



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 01:12 PM UTC

PDB ID : 2J8L / pdb_00002j8l
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

<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

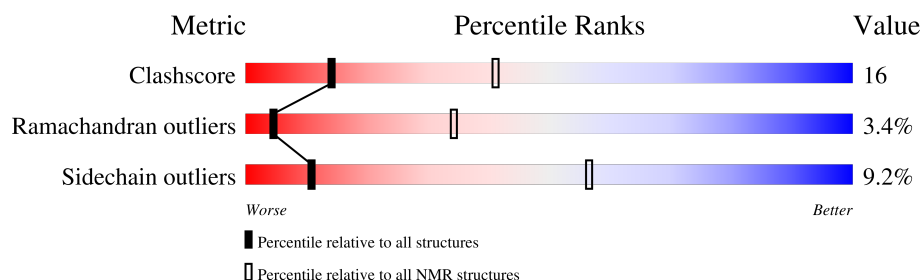
1 Overall quality at a glance

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	90	
1	B	90	

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)	1.95	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.

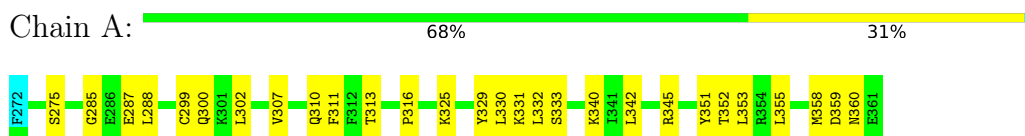
Mol	Chain	Residues	Atoms						Trace
1	A	90	Total	C	H	N	O	S	0
			1242	431	549	121	133	8	
1	B	90	Total	C	H	N	O	S	0
			1242	431	549	121	133	8	

4 Residue-property plots

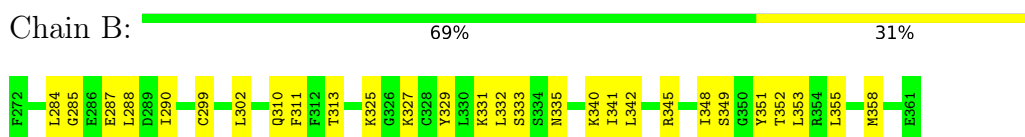
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: COAGULATION FACTOR XI



- Molecule 1: COAGULATION FACTOR XI

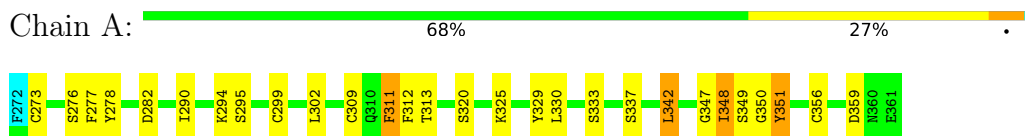


4.2 Scores per residue for each member of the ensemble

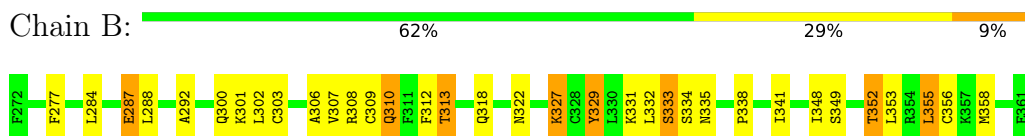
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: COAGULATION FACTOR XI

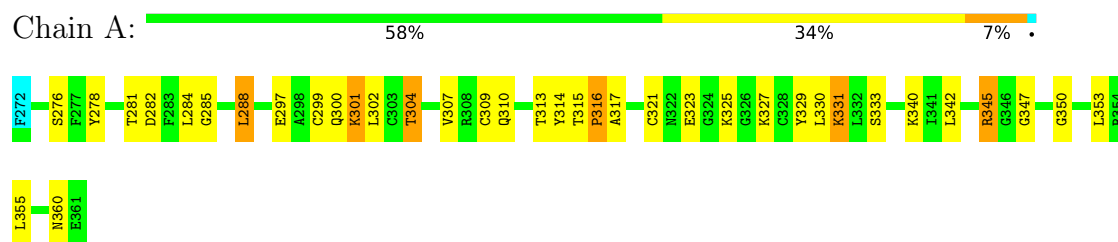


- Molecule 1: COAGULATION FACTOR XI

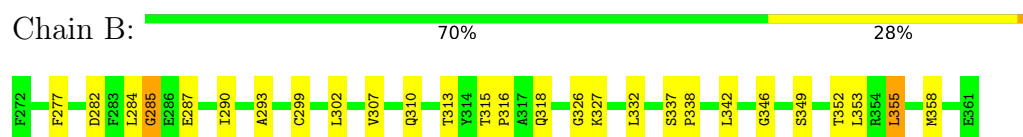


4.2.2 Score per residue for model 2

- Molecule 1: COAGULATION FACTOR XI

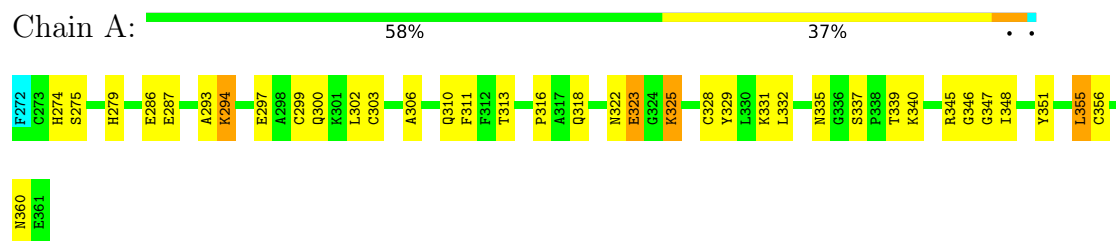


- Molecule 1: COAGULATION FACTOR XI

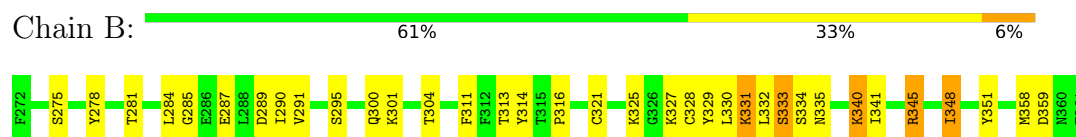


4.2.3 Score per residue for model 3

- Molecule 1: COAGULATION FACTOR XI

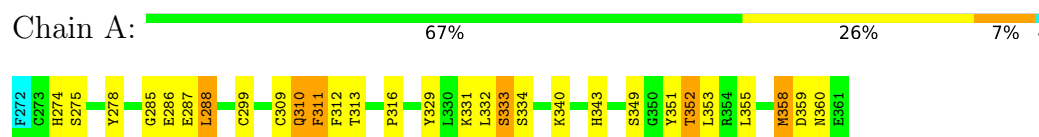


- Molecule 1: COAGULATION FACTOR XI

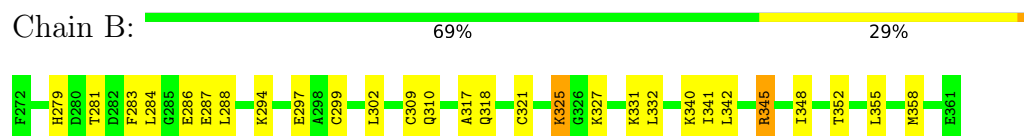


4.2.4 Score per residue for model 4

- Molecule 1: COAGULATION FACTOR XI

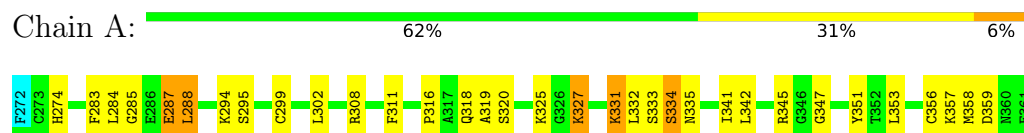


- Molecule 1: COAGULATION FACTOR XI

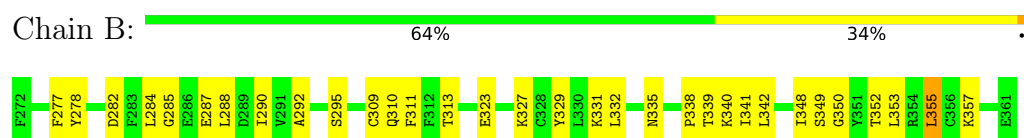


4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: COAGULATION FACTOR XI

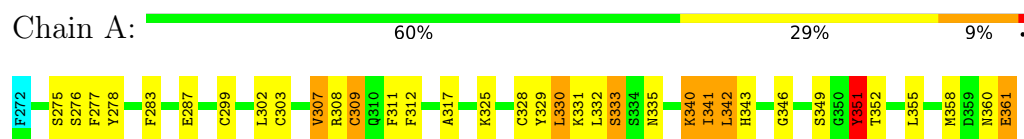


- Molecule 1: COAGULATION FACTOR XI

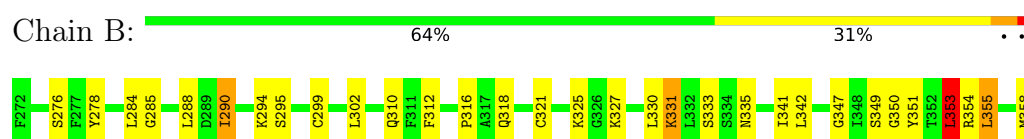


4.2.6 Score per residue for model 6

- Molecule 1: COAGULATION FACTOR XI

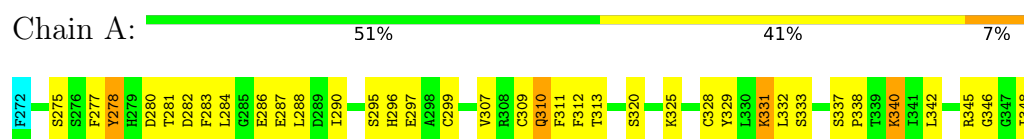


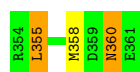
- Molecule 1: COAGULATION FACTOR XI



4.2.7 Score per residue for model 7

- Molecule 1: COAGULATION FACTOR XI





• Molecule 1: COAGULATION FACTOR XI

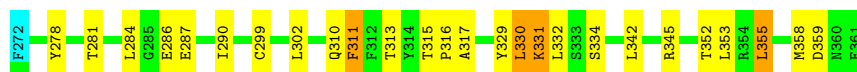
Chain B: 64% 31% .



4.2.8 Score per residue for model 8

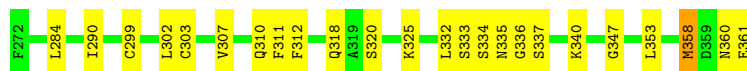
• Molecule 1: COAGULATION FACTOR XI

Chain A: 70% 24% . .



• Molecule 1: COAGULATION FACTOR XI

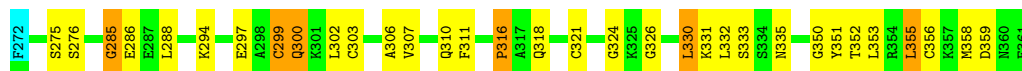
Chain B: 73% 26% .



4.2.9 Score per residue for model 9

• Molecule 1: COAGULATION FACTOR XI

Chain A: 62% 30% 7% .



• Molecule 1: COAGULATION FACTOR XI

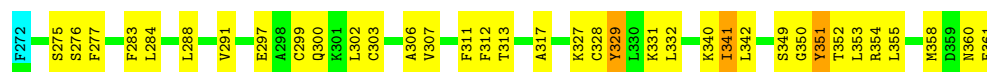
Chain B: 61% 31% 8%



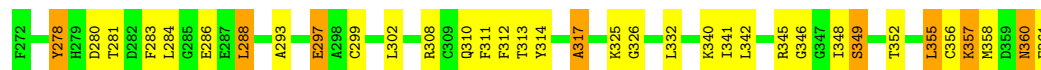
4.2.10 Score per residue for model 10

• Molecule 1: COAGULATION FACTOR XI

Chain A: 59% 37% . .



• Molecule 1: COAGULATION FACTOR XI

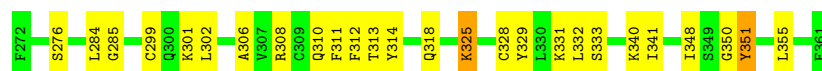


4.2.11 Score per residue for model 11

• Molecule 1: COAGULATION FACTOR XI

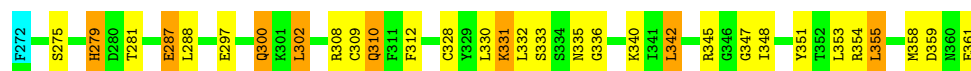


• Molecule 1: COAGULATION FACTOR XI



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

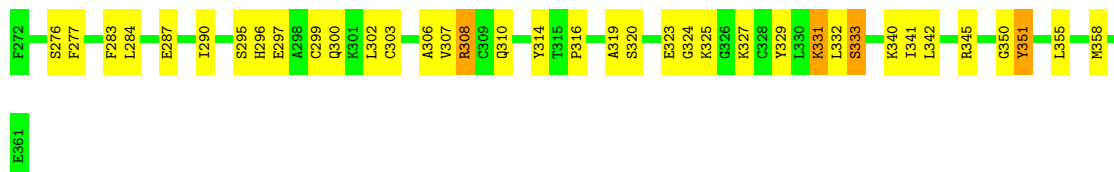
• Molecule 1: COAGULATION FACTOR XI





• Molecule 1: COAGULATION FACTOR XI

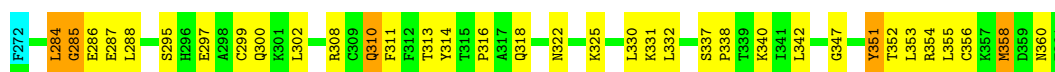
Chain B: 59% 37% .



4.2.14 Score per residue for model 14

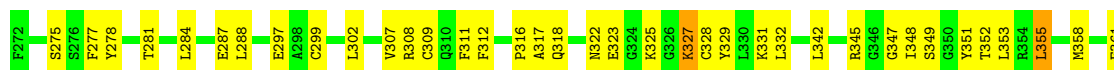
• Molecule 1: COAGULATION FACTOR XI

Chain A: 60% 33% 6% .



• Molecule 1: COAGULATION FACTOR XI

Chain B: 59% 39% .



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.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.41±0.02	0±0/695 (0.0± 0.0%)	0.70±0.04	0±0/933 (0.0± 0.0%)
1	B	0.41±0.02	0±0/707 (0.0± 0.0%)	0.69±0.03	0±0/949 (0.0± 0.0%)
All	All	0.41	0/19628 (0.0%)	0.69	1/26348 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	351	TYR	N-CA-C	6.13	119.19	108.52	6	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	682	538	650	22±4
1	B	693	549	658	22±5
All	All	19250	15218	18312	587

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 16.

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
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:A:313:THR:HB	1:A:329:TYR:HB2	0.79	1.52	3	3
1:B:355:LEU:H	1:B:355:LEU:HD13	0.79	1.37	7	5
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:301:LYS:HA	1:B:304:THR:HG22	0.75	1.59	3	1
1:B:284:LEU:HB2	1:B:288:LEU:HD11	0.75	1.57	9	1
1:A:355:LEU:H	1:A:355:LEU:HD13	0.75	1.42	7	3
1:B:291:VAL:HA	1:B:328:CYS:O	0.74	1.83	3	1
1:B:290:ILE:HG12	1:B:291:VAL:H	0.73	1.43	3	1
1:B:325:LYS:HA	1:B:325:LYS:HE3	0.73	1.60	4	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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
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:358:MET:HE3	1:A:358:MET:HA	0.64	1.69	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:279:HIS:HB3	1:B:348:ILE:HG12	0.61	1.71	4	1
1:B:316:PRO:HD3	1:B:347:GLY:HA3	0.61	1.71	14	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:355:LEU:HD13	1:B:356:CYS:N	0.60	2.11	10	1
1:B:327:LYS:HD2	1:B:329:TYR:CE1	0.60	2.32	12	1
1:B:332:LEU:HG	1:B:333:SER:N	0.59	2.12	13	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:297:GLU:O	1:B:300:GLN:HG3	0.59	1.98	9	2
1:B:313:THR:OG1	1:B:331:LYS:HE2	0.59	1.97	11	1
1:B:358:MET:HE3	1:B:358:MET:HA	0.59	1.73	8	1
1:A:352:THR:O	1:A:355:LEU:HD12	0.59	1.96	9	1
1:B:290:ILE:HG12	1:B:291:VAL:N	0.59	2.11	3	1
1:A:330:LEU:H	1:A:330:LEU:HD13	0.59	1.58	9	1
1:A:311:PHE:HA	1:A:351:TYR:CB	0.58	2.22	1	1
1:B:352:THR:O	1:B:355:LEU:HD12	0.58	1.97	10	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:279:HIS:HE1	1:A:313:THR:HG23	0.58	1.57	3	1
1:A:284:LEU:HB3	1:A:340:LYS:HB2	0.58	1.74	14	1
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:B:329:TYR:HB3	1:B:331:LYS:HE3	0.58	1.73	3	1
1:A:288:LEU:HB2	1:A:330:LEU:O	0.58	1.98	14	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: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:284:LEU:HG	1:B:288:LEU:HD13	0.57	1.75	12	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:286:GLU:HA	1:B:340:LYS:HE2	0.56	1.75	4	1
1:A:288:LEU:HD12	1:A:331:LYS:HE2	0.56	1.78	11	1
1:B:332:LEU:HD21	1:B:358:MET:HE1	0.56	1.76	3	1
1:B:357:LYS:HA	1:B:357:LYS:HE2	0.56	1.78	10	1
1:A:287:GLU:O	1:A:331:LYS:HA	0.56	2.00	6	4
1:A:276:SER:HB2	1:A:278:TYR:CE2	0.56	2.36	6	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:352:THR:HG22	1:A:355:LEU:HD23	0.56	1.78	14	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:B:355:LEU:HD12	1:B:356:CYS:N	0.55	2.17	1	1
1:A:299:CYS:HB3	1:A:312:PHE:CE2	0.55	2.35	7	1
1:A:352:THR:HB	1:A:355:LEU:CD1	0.55	2.32	4	1
1:A:332:LEU:HD11	1:A:358:MET:SD	0.55	2.41	10	1
1:A:340:LYS:HE2	1:B:286:GLU:HG3	0.55	1.78	12	1
1:B:279:HIS:CD2	1:B:348:ILE:HG12	0.55	2.37	9	1
1:B:283:PHE:CD2	1:B:341:ILE:HG22	0.55	2.37	10	1
1:A:284:LEU:HD21	1:B:284:LEU:HD21	0.55	1.77	14	1
1:B:280:ASP:O	1:B:344:GLY:HA2	0.55	2.02	9	1
1:A:332:LEU:HD11	1:A:358:MET:HG2	0.55	1.79	12	1
1:A:290:ILE:HD11	1:B:345:ARG:HB2	0.55	1.79	13	1
1:A:345:ARG:NE	1:A:345:ARG:HA	0.55	2.17	8	2
1:B:355:LEU:O	1:B:358:MET:HG2	0.54	2.02	7	2
1:B:310:GLN:HA	1:B:310:GLN:OE1	0.54	2.02	2	1
1:A:276:SER:O	1:A:351:TYR:HA	0.54	2.02	6	1
1:A:309:CYS:HB3	1:A:330:LEU:HD23	0.54	1.79	12	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:334:SER:HB2	1:A:358:MET:HE2	0.53	1.80	8	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:325:LYS:HA	1:B:325:LYS:CE	0.53	2.27	4	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:306:ALA:HB1	1:B:308:ARG:HH11	0.53	1.63	11	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:A:288:LEU:HB2	1:B:342:LEU:HD23	0.52	1.81	5	1
1:B:287:GLU:C	1:B:288:LEU:HD12	0.52	2.29	5	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:291:VAL:CA	1:B:328:CYS:O	0.52	2.56	3	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:A:345:ARG:HA	1:A:345:ARG:HE	0.52	1.65	13	2
1:B:291:VAL:HA	1:B:328:CYS:H	0.52	1.63	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: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: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
1:A:302:LEU:HD13	1:A:330:LEU:HG	0.51	1.82	11	1
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:288:LEU:HB2	1:B:342:LEU:HD21	0.51	1.81	4	1
1:A:287:GLU:HG3	1:A:331:LYS:HB2	0.51	1.81	14	1
1:A:279:HIS:NE2	1:A:346:GLY:HA3	0.51	2.20	3	1
1:A:355:LEU:HD13	1:A:356:CYS:H	0.51	1.65	9	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:311:PHE:CZ	1:A:331:LYS:HG3	0.50	2.41	5	1
1:A:310:GLN:HA	1:A:355:LEU:CB	0.50	2.34	9	1
1:A:329:TYR:OH	1:A:331:LYS:HD2	0.50	2.05	11	1
1:A:329:TYR:CE2	1:A:331:LYS:HE3	0.50	2.41	6	1
1:B:345:ARG:NE	1:B:345:ARG:HA	0.50	2.21	10	2
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:B:315:THR:O	1:B:327:LYS:HB2	0.50	2.07	2	1
1:A:311:PHE:HA	1:A:351:TYR:CD1	0.50	2.42	14	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:A:282:ASP:HB3	1:A:342:LEU:HD22	0.49	1.83	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:278:TYR:CD2	1:B:281:THR:HB	0.49	2.43	14	2
1:B:345:ARG:HA	1:B:345:ARG:HE	0.49	1.66	4	2
1:B:297:GLU:CD	1:B:297:GLU:H	0.49	2.15	10	1
1:B:309:CYS:H	1:B:355:LEU:HD12	0.49	1.66	14	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:277:PHE:CD1	1:B:350:GLY:HA3	0.49	2.42	5	1
1:B:313:THR:CG2	1:B:329:TYR:HB2	0.49	2.36	7	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:B:291:VAL:HA	1:B:328:CYS:N	0.49	2.22	3	1
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: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:312:PHE:CD1	1:A:328:CYS:HB2	0.49	2.42	10	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: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:A:302:LEU:HD13	1:A:330:LEU:HD12	0.49	1.85	1	1
1:B:311:PHE:O	1:B:331:LYS:HG2	0.49	2.07	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:310:GLN:HG2	1:A:311:PHE:CE2	0.48	2.43	7	1
1:A:333:SER:HB2	1:A:337:SER:HB3	0.48	1.84	1	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:A:353:LEU:HG	1:A:354:ARG:N	0.48	2.23	14	1
1:B:334:SER:CB	1:B:359:ASP:HA	0.48	2.15	3	1
1:B:313:THR:HG22	1:B:329:TYR:HB2	0.48	1.84	7	1
1:B:323:GLU:HG3	1:B:324:GLY:N	0.48	2.23	7	1
1:B:284:LEU:HG	1:B:342:LEU:HD11	0.48	1.84	9	1
1:A:286:GLU:HG3	1:B:340:LYS:HE2	0.48	1.85	7	1
1:B:312:PHE:CE1	1:B:328:CYS:HB3	0.48	2.43	11	1
1:A:332:LEU:HD11	1:A:358:MET:HG3	0.48	1.85	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:310:GLN:NE2	1:B:358:MET:HE3	0.48	2.24	4	1
1:A:318:GLN:HB2	1:A:322:ASN:O	0.48	2.08	14	1
1:A:345:ARG:HD3	1:A:345:ARG:H	0.48	1.68	3	1
1:A:287:GLU:HG3	1:B:340:LYS:HD3	0.48	1.85	5	1
1:A:315:THR:HG23	1:A:327:LYS:CG	0.48	2.39	2	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:342:LEU:N	1:A:342:LEU:HD13	0.48	2.24	12	3
1:A:299:CYS:HB3	1:A:312:PHE:CZ	0.48	2.37	4	1
1:B:355:LEU:HD13	1:B:355:LEU:N	0.48	2.19	9	1
1:B:312:PHE:CZ	1:B:328:CYS:HB2	0.48	2.43	14	1
1:A:299:CYS:O	1:A:302:LEU:HD22	0.47	2.09	2	2
1:A:334:SER:HA	1:A:359:ASP:HA	0.47	1.85	5	1
1:B:293:ALA:HB1	1:B:314:TYR:CE1	0.47	2.42	10	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:A:283:PHE:O	1:A:331:LYS:HE3	0.47	2.08	7	1
1:A:330:LEU:H	1:A:330:LEU:CD1	0.47	2.22	9	1
1:B:284:LEU:HB3	1:B:340:LYS:HG3	0.47	1.86	11	1
1:B:310:GLN:HA	1:B:355:LEU:HB3	0.47	1.85	13	1
1:B:292:ALA:CB	1:B:327:LYS:HA	0.47	2.39	5	1
1:A:276:SER:C	1:A:351:TYR:HA	0.47	2.35	6	1
1:B:332:LEU:HG	1:B:333:SER:O	0.47	2.09	8	1
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:A:313:THR:HB	1:A:329:TYR:CE1	0.47	2.44	7	2
1:B:332:LEU:HD12	1:B:358:MET:HE1	0.47	1.86	14	2
1:B:313:THR:CB	1:B:349:SER:HA	0.47	2.39	1	1
1:A:303:CYS:HA	1:A:306:ALA:O	0.47	2.10	3	2
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:284:LEU:HA	1:A:331:LYS:CE	0.47	2.38	7	1
1:B:335:ASN:ND2	1:B:360:ASN:HA	0.47	2.25	9	1
1:A:277:PHE:CD1	1:A:350:GLY:HA3	0.47	2.45	10	1
1:B:360:ASN:HD22	1:B:360:ASN:C	0.47	2.18	10	1
1:B:312:PHE:HB2	1:B:351:TYR:CE2	0.47	2.44	11	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:354:ARG:N	1:A:354:ARG:HD2	0.47	2.25	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:286:GLU:O	1:A:332:LEU:HB3	0.47	2.09	14	1
1:A:335:ASN:C	1:A:335:ASN:HD22	0.47	2.18	3	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:332:LEU:HG	1:A:358:MET:HE1	0.46	1.87	5	2
1:B:342:LEU:HD12	1:B:342:LEU:N	0.46	2.26	2	1
1:B:334:SER:OG	1:B:358:MET:HE2	0.46	2.11	3	1
1:A:331:LYS:N	1:A:331:LYS:HD3	0.46	2.26	8	1
1:A:336:GLY:H	1:A:361:GLU:C	0.46	2.18	12	1
1:B:333:SER:O	1:B:335:ASN:N	0.46	2.48	1	1
1:A:333:SER:HB2	1:A:359:ASP:HB3	0.46	1.85	12	1
1:B:309:CYS:O	1:B:355:LEU:HB2	0.46	2.09	4	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: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:A:279:HIS:C	1:A:281:THR:N	0.46	2.74	12	1
1:A:333:SER:HA	1:A:359:ASP:OD1	0.46	2.11	1	1
1:A:340:LYS:HG3	1:B:286:GLU:O	0.46	2.11	10	1
1:B:299:CYS:O	1:B:302:LEU:HD22	0.46	2.11	11	1
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:311:PHE:CE1	1:A:331:LYS:HG2	0.46	2.46	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:360:ASN:C	1:A:360:ASN:HD22	0.46	2.18	7	1
1:A:352:THR:O	1:A:353:LEU:HB2	0.46	2.11	8	1
1:A:283:PHE:HB2	1:A:311:PHE:CZ	0.45	2.45	5	1
1:A:284:LEU:HG	1:B:284:LEU:HD13	0.45	1.88	8	1
1:A:274:HIS:HD2	1:A:351:TYR:HB3	0.45	1.71	4	1
1:A:277:PHE:HA	1:A:349:SER:O	0.45	2.10	1	1
1:B:352:THR:C	1:B:353:LEU:HD22	0.45	2.36	1	2
1:A:351:TYR:CD2	1:A:351:TYR:N	0.45	2.83	6	1
1:B:299:CYS:HB3	1:B:312:PHE:CZ	0.45	2.46	14	1
1:B:311:PHE:HD2	1:B:331:LYS:HE3	0.45	1.71	5	1
1:A:294:LYS:HG2	1:A:324:GLY:O	0.45	2.12	9	1
1:A:287:GLU:HG3	1:B:340:LYS:CD	0.45	2.41	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:283:PHE:O	1:A:331:LYS:HD2	0.45	2.11	6	2
1:B:353:LEU:HD12	1:B:354:ARG:N	0.45	2.26	6	1
1:A:355:LEU:H	1:A:355:LEU:CD1	0.45	2.23	13	2
1:A:309:CYS:SG	1:A:355:LEU:HD22	0.45	2.52	2	1
1:A:296:HIS:HA	1:A:328:CYS:SG	0.45	2.51	7	1
1:A:354:ARG:HD2	1:A:354:ARG:H	0.45	1.71	11	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: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:330:LEU:HD13	1:A:330:LEU:N	0.45	2.27	8	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:314:TYR:O	1:A:347:GLY:HA3	0.45	2.12	2	1
1:A:280:ASP:HA	1:A:346:GLY:O	0.45	2.12	7	1
1:B:353:LEU:H	1:B:353:LEU:HD23	0.45	1.71	8	1
1:B:291:VAL:CA	1:B:328:CYS:N	0.45	2.79	3	1
1:A:327:LYS:HE3	1:A:327:LYS:HA	0.45	1.88	5	1
1:B:284:LEU:O	1:B:339:THR:HA	0.45	2.11	5	1
1:B:290:ILE:HD11	1:B:327:LYS:HE3	0.45	1.87	6	1
1:A:297:GLU:O	1:A:300:GLN:HB3	0.45	2.11	10	1
