2.15	1	1
1:B:281:THR:HB	1:B:283:PHE:CE1	0.41	2.50	4	1
1:B:298:ALA:O	1:B:301:LYS:HG3	0.41	2.15	9	1
1:A:355:LEU:N	1:A:355:LEU:HD13	0.41	2.21	7	1
1:A:360:ASN:C	1:A:360:ASN:HD22	0.41	2.18	7	1
1:B:308:ARG:HB3	1:B:355:LEU:HA	0.41	1.93	1	1
1:A:310:GLN:HB2	1:A:358:MET:HE3	0.41	1.93	5	1
1:B:340:LYS:HD2	1:B:340:LYS:N	0.41	2.31	7	1
1:A:288:LEU:HD23	1:B:283:PHE:CE1	0.41	2.51	12	1
1:A:285:GLY:HA2	1:A:338:PRO:O	0.41	2.16	13	1
1:B:325:LYS:O	1:B:327:LYS:HD2	0.41	2.16	13	1
1:B:332:LEU:O	1:B:333:SER:HB2	0.41	2.16	13	1
1:A:276:SER:N	1:A:351:TYR:HB2	0.41	2.31	6	1
1:A:356:CYS:HA	1:A:359:ASP:OD1	0.41	2.16	11	1
1:B:336:GLY:CA	1:B:361:GLU:HA	0.41	2.29	8	1
1:B:352:THR:C	1:B:353:LEU:HD22	0.41	2.36	1	1
1:A:316:PRO:HA	1:A:325:LYS:O	0.41	2.16	2	1
1:B:345:ARG:CZ	1:B:345:ARG:HA	0.41	2.46	9	1
1:A:286:GLU:HB2	1:A:337:SER:HB2	0.41	1.92	3	1
1:A:283:PHE:HE2	1:A:341:ILE:HG22	0.41	1.75	5	1
1:A:311:PHE:HD2	1:A:331:LYS:HB2	0.40	1.76	4	1
1:B:327:LYS:HD2	1:B:327:LYS:N	0.40	2.30	4	1
1:A:286:GLU:HG2	1:A:335:ASN:ND2	0.40	2.32	9	1
1:B:285:GLY:HA3	1:B:333:SER:HA	0.40	1.94	11	1
1:A:314:TYR:OH	1:A:325:LYS:HD2	0.40	2.15	14	1
1:B:300:GLN:HA	1:B:312:PHE:CE2	0.40	2.52	1	1
1:A:288:LEU:N	1:A:288:LEU:HD22	0.40	2.31	5	1
1:A:282:ASP:HB3	1:A:284:LEU:HD11	0.40	1.93	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:299:CYS:O	1:B:302:LEU:HB3	0.40	2.17	2	1
1:B:341:ILE:N	1:B:341:ILE:HD12	0.40	2.32	5	1
1:A:332:LEU:O	1:A:333:SER:HB3	0.40	2.16	6	1
1:B:288:LEU:HD21	1:B:329:TYR:HD1	0.40	1.75	7	1
1:B:341:ILE:HD12	1:B:341:ILE:H	0.40	1.77	1	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	88/90 (98%)	70±3 (80±4%)	14±3 (16±3%)	3±2 (4±2%)	7	34
1	B	88/90 (98%)	72±2 (82±3%)	14±2 (15±3%)	3±2 (3±2%)	9	42
All	All	2464/2520 (98%)	1990 (81%)	390 (16%)	84 (3%)	7	38

All 45 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	316	PRO	5
1	A	295	SER	5
1	A	307	VAL	5
1	A	317	ALA	4
1	B	295	SER	4
1	B	323	GLU	4
1	B	321	CYS	3
1	B	317	ALA	3
1	A	320	SER	2
1	B	322	ASN	2
1	B	306	ALA	2
1	A	347	GLY	2
1	A	333	SER	2
1	B	318	GLN	2
1	B	353	LEU	2
1	B	334	SER	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	285	GLY	2
1	A	274	HIS	2
1	A	353	LEU	2
1	A	321	CYS	2
1	B	333	SER	2
1	B	338	PRO	2
1	A	322	ASN	1
1	A	273	CYS	1
1	A	306	ALA	1
1	A	346	GLY	1
1	A	360	ASN	1
1	A	309	CYS	1
1	B	347	GLY	1
1	B	320	SER	1
1	A	279	HIS	1
1	B	324	GLY	1
1	A	323	GLU	1
1	A	319	ALA	1
1	B	274	HIS	1
1	A	338	PRO	1
1	B	352	THR	1
1	A	318	GLN	1
1	B	307	VAL	1
1	A	275	SER	1
1	B	309	CYS	1
1	B	285	GLY	1
1	A	354	ARG	1
1	B	325	LYS	1
1	A	310	GLN	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	75/76 (99%)	67±2 (89±2%)	8±2 (11±2%)	12	55
1	B	76/76 (100%)	69±2 (90±3%)	7±2 (10±3%)	14	59
All	All	2114/2128 (99%)	1898 (90%)	216 (10%)	13	57

All 85 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	B	355	LEU	8
1	A	355	LEU	7
1	A	329	TYR	6
1	A	360	ASN	6
1	A	325	LYS	6
1	A	331	LYS	6
1	B	311	PHE	6
1	B	325	LYS	6
1	A	342	LEU	6
1	A	340	LYS	5
1	A	351	TYR	5
1	B	331	LYS	5
1	B	335	ASN	4
1	B	329	TYR	4
1	A	353	LEU	4
1	A	288	LEU	4
1	A	311	PHE	4
1	B	290	ILE	4
1	B	300	GLN	4
1	B	351	TYR	4
1	B	340	LYS	4
1	A	335	ASN	4
1	B	318	GLN	3
1	A	341	ILE	3
1	A	327	LYS	3
1	A	310	GLN	3
1	B	301	LYS	3
1	B	302	LEU	3
1	A	343	HIS	3
1	A	294	LYS	3
1	B	294	LYS	3
1	B	358	MET	3
1	B	345	ARG	3
1	B	312	PHE	2
1	A	300	GLN	2
1	B	278	TYR	2
1	A	358	MET	2
1	A	356	CYS	2
1	B	360	ASN	2
1	A	278	TYR	2
1	A	297	GLU	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	353	LEU	2
1	B	341	ILE	2
1	B	308	ARG	2
1	B	348	ILE	2
1	A	330	LEU	2
1	B	327	LYS	2
1	A	308	ARG	2
1	B	287	GLU	2
1	A	287	GLU	2
1	A	345	ARG	2
1	B	310	GLN	2
1	A	299	CYS	1
1	B	314	TYR	1
1	A	277	PHE	1
1	A	302	LEU	1
1	B	288	LEU	1
1	B	321	CYS	1
1	A	281	THR	1
1	A	290	ILE	1
1	B	361	GLU	1
1	A	304	THR	1
1	A	348	ILE	1
1	B	337	SER	1
1	A	359	ASP	1
1	A	323	GLU	1
1	A	309	CYS	1
1	A	334	SER	1
1	B	357	LYS	1
1	B	352	THR	1
1	A	333	SER	1
1	A	352	THR	1
1	B	283	PHE	1
1	B	342	LEU	1
1	B	284	LEU	1
1	A	361	GLU	1
1	B	323	GLU	1
1	A	321	CYS	1
1	B	309	CYS	1
1	B	313	THR	1
1	B	333	SER	1
1	A	301	LYS	1
1	A	354	ARG	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	280	ASP	1
1	A	284	LEU	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](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided