Full wwPDB NMR Structure Validation Report (i)

Feb 12, 2017 – 10:01 pm GMT

PDB ID : 2H25
Title : Solution Structure of Maltose Binding Protein complexed with beta-cyclodextrin
Authors : Xu, Y.; Lin, Z.; Zheng, Y.; Yang, D.
Deposited on : 2006-05-18

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 (i) symbol.

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

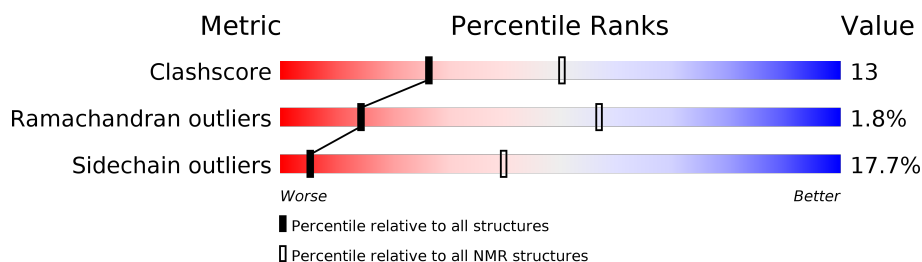|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (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 is 90%.

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	Percentile Ranks	Value
Clashscore		13
Ramachandran outliers		1.8%
Sidechain outliers		17.7%

Worse   *Better*

▌ Percentile relative to all structures

▯ Percentile relative to all NMR structures

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	370	65% 33% •

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:370 (369)	0.81	10

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

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

The models can be grouped into 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 4, 6, 7, 8, 10
2	5, 9
Single-model clusters	2; 3

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 5735 atoms, of which 2858 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	370	5735	1851	2858	469	551	6	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	THR	ILE	CONFLICT	UNP P0AEX9

4 Residue-property plots ⓘ

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Maltose-binding periplasmic protein
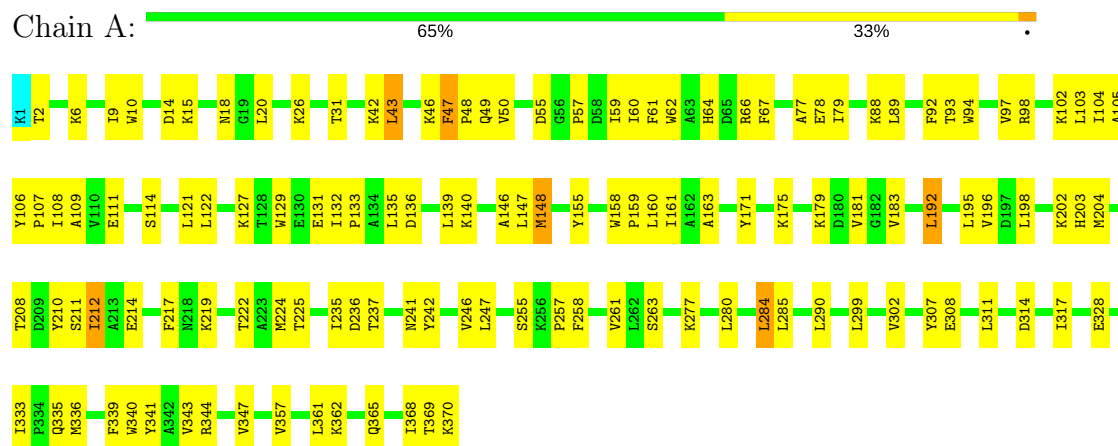
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Maltose-binding periplasmic protein
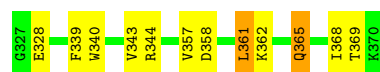
4.2.2 Score per residue for model 2

• Molecule 1: Maltose-binding periplasmic protein

4.2.3 Score per residue for model 3

• Molecule 1: Maltose-binding periplasmic protein

4.2.4 Score per residue for model 4

• Molecule 1: Maltose-binding periplasmic protein
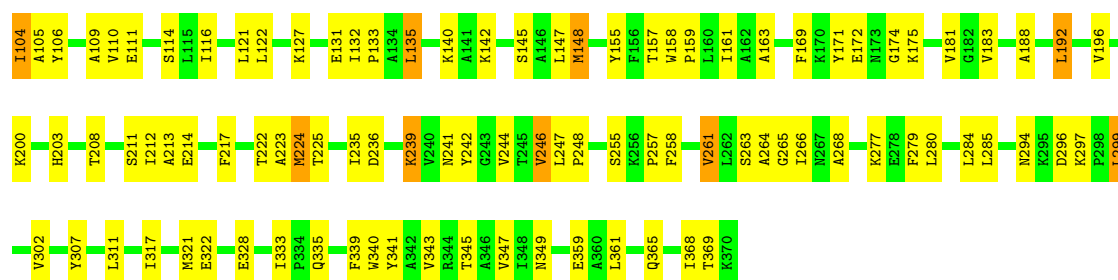
4.2.5 Score per residue for model 5

• Molecule 1: Maltose-binding periplasmic protein

Chain A:
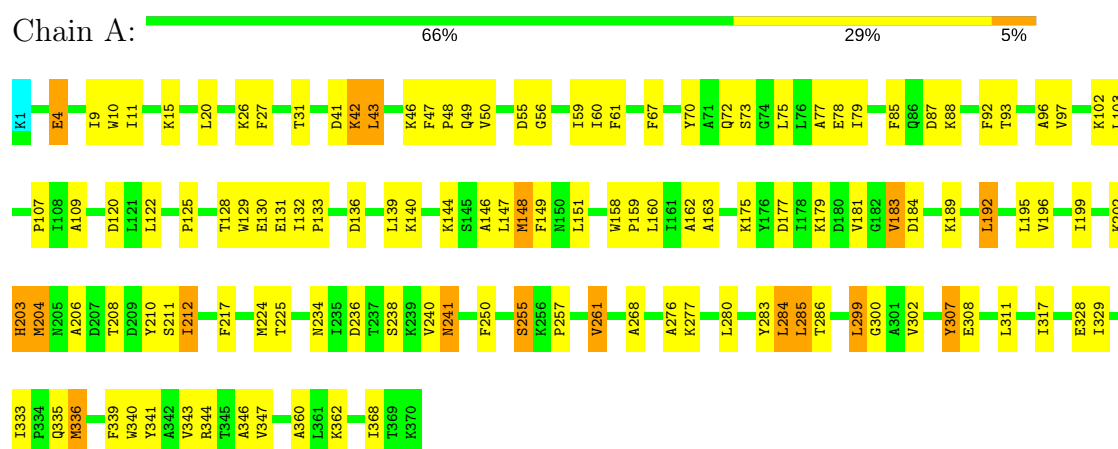
4.2.6 Score per residue for model 6

• Molecule 1: Maltose-binding periplasmic protein

Chain A:
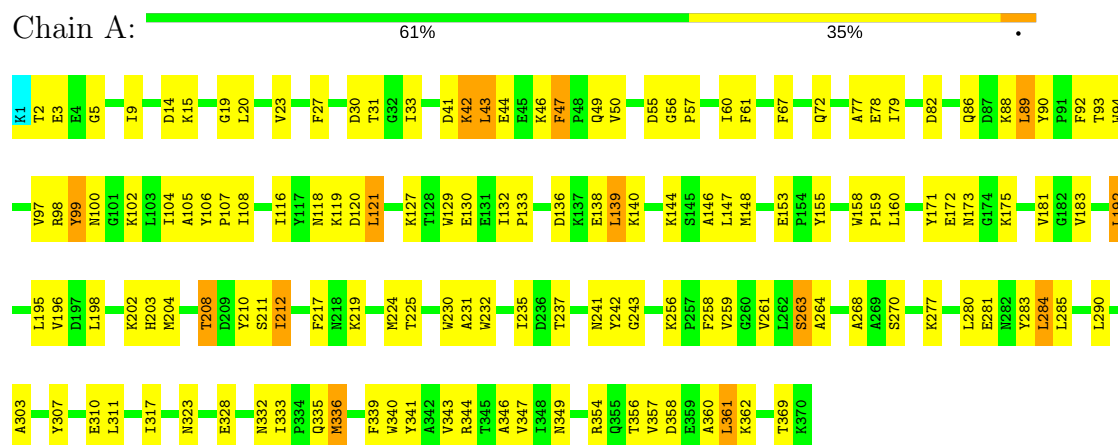
4.2.7 Score per residue for model 7

• Molecule 1: Maltose-binding periplasmic protein
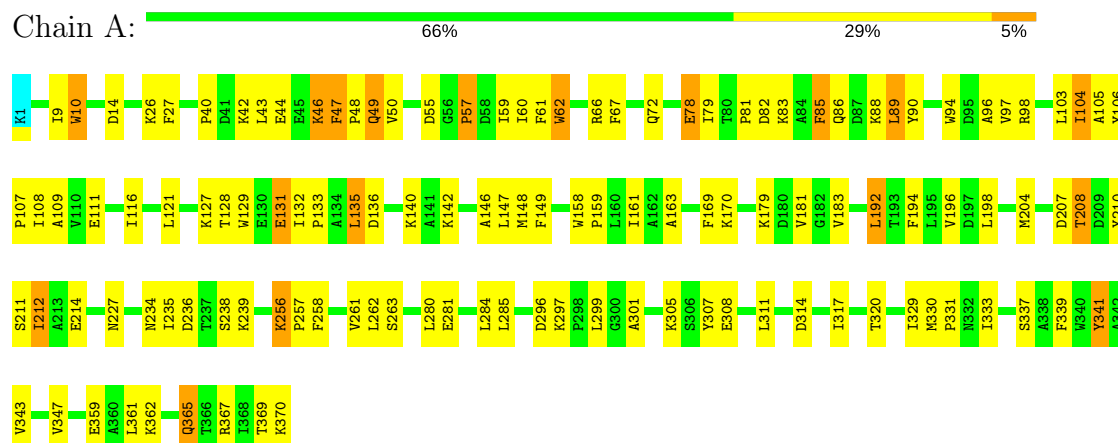
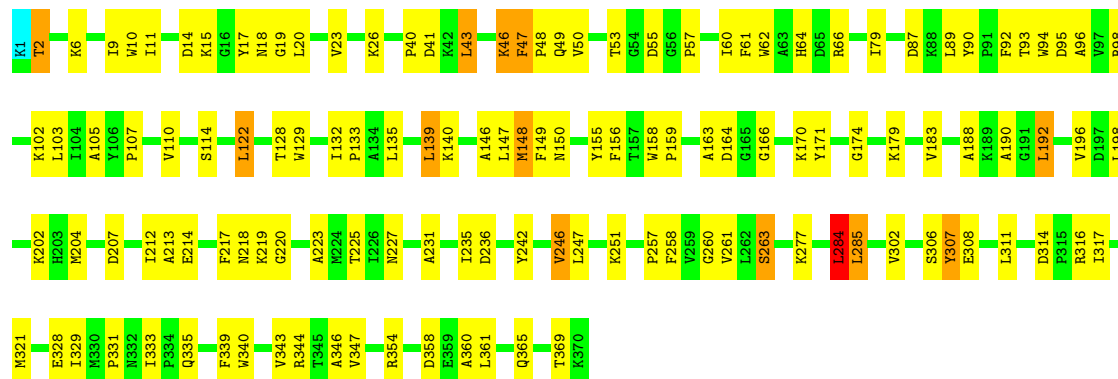### 4.2.8 Score per residue for model 8
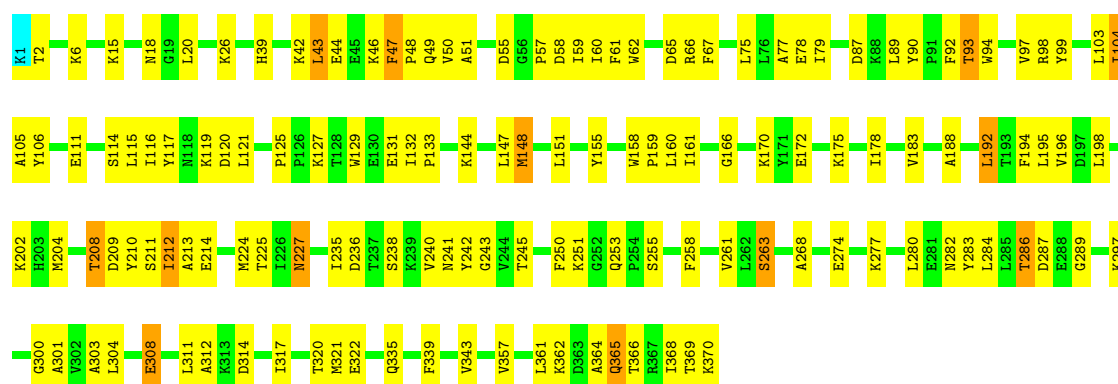
• Molecule 1: Maltose-binding periplasmic protein
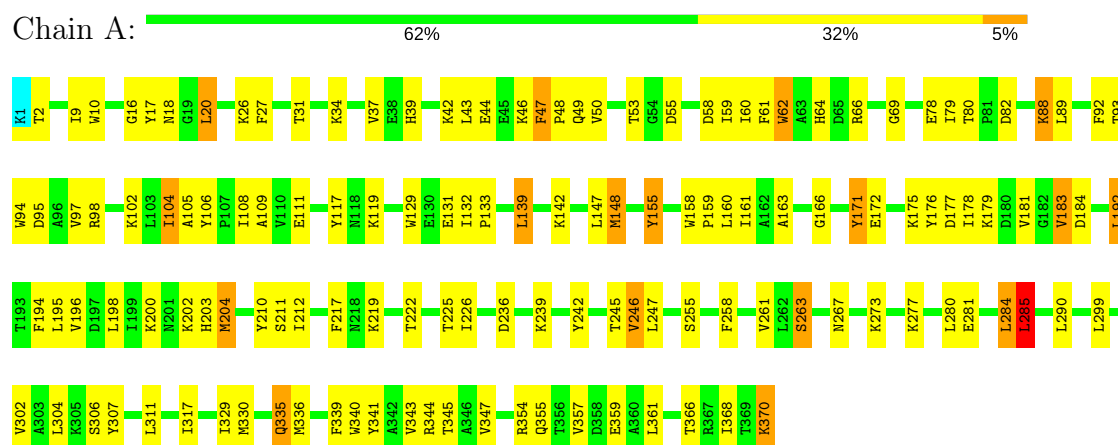
4.2.9 Score per residue for model 9

• Molecule 1: Maltose-binding periplasmic protein

M204 Y210 S211 I212 A213 E214 F217 N218 K219 T222 A223 M224 T225 W230 D236 T237 N241 L247 P248 Q253 F258 V261 L262 S263 I266 S270 P271 L275 L280 L284 L285 T286 L290 L299 V302 A303 L304 Y307 E310 L311

I317 T320 K326 P331 S337 A338 F339 W340 Y341 A342 V343 R344 T345 A346 V347 I348 N349 S352 E359 K362 D363 A364 Q365 I368 T369 K370
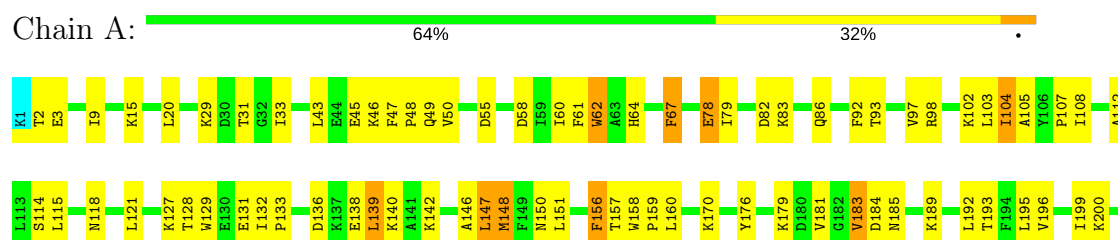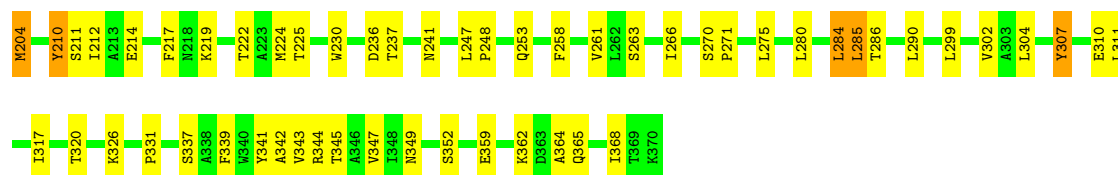
4.2.10 Score per residue for model 10 (medoid)

• Molecule 1: Maltose-binding periplasmic protein

Chain A:

66% 28% 5%

K1 T2 E3 K6 I9 W10 K15 G16 Y17 N18 G19 L20 A21 E22 K26 F27 E28 D41 K42 L43 K46 F47 P48 Q49 V50 P57 I60 F61 S73 E78 I79 T80 L89 F92 T93 W94 D95 A96 V97 K102 L103 I104 A105 Y106 P107 I108 A109

V110 E111 L121 K127 T128 W129 E130 E131 I132 P133 A134 L135 D136 L139 K140 A146 L147 M148 L151 Q152 E153 P154 Y155 F156 T157 W158 P159 L160 I161 A162 A163 D164 A168 V181 G182 V183 K189 L192 T193 F194 L195 V196 D197 L198 I199 K202 H203 M204 D207

T208 D209 Y210 S211 I212 A213 E214 E221 T222 A223 M224 T225 S233 N234 I235 D236 T237 Y242 V246 L247 S255 K256 P257 F258 V261 L262 S263 N272 K273 E274 L275 A276 K277 L284 L290 E291 V302 A303 L304 Y307 E308 L311 D314 I317 Q335

F339 V343 V347 S352 G353 R354 V357 L361 Q365 T369 K370

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing.*

Of the 40 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 7114
Number of chemical shift lists	1
Total number of shifts	4389
Number of shifts mapped to atoms	4389
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

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	2868	2843	2840	72±6
All	All	28680	28430	28400	721

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:280:LEU:HD22	1:A:284:LEU:HD22	0.84	1.48	3	2
1:A:51:ALA:HB1	1:A:75:LEU:HD22	0.83	1.49	4	2
1:A:183:VAL:HG12	1:A:361:LEU:CD2	0.83	2.03	1	2
1:A:280:LEU:HD23	1:A:284:LEU:HD22	0.81	1.53	1	5
1:A:161:ILE:HG21	1:A:192:LEU:HD12	0.81	1.50	4	1
1:A:169:PHE:CE2	1:A:333:ILE:HD11	0.80	2.11	4	2
1:A:92:PHE:CE1	1:A:93:THR:HG23	0.80	2.11	6	2
1:A:125:PRO:CB	1:A:245:THR:HG21	0.79	2.07	3	1
1:A:129:TRP:CE3	1:A:132:ILE:HD12	0.79	2.12	1	8
1:A:46:LYS:O	1:A:50:VAL:HG22	0.79	1.78	8	6
1:A:192:LEU:O	1:A:196:VAL:HG23	0.77	1.79	1	10
1:A:67:PHE:CD2	1:A:105:ALA:HB2	0.77	2.15	7	1
1:A:9:ILE:HG21	1:A:20:LEU:HD21	0.77	1.55	9	3
1:A:183:VAL:HG12	1:A:361:LEU:HD22	0.76	1.57	6	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:192:LEU:HD12	1:A:357:VAL:HG22	0.76	1.58	10	1
1:A:339:PHE:CE1	1:A:343:VAL:HG21	0.76	2.15	9	5
1:A:161:ILE:HD13	1:A:192:LEU:HD12	0.76	1.55	7	3
1:A:116:ILE:HD12	1:A:227:ASN:HB2	0.75	1.58	3	2
1:A:112:ALA:HB3	1:A:320:THR:HG23	0.75	1.59	9	1
1:A:135:LEU:HD23	1:A:139:LEU:HD12	0.75	1.58	1	1
1:A:343:VAL:O	1:A:347:VAL:HG23	0.75	1.81	6	7
1:A:9:ILE:HG21	1:A:20:LEU:CD2	0.74	2.12	4	5
1:A:183:VAL:HG12	1:A:361:LEU:HD23	0.74	1.57	1	1
1:A:209:ASP:OD2	1:A:212:ILE:HD11	0.74	1.81	3	2
1:A:183:VAL:O	1:A:361:LEU:HD13	0.73	1.82	6	1
1:A:339:PHE:O	1:A:343:VAL:HG23	0.73	1.83	6	7
1:A:181:VAL:CG1	1:A:183:VAL:HG23	0.73	2.13	7	2
1:A:157:THR:O	1:A:161:ILE:HD12	0.73	1.84	10	1
1:A:43:LEU:HD11	1:A:62:TRP:CZ3	0.73	2.19	3	1
1:A:227:ASN:ND2	1:A:231:ALA:HB2	0.72	1.98	2	1
1:A:147:LEU:HD12	1:A:224:MET:CB	0.72	2.14	10	1
1:A:365:GLN:O	1:A:369:THR:HG22	0.72	1.85	1	1
1:A:280:LEU:HD23	1:A:284:LEU:CD2	0.72	2.14	5	2
1:A:89:LEU:HD12	1:A:94:TRP:CZ2	0.72	2.20	10	4
1:A:235:ILE:HG21	1:A:242:TYR:CD1	0.72	2.20	2	4
1:A:59:ILE:HD13	1:A:280:LEU:HD21	0.72	1.62	3	2
1:A:106:TYR:OH	1:A:266:ILE:HD11	0.71	1.85	1	1
1:A:280:LEU:HD22	1:A:284:LEU:CD2	0.71	2.13	3	1
1:A:105:ALA:HB1	1:A:263:SER:HB2	0.70	1.63	6	5
1:A:64:HIS:CD2	1:A:96:ALA:HB1	0.70	2.21	2	1
1:A:97:VAL:HB	1:A:105:ALA:HB3	0.70	1.62	9	2
1:A:285:LEU:CD2	1:A:304:LEU:HD13	0.69	2.18	9	2
1:A:77:ALA:HB2	1:A:267:ASN:O	0.69	1.87	1	1
1:A:79:ILE:HD11	1:A:103:LEU:CB	0.69	2.18	7	5
1:A:181:VAL:HG12	1:A:183:VAL:HG23	0.68	1.64	7	3
1:A:339:PHE:CZ	1:A:343:VAL:HG21	0.68	2.23	10	6
1:A:115:LEU:HD11	1:A:147:LEU:HD11	0.68	1.66	3	1
1:A:116:ILE:HG22	1:A:217:PHE:CZ	0.68	2.24	4	1
1:A:232:TRP:HA	1:A:235:ILE:HD12	0.68	1.65	6	1
1:A:158:TRP:CE2	1:A:162:ALA:HB2	0.67	2.24	5	1
1:A:169:PHE:CD2	1:A:333:ILE:HD11	0.67	2.24	7	1
1:A:131:GLU:O	1:A:135:LEU:HD12	0.67	1.89	7	2
1:A:311:LEU:O	1:A:317:ILE:HD12	0.67	1.89	1	3
1:A:346:ALA:HB1	1:A:360:ALA:HB1	0.67	1.65	2	3
1:A:159:PRO:O	1:A:163:ALA:HB2	0.67	1.90	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:148:MET:HB2	1:A:208:THR:HG21	0.66	1.66	5	2
1:A:11:ILE:HD11	1:A:15:LYS:HD3	0.66	1.65	5	1
1:A:365:GLN:HA	1:A:368:ILE:HD12	0.66	1.68	9	1
1:A:94:TRP:CZ3	1:A:103:LEU:HD11	0.66	2.26	7	1
1:A:333:ILE:HD12	1:A:335:GLN:HB2	0.66	1.68	6	3
1:A:60:ILE:HD11	1:A:62:TRP:CE3	0.66	2.26	7	3
1:A:139:LEU:HD13	1:A:146:ALA:HA	0.66	1.68	5	5
1:A:106:TYR:CE1	1:A:266:ILE:HD12	0.65	2.26	4	1
1:A:259:VAL:HG23	1:A:328:GLU:O	0.65	1.90	6	1
1:A:217:PHE:CG	1:A:225:THR:HG21	0.65	2.27	8	3
1:A:304:LEU:HD23	1:A:307:TYR:HB2	0.64	1.69	9	2
1:A:77:ALA:HB2	1:A:268:ALA:HA	0.64	1.70	5	4
1:A:122:LEU:HD22	1:A:223:ALA:HB1	0.64	1.68	2	1
1:A:50:VAL:O	1:A:53:THR:HG22	0.63	1.93	2	1
1:A:285:LEU:HD23	1:A:304:LEU:HD13	0.63	1.69	8	1
1:A:311:LEU:HB3	1:A:317:ILE:HG21	0.63	1.71	10	10
1:A:122:LEU:CD2	1:A:223:ALA:HB1	0.63	2.24	2	1
1:A:19:GLY:O	1:A:23:VAL:HG23	0.63	1.94	6	2
1:A:339:PHE:CE2	1:A:368:ILE:HD13	0.62	2.29	5	1
1:A:280:LEU:CD2	1:A:284:LEU:HD22	0.62	2.24	3	5
1:A:105:ALA:HB1	1:A:263:SER:HB3	0.62	1.69	4	1
1:A:234:ASN:OD1	1:A:235:ILE:HG23	0.62	1.93	7	1
1:A:79:ILE:HD11	1:A:103:LEU:HB3	0.61	1.70	3	5
1:A:77:ALA:HB2	1:A:268:ALA:CA	0.61	2.26	5	2
1:A:109:ALA:HB2	1:A:299:LEU:HD12	0.61	1.71	5	1
1:A:108:ILE:HD13	1:A:284:LEU:O	0.61	1.95	8	1
1:A:47:PHE:CE2	1:A:60:ILE:HG21	0.61	2.31	5	1
1:A:213:ALA:HB1	1:A:225:THR:HG23	0.61	1.73	2	1
1:A:302:VAL:HG21	1:A:307:TYR:HB3	0.60	1.73	2	3
1:A:161:ILE:CD1	1:A:192:LEU:HD12	0.60	2.26	7	1
1:A:135:LEU:CD2	1:A:139:LEU:HD12	0.60	2.26	1	1
1:A:136:ASP:OD1	1:A:146:ALA:HB3	0.60	1.96	1	1
1:A:147:LEU:HD11	1:A:226:ILE:HG13	0.60	1.73	8	1
1:A:64:HIS:CD2	1:A:261:VAL:HG12	0.60	2.31	9	3
1:A:181:VAL:HG21	1:A:365:GLN:HA	0.60	1.73	10	2
1:A:104:ILE:O	1:A:104:ILE:HD12	0.60	1.95	4	2
1:A:147:LEU:HD12	1:A:224:MET:HB3	0.60	1.71	10	1
1:A:85:PHE:CZ	1:A:285:LEU:HD22	0.60	2.31	7	2
1:A:64:HIS:ND1	1:A:261:VAL:HG12	0.59	2.12	2	1
1:A:116:ILE:HD12	1:A:227:ASN:CB	0.59	2.27	3	1
1:A:139:LEU:HD22	1:A:223:ALA:HB2	0.59	1.73	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:164:ASP:OD2	1:A:190:ALA:HB3	0.59	1.98	2	1
1:A:198:LEU:HD13	1:A:204:MET:CE	0.59	2.28	8	1
1:A:183:VAL:CG1	1:A:361:LEU:HD22	0.59	2.26	6	4
1:A:160:LEU:CD2	1:A:195:LEU:HD13	0.59	2.27	6	2
1:A:148:MET:CG	1:A:213:ALA:HB2	0.58	2.28	2	1
1:A:110:VAL:HG13	1:A:260:GLY:O	0.58	1.98	2	1
1:A:132:ILE:HD13	1:A:147:LEU:HD22	0.58	1.75	2	4
1:A:300:GLY:O	1:A:311:LEU:HD13	0.58	1.99	5	2
1:A:104:ILE:HD12	1:A:104:ILE:O	0.58	1.98	8	2
1:A:2:THR:HG22	1:A:55:ASP:O	0.58	1.98	6	1
1:A:148:MET:SD	1:A:208:THR:HG23	0.58	2.39	3	1
1:A:115:LEU:HD11	1:A:147:LEU:CD1	0.57	2.30	3	2
1:A:151:LEU:CD2	1:A:195:LEU:HD21	0.57	2.29	9	1
1:A:129:TRP:CZ2	1:A:160:LEU:HD13	0.57	2.35	6	1
1:A:109:ALA:CB	1:A:299:LEU:HD22	0.57	2.30	8	2
1:A:97:VAL:CG1	1:A:105:ALA:HB3	0.57	2.30	8	3
1:A:92:PHE:CD1	1:A:93:THR:HG23	0.57	2.35	6	1
1:A:160:LEU:HD11	1:A:194:PHE:CD2	0.56	2.34	10	2
1:A:192:LEU:HD23	1:A:196:VAL:CG2	0.56	2.30	4	1
1:A:109:ALA:HB2	1:A:299:LEU:CD1	0.56	2.30	5	1
1:A:9:ILE:N	1:A:9:ILE:HD12	0.56	2.14	7	1
1:A:108:ILE:HD12	1:A:284:LEU:HD23	0.56	1.77	10	1
1:A:311:LEU:CB	1:A:317:ILE:HG21	0.56	2.30	6	2
1:A:129:TRP:CH2	1:A:160:LEU:HD13	0.56	2.36	3	1
1:A:339:PHE:CE2	1:A:343:VAL:HG21	0.56	2.36	1	4
1:A:307:TYR:CE2	1:A:311:LEU:HD11	0.56	2.36	7	3
1:A:154:PRO:CB	1:A:343:VAL:HG12	0.55	2.31	1	1
1:A:195:LEU:HA	1:A:198:LEU:HD12	0.55	1.78	8	1
1:A:23:VAL:HG12	1:A:279:PHE:CZ	0.55	2.35	4	1
1:A:196:VAL:HG12	1:A:200:LYS:HD2	0.55	1.76	4	2
1:A:108:ILE:CG2	1:A:290:LEU:HD21	0.55	2.31	9	1
1:A:9:ILE:HD12	1:A:37:VAL:HG22	0.55	1.78	8	1
1:A:108:ILE:HD12	1:A:262:LEU:O	0.55	2.02	7	1
1:A:168:ALA:HB2	1:A:339:PHE:CZ	0.55	2.36	1	1
1:A:365:GLN:O	1:A:369:THR:HG23	0.55	2.02	3	5
1:A:105:ALA:HB1	1:A:263:SER:CB	0.55	2.32	3	4
1:A:181:VAL:HG11	1:A:368:ILE:HD12	0.55	1.79	4	1
1:A:92:PHE:CE1	1:A:93:THR:HG22	0.55	2.37	5	4
1:A:181:VAL:HG11	1:A:368:ILE:HD13	0.54	1.79	1	1
1:A:160:LEU:HD23	1:A:195:LEU:HD13	0.54	1.79	9	1
1:A:147:LEU:HD12	1:A:224:MET:HB2	0.53	1.79	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:178:ILE:HG21	1:A:335:GLN:OE1	0.53	2.03	8	1
1:A:122:LEU:HD22	1:A:224:MET:SD	0.53	2.42	5	1
1:A:9:ILE:HD13	1:A:20:LEU:HD12	0.53	1.79	2	2
1:A:27:PHE:CE1	1:A:31:THR:HG21	0.53	2.39	8	2
1:A:217:PHE:CD2	1:A:225:THR:HG21	0.53	2.39	9	3
1:A:345:THR:HG22	1:A:349:ASN:OD1	0.53	2.03	4	1
1:A:235:ILE:HG21	1:A:242:TYR:CE1	0.53	2.39	6	2
1:A:125:PRO:HB2	1:A:245:THR:HG21	0.53	1.77	3	1
1:A:302:VAL:HG21	1:A:307:TYR:CD2	0.53	2.39	4	2
1:A:59:ILE:HD11	1:A:276:ALA:HB1	0.53	1.80	5	1
1:A:236:ASP:O	1:A:237:THR:HG23	0.52	2.03	10	1
1:A:147:LEU:HD13	1:A:224:MET:HB2	0.52	1.80	4	1
1:A:208:THR:HA	1:A:212:ILE:HD12	0.52	1.80	7	4
1:A:115:LEU:HD22	1:A:248:PRO:HD3	0.52	1.79	9	1
1:A:114:SER:HB3	1:A:244:VAL:HG13	0.52	1.82	4	1
1:A:97:VAL:HG23	1:A:103:LEU:CD2	0.52	2.35	7	1
1:A:272:ASN:ND2	1:A:275:LEU:HD12	0.52	2.20	1	2
1:A:64:HIS:HD2	1:A:261:VAL:HG12	0.52	1.64	1	2
1:A:106:TYR:HB2	1:A:264:ALA:HB3	0.52	1.80	4	1
1:A:181:VAL:HG12	1:A:183:VAL:H	0.52	1.65	9	4
1:A:107:PRO:HB3	1:A:261:VAL:HG21	0.52	1.82	2	3
1:A:97:VAL:O	1:A:97:VAL:HG23	0.51	2.04	5	1
1:A:79:ILE:HD11	1:A:103:LEU:HB2	0.51	1.82	5	3
1:A:59:ILE:HG21	1:A:280:LEU:HD11	0.51	1.82	7	1
1:A:149:PHE:CZ	1:A:195:LEU:HD11	0.51	2.40	5	1
1:A:2:THR:HG23	1:A:57:PRO:HA	0.51	1.83	2	1
1:A:11:ILE:HD11	1:A:15:LYS:CD	0.51	2.35	5	1
1:A:148:MET:SD	1:A:222:THR:HG21	0.51	2.45	4	4
1:A:98:ARG:HB3	1:A:103:LEU:HD23	0.51	1.82	2	1
1:A:109:ALA:O	1:A:261:VAL:HG12	0.51	2.06	5	3
1:A:89:LEU:HD13	1:A:94:TRP:CZ2	0.51	2.41	3	3
1:A:120:ASP:HB3	1:A:121:LEU:HD23	0.51	1.82	6	1
1:A:301:ALA:HB2	1:A:321:MET:CG	0.51	2.36	3	1
1:A:47:PHE:CE2	1:A:60:ILE:HD12	0.51	2.41	2	1
1:A:342:ALA:HB1	1:A:364:ALA:HA	0.51	1.83	9	1
1:A:64:HIS:CB	1:A:96:ALA:HB1	0.50	2.36	1	1
1:A:302:VAL:HG11	1:A:307:TYR:CD2	0.50	2.41	4	3
1:A:151:LEU:HD21	1:A:195:LEU:HD21	0.50	1.82	9	1
1:A:60:ILE:HD11	1:A:62:TRP:HE3	0.50	1.65	8	1
1:A:343:VAL:HG12	1:A:347:VAL:CG2	0.50	2.36	9	1
1:A:92:PHE:HB2	1:A:329:ILE:HD11	0.50	1.82	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:339:PHE:CD2	1:A:368:ILE:HD12	0.50	2.42	8	1
1:A:194:PHE:CZ	1:A:198:LEU:HD11	0.50	2.42	3	1
1:A:155:TYR:CZ	1:A:340:TRP:CH2	0.50	3.00	8	2
1:A:155:TYR:CD1	1:A:258:PHE:CE2	0.50	3.00	2	1
1:A:61:PHE:CE2	1:A:264:ALA:HB2	0.50	2.41	6	1
1:A:61:PHE:CE2	1:A:284:LEU:HD21	0.50	2.41	6	1
1:A:149:PHE:O	1:A:208:THR:HG22	0.50	2.07	7	1
1:A:108:ILE:HG23	1:A:285:LEU:CD2	0.50	2.37	1	1
1:A:110:VAL:HG22	1:A:261:VAL:HG13	0.50	1.83	4	1
1:A:92:PHE:CE2	1:A:93:THR:HG23	0.50	2.42	4	2
1:A:339:PHE:CD2	1:A:368:ILE:HD13	0.50	2.42	5	1
1:A:158:TRP:CD1	1:A:258:PHE:CZ	0.50	3.00	9	2
1:A:155:TYR:CE1	1:A:340:TRP:CH2	0.50	3.00	2	1
1:A:158:TRP:CD1	1:A:258:PHE:CE2	0.50	3.00	6	2
1:A:155:TYR:CE1	1:A:258:PHE:CD1	0.50	3.00	10	1
1:A:283:TYR:O	1:A:286:THR:HG22	0.50	2.07	3	1
1:A:78:GLU:HA	1:A:104:ILE:HG22	0.49	1.84	6	1
1:A:155:TYR:CZ	1:A:258:PHE:CE1	0.49	3.00	1	1
1:A:155:TYR:CD2	1:A:258:PHE:CD2	0.49	3.00	1	2
1:A:155:TYR:CD2	1:A:258:PHE:CE2	0.49	3.00	4	1
1:A:158:TRP:N	1:A:159:PRO:HD2	0.49	2.22	7	5
1:A:155:TYR:CZ	1:A:258:PHE:CD1	0.49	3.00	3	1
1:A:85:PHE:O	1:A:89:LEU:HD12	0.49	2.08	7	1
1:A:60:ILE:HG22	1:A:265:GLY:O	0.49	2.07	4	1
1:A:59:ILE:HG21	1:A:280:LEU:HD21	0.49	1.85	8	1
1:A:213:ALA:O	1:A:225:THR:HG21	0.49	2.08	4	1
1:A:194:PHE:CZ	1:A:250:PHE:CE1	0.49	3.01	3	1
1:A:139:LEU:HD22	1:A:145:SER:O	0.49	2.07	1	1
1:A:155:TYR:CZ	1:A:340:TRP:CZ2	0.49	3.00	1	1
1:A:158:TRP:N	1:A:159:PRO:CD	0.49	2.76	5	7
1:A:108:ILE:O	1:A:303:ALA:HB3	0.49	2.07	6	1
1:A:194:PHE:CD1	1:A:250:PHE:CZ	0.49	3.00	3	1
1:A:171:TYR:CE2	1:A:176:TYR:CE2	0.49	3.00	8	1
1:A:132:ILE:N	1:A:133:PRO:CD	0.48	2.76	8	7
1:A:238:SER:HB3	1:A:240:VAL:HG23	0.48	1.85	5	2
1:A:108:ILE:HG22	1:A:290:LEU:HD21	0.48	1.85	9	2
1:A:103:LEU:O	1:A:104:ILE:HG23	0.48	2.08	10	5
1:A:27:PHE:CD2	1:A:283:TYR:CE1	0.48	3.01	6	1
1:A:94:TRP:CH2	1:A:103:LEU:HD11	0.48	2.43	7	1
1:A:155:TYR:CE1	1:A:258:PHE:CD2	0.48	3.00	6	1
1:A:60:ILE:CG1	1:A:61:PHE:N	0.48	2.76	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:132:ILE:N	1:A:133:PRO:HD2	0.48	2.23	5	3
1:A:163:ALA:HB2	1:A:255:SER:HA	0.48	1.84	10	1
1:A:166:GLY:HA3	1:A:188:ALA:HB2	0.48	1.86	3	1
1:A:357:VAL:CG1	1:A:358:ASP:N	0.48	2.77	1	2
1:A:76:LEU:HD13	1:A:104:ILE:HD13	0.48	1.85	4	1
1:A:11:ILE:HD11	1:A:15:LYS:HE3	0.48	1.83	2	1
1:A:90:TYR:CD1	1:A:92:PHE:CZ	0.48	3.01	6	1
1:A:121:LEU:HD11	1:A:223:ALA:HA	0.48	1.85	4	1
1:A:155:TYR:CE1	1:A:258:PHE:CG	0.48	3.01	6	1
1:A:43:LEU:HD12	1:A:47:PHE:CD1	0.48	2.43	6	1
1:A:90:TYR:CZ	1:A:321:MET:HE2	0.48	2.44	2	1
1:A:266:ILE:HD11	1:A:280:LEU:HD12	0.48	1.84	9	1
1:A:115:LEU:CD1	1:A:147:LEU:HD11	0.48	2.38	3	1
1:A:40:PRO:HG2	1:A:43:LEU:HD22	0.48	1.86	2	2
1:A:97:VAL:HG21	1:A:107:PRO:CG	0.48	2.38	10	1
1:A:345:THR:HG22	1:A:349:ASN:ND2	0.48	2.23	9	1
1:A:90:TYR:CD1	1:A:92:PHE:CE2	0.48	3.02	6	1
1:A:183:VAL:O	1:A:188:ALA:HB3	0.47	2.09	3	2
1:A:151:LEU:HD13	1:A:206:ALA:HA	0.47	1.87	5	1
1:A:79:ILE:HG21	1:A:106:TYR:CE1	0.47	2.44	6	2
1:A:160:LEU:HD21	1:A:194:PHE:HB3	0.47	1.86	8	1
1:A:166:GLY:CA	1:A:188:ALA:HB2	0.47	2.39	2	1
1:A:89:LEU:HD23	1:A:303:ALA:HB1	0.47	1.84	3	1
1:A:37:VAL:HG12	1:A:39:HIS:CE1	0.47	2.44	8	1
1:A:343:VAL:HG12	1:A:347:VAL:HG23	0.47	1.86	9	1
1:A:2:THR:HG23	1:A:2:THR:O	0.47	2.09	3	1
1:A:261:VAL:HG13	1:A:261:VAL:O	0.47	2.09	7	1
1:A:183:VAL:O	1:A:361:LEU:HD22	0.47	2.09	8	1
1:A:151:LEU:HD21	1:A:195:LEU:HD11	0.47	1.85	10	1