1:B:284:LEU:CB	1:B:288:LEU:HD21	0.44	2.43	4	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:B:316:PRO:HD3	1:B:347:GLY:CA	0.44	2.41	6	1
1:A:327:LYS:C	1:A:327:LYS:HD2	0.44	2.38	10	1
1:B:313:THR:HG22	1:B:349:SER:HB3	0.44	1.89	10	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: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:B:312:PHE:O	1:B:349:SER:HA	0.44	2.13	6	1
1:A:291:VAL:HB	1:A:328:CYS:SG	0.44	2.53	10	1
1:B:291:VAL:HG12	1:B:328:CYS:C	0.44	2.37	3	1
1:A:278:TYR:HD1	1:A:281:THR:HB	0.44	1.73	8	1
1:A:284:LEU:HD11	1:B:340:LYS:HD2	0.44	1.89	10	1
1:B:317:ALA:HB3	1:B:326:GLY:CA	0.44	2.43	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:287:GLU:HA	1:B:340:LYS:HG2	0.43	1.89	7	1
1:B:301:LYS:HD3	1:B:301:LYS:C	0.43	2.38	9	1
1:A:341:ILE:H	1:A:341:ILE:HD13	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: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:A:342:LEU:HD21	1:B:288:LEU:HB3	0.43	1.89	7	1
1:B:318:GLN:HB3	1:B:325:LYS:HD3	0.43	1.91	8	1
1:B:324:GLY:O	1:B:325:LYS:HG3	0.43	2.13	12	1
1:B:303:CYS:HA	1:B:307:VAL:CB	0.43	2.27	13	1
1:B:308:ARG:HG2	1:B:358:MET:SD	0.43	2.53	14	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:289:ASP:HB3	1:B:330:LEU:HB3	0.43	1.90	3	1
1:A:335:ASN:C	1:A:361:GLU:HA	0.43	2.39	6	1
1:B:311:PHE:CD2	1:B:331:LYS:HG3	0.43	2.49	12	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
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:A:282:ASP:OD2	1:A:331:LYS:NZ	0.42	2.50	2	1
1:A:335:ASN:HB3	1:A:358:MET:O	0.42	2.14	6	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:294:LYS:HA	1:A:326:GLY:HA3	0.42	1.90	9	1
1:B:291:VAL:HA	1:B:328:CYS:C	0.42	2.39	3	1
1:A:360:ASN:C	1:A:361:GLU:HG3	0.42	2.38	6	1
1:A:285:GLY:HA3	1:A:333:SER:OG	0.42	2.15	2	2
1:A:342:LEU:HB3	1:A:345:ARG:HB2	0.42	1.91	7	1
1:A:342:LEU:N	1:A:342:LEU:HD23	0.42	2.28	13	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:B:285:GLY:HA2	1:B:338:PRO:HA	0.42	1.91	2	1
1:A:345:ARG:H	1:A:345:ARG:CD	0.42	2.28	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:313:THR:HB	1:A:329:TYR:CG	0.42	2.49	11	1
1:A:294:LYS:HG3	1:A:325:LYS:HG3	0.42	1.91	3	1
1:A:313:THR:HG22	1:A:349:SER:CB	0.42	2.42	10	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:288:LEU:HD21	1:B:284:LEU:HD23	0.42	1.92	2	1
1:A:310:GLN:CD	1:A:333:SER:H	0.42	2.22	2	1
1:A:315:THR:HB	1:A:316:PRO:CD	0.42	2.45	8	1
1:A:311:PHE:HB3	1:A:351:TYR:HB3	0.42	1.91	5	1
1:B:288:LEU:C	1:B:288:LEU:HD22	0.42	2.40	10	1
1:A:297:GLU:H	1:A:297:GLU:CD	0.42	2.23	12	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:A:278:TYR:CE2	1:A:349:SER:HB3	0.41	2.50	7	1
1:B:316:PRO:O	1:B:325:LYS:HA	0.41	2.15	3	1
1:B:294:LYS:HG2	1:B:325:LYS:HG3	0.41	1.92	7	1
1:B:335:ASN:CG	1:B:336:GLY:H	0.41	2.23	8	1
1:A:284:LEU:HB2	1:A:342:LEU:CD1	0.41	2.45	2	1
1:A:301:LYS:HA	1:A:304:THR:OG1	0.41	2.16	2	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: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:303:CYS:SG	1:A:330:LEU:HD11	0.41	2.55	6	1
1:B:284:LEU:O	1:B:340:LYS:HG2	0.41	2.15	3	1
1:A:294:LYS:NZ	1:A:294:LYS:HB2	0.41	2.30	5	1
1:B:288:LEU:HG	1:B:331:LYS:CB	0.41	2.43	6	1
1:A:332:LEU:HD21	1:A:358:MET:HE1	0.41	1.92	8	1
1:B:342:LEU:CD2	1:B:345:ARG:HB2	0.41	2.45	12	1
1:B:292:ALA:HB3	1:B:327:LYS:HG2	0.41	1.92	5	1
1:A:342:LEU:HD13	1:A:342:LEU:H	0.41	1.75	1	1
1:A:309:CYS:O	1:A:355:LEU:HG	0.41	2.15	7	2
1:A:352:THR:CG2	1:A:355:LEU:HD11	0.41	2.44	6	1
1:B:355:LEU:HD22	1:B:355:LEU:C	0.41	2.41	10	1
1:B:342:LEU:HD13	1:B:345:ARG:HH21	0.41	1.74	14	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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:298:ALA:O	1:B:301:LYS:HG3	0.41	2.15	9	1
1:B:357:LYS:O	1:B:361:GLU:HG2	0.41	2.16	10	1
1:A:310:GLN:O	1:A:355:LEU:HD13	0.41	2.15	12	1
1:B:308:ARG:HB3	1:B:355:LEU:HA	0.41	1.93	1	1
1:A:355:LEU:HD13	1:A:355:LEU:N	0.41	2.21	7	1
1:A:276:SER:N	1:A:351:TYR:HB2	0.41	2.31	6	1
1:B:284:LEU:C	1:B:284:LEU:HD12	0.41	2.41	6	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:316:PRO:HA	1:A:325:LYS:O	0.41	2.16	2	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:287:GLU:C	1:A:288:LEU:HD12	0.41	2.41	7	1
1:B:336:GLY:CA	1:B:361:GLU:HA	0.41	2.29	8	1
1:B:345:ARG:HA	1:B:345:ARG:CZ	0.41	2.46	9	1
1:B:310:GLN:CD	1:B:358:MET:HE3	0.41	2.40	10	1
1:A:355:LEU:HD22	1:A:355:LEU:C	0.41	2.41	11	1
1:A:356:CYS:HA	1:A:359:ASP:OD1	0.41	2.16	11	1
1:A:339:THR:C	1:A:340:LYS:HD2	0.40	2.41	3	1
1:A:311:PHE:HD2	1:A:331:LYS:HB2	0.40	1.76	4	1
1:B:327:LYS:N	1:B:327:LYS:HD2	0.40	2.30	4	1
1:A:330:LEU:C	1:A:330:LEU:HD23	0.40	2.41	1	1
1:A:286:GLU:HG2	1:A:335:ASN:ND2	0.40	2.32	9	1
1:A:316:PRO:C	1:A:318:GLN:H	0.40	2.24	9	1
1:A:359:ASP:C	1:A:360:ASN:HD22	0.40	2.25	13	1
1:B:300:GLN:HA	1:B:312:PHE:CE2	0.40	2.52	1	1
1:A:288:LEU:HD22	1:A:288:LEU:N	0.40	2.31	5	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: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:A:282:ASP:HB3	1:A:284:LEU:HD11	0.40	1.93	7	1
1:A:355:LEU:HD12	1:A:355:LEU:C	0.40	2.42	14	1
1:B:341:ILE:H	1:B:341:ILE:HD12	0.40	1.77	1	1
1:B:288:LEU:HD21	1:B:329:TYR:HD1	0.40	1.75	7	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%)	4	31
1	B	88/90 (98%)	72±2 (82±3%)	14±2 (15±3%)	3±2 (3±2%)	5	38
All	All	2464/2520 (98%)	1990 (81%)	390 (16%)	84 (3%)	4	34

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	295	SER	5
1	A	307	VAL	5
1	A	316	PRO	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	A	347	GLY	2
1	B	306	ALA	2
1	B	318	GLN	2
1	B	322	ASN	2
1	B	334	SER	2
1	B	338	PRO	2
1	A	321	CYS	2
1	A	353	LEU	2
1	A	274	HIS	2
1	B	333	SER	2
1	A	333	SER	2
1	B	353	LEU	2
1	A	285	GLY	2
1	A	273	CYS	1
1	B	309	CYS	1
1	B	352	THR	1
1	A	323	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	B	285	GLY	1
1	B	307	VAL	1
1	A	322	ASN	1
1	A	360	ASN	1
1	A	318	GLN	1
1	A	319	ALA	1
1	A	309	CYS	1
1	A	346	GLY	1
1	A	310	GLN	1
1	B	320	SER	1
1	B	347	GLY	1
1	A	306	ALA	1
1	A	275	SER	1
1	B	325	LYS	1
1	A	279	HIS	1
1	A	354	ARG	1
1	B	274	HIS	1
1	B	324	GLY	1
1	A	338	PRO	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	75/76 (99%)	68±2 (91±3%)	7±2 (9±3%)	11	57
1	B	76/76 (100%)	69±2 (91±3%)	7±2 (9±3%)	11	56
All	All	2114/2128 (99%)	1920 (91%)	194 (9%)	11	56

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	9
1	A	355	LEU	7
1	A	331	LYS	6
1	B	325	LYS	6
1	A	342	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	B	331	LYS	5
1	A	311	PHE	4
1	A	351	TYR	4
1	A	288	LEU	4
1	A	360	ASN	4
1	A	325	LYS	4
1	B	335	ASN	4
1	B	341	ILE	4
1	B	345	ARG	4
1	A	340	LYS	4
1	A	353	LEU	4
1	B	297	GLU	4
1	B	290	ILE	4
1	B	301	LYS	3
1	B	302	LEU	3
1	B	329	TYR	3
1	B	340	LYS	3
1	A	310	GLN	3
1	A	330	LEU	3
1	A	341	ILE	3
1	B	318	GLN	3
1	B	360	ASN	3
1	B	311	PHE	3
1	A	356	CYS	2
1	B	287	GLU	2
1	B	327	LYS	2
1	A	278	TYR	2
1	B	353	LEU	2
1	B	300	GLN	2
1	B	348	ILE	2
1	A	333	SER	2
1	A	343	HIS	2
1	A	358	MET	2
1	B	294	LYS	2
1	A	287	GLU	2
1	A	308	ARG	2
1	B	357	LYS	2
1	B	321	CYS	2
1	B	358	MET	2
1	B	308	ARG	2
1	B	312	PHE	2
1	A	300	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	329	TYR	2
1	B	351	TYR	2
1	A	290	ILE	1
1	A	309	CYS	1
1	A	348	ILE	1
1	B	284	LEU	1
1	B	310	GLN	1
1	B	313	THR	1
1	B	333	SER	1
1	A	281	THR	1
1	A	301	LYS	1
1	A	304	THR	1
1	A	345	ARG	1
1	B	337	SER	1
1	B	352	THR	1
1	A	294	LYS	1
1	A	323	GLU	1
1	A	352	THR	1
1	A	327	LYS	1
1	A	334	SER	1
1	A	335	ASN	1
1	A	357	LYS	1
1	B	309	CYS	1
1	B	323	GLU	1
1	A	277	PHE	1
1	A	361	GLU	1
1	B	342	LEU	1
1	A	297	GLU	1
1	A	299	CYS	1
1	A	359	ASP	1
1	B	278	TYR	1
1	B	288	LEU	1
1	B	349	SER	1
1	A	354	ARG	1
1	A	302	LEU	1
1	B	283	PHE	1
1	A	284	LEU	1
1	B	361	GLU	1

6.3.3 RNA ⓘ

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 oligosaccharides 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