1:A:136:ASP:HA	1:A:146:ALA:HB2	0.47	1.86	7	3
1:A:194:PHE:CE1	1:A:250:PHE:CE1	0.47	3.02	3	1
1:A:64:HIS:NE2	1:A:329:ILE:HG22	0.47	2.25	2	1
1:A:192:LEU:HD22	1:A:357:VAL:HG23	0.47	1.87	1	1
1:A:155:TYR:CE1	1:A:258:PHE:CZ	0.47	3.03	2	1
1:A:154:PRO:CG	1:A:343:VAL:HG12	0.47	2.40	1	1
1:A:171:TYR:CD2	1:A:176:TYR:CZ	0.47	3.03	8	1
1:A:199:ILE:HG23	1:A:204:MET:O	0.46	2.10	9	3
1:A:115:LEU:HD12	1:A:225:THR:O	0.46	2.10	3	1
1:A:97:VAL:HG11	1:A:107:PRO:CG	0.46	2.40	7	1
1:A:10:TRP:CE3	1:A:43:LEU:HD13	0.46	2.45	1	1
1:A:139:LEU:HD13	1:A:139:LEU:H	0.46	1.70	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:ALA:HB2	1:A:329:ILE:HG21	0.46	1.86	7	1
1:A:181:VAL:HG12	1:A:183:VAL:CG2	0.46	2.41	1	2
1:A:116:ILE:HG22	1:A:217:PHE:CE2	0.46	2.45	4	1
1:A:47:PHE:CZ	1:A:60:ILE:HG21	0.46	2.45	3	1
1:A:198:LEU:HD13	1:A:204:MET:HE2	0.46	1.86	8	1
1:A:97:VAL:CG2	1:A:103:LEU:HD22	0.46	2.40	7	1
1:A:2:THR:O	1:A:2:THR:HG23	0.46	2.09	9	1
1:A:161:ILE:HG12	1:A:192:LEU:HD12	0.46	1.88	8	1
1:A:77:ALA:HB2	1:A:267:ASN:C	0.46	2.31	1	1
1:A:92:PHE:CE1	1:A:93:THR:CG2	0.46	2.99	8	4
1:A:290:LEU:HD13	1:A:307:TYR:CD2	0.46	2.46	10	1
1:A:78:GLU:CG	1:A:79:ILE:N	0.46	2.79	8	2
1:A:148:MET:HG3	1:A:213:ALA:HB2	0.46	1.87	2	1
1:A:139:LEU:HD22	1:A:139:LEU:N	0.46	2.25	8	2
1:A:27:PHE:CD2	1:A:283:TYR:CD1	0.46	3.04	6	1
1:A:166:GLY:HA2	1:A:188:ALA:HB2	0.46	1.87	2	1
1:A:42:LYS:C	1:A:43:LEU:HD23	0.45	2.32	4	1
1:A:49:GLN:CG	1:A:50:VAL:N	0.45	2.79	4	8
1:A:210:TYR:CD1	1:A:211:SER:N	0.45	2.84	10	1
1:A:92:PHE:CE2	1:A:93:THR:CG2	0.45	2.99	4	2
1:A:151:LEU:HD22	1:A:195:LEU:HD21	0.45	1.88	10	2
1:A:89:LEU:CD1	1:A:94:TRP:CZ2	0.45	2.99	4	2
1:A:47:PHE:N	1:A:48:PRO:CD	0.45	2.79	9	5
1:A:160:LEU:HD11	1:A:194:PHE:CE2	0.45	2.46	10	1
1:A:5:GLY:O	1:A:33:ILE:HG23	0.45	2.12	6	1
1:A:10:TRP:CE3	1:A:43:LEU:CD1	0.45	3.00	2	1
1:A:109:ALA:HB2	1:A:299:LEU:HD13	0.45	1.88	7	1
1:A:40:PRO:O	1:A:43:LEU:HD22	0.45	2.11	2	1
1:A:70:TYR:O	1:A:75:LEU:HD12	0.45	2.12	5	1
1:A:116:ILE:HG23	1:A:242:TYR:HB2	0.45	1.88	4	1
1:A:194:PHE:CE2	1:A:198:LEU:HD11	0.45	2.47	7	3
1:A:286:THR:HG23	1:A:289:GLY:HA3	0.45	1.89	3	1
1:A:44:GLU:CG	1:A:62:TRP:CH2	0.45	3.00	8	1
1:A:94:TRP:CZ3	1:A:103:LEU:CD1	0.45	2.98	7	1
1:A:10:TRP:CG	1:A:57:PRO:CG	0.45	3.00	10	1
1:A:217:PHE:CD2	1:A:225:THR:CG2	0.45	3.00	9	1
1:A:92:PHE:CD1	1:A:93:THR:N	0.45	2.85	3	3
1:A:17:TYR:CD1	1:A:18:ASN:N	0.45	2.85	10	4
1:A:47:PHE:CB	1:A:48:PRO:HD3	0.45	2.42	3	2
1:A:213:ALA:CB	1:A:225:THR:HG23	0.45	2.42	2	1
1:A:109:ALA:CB	1:A:299:LEU:HD13	0.45	2.41	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:47:PHE:CE2	1:A:57:PRO:CG	0.44	2.99	6	1
1:A:235:ILE:HG21	1:A:242:TYR:HD1	0.44	1.65	3	1
1:A:79:ILE:HD12	1:A:81:PRO:HD3	0.44	1.89	7	1
1:A:339:PHE:CE1	1:A:343:VAL:CG2	0.44	3.00	10	4
1:A:90:TYR:CZ	1:A:321:MET:CE	0.44	3.00	2	1
1:A:157:THR:HG21	1:A:347:VAL:HG11	0.44	1.87	4	1
1:A:129:TRP:CZ3	1:A:132:ILE:HD12	0.44	2.47	5	1
1:A:147:LEU:HB2	1:A:224:MET:HE2	0.44	1.89	6	1
1:A:61:PHE:N	1:A:61:PHE:CD1	0.44	2.85	10	2
1:A:106:TYR:CE1	1:A:264:ALA:HB3	0.44	2.47	1	1
1:A:171:TYR:CD1	1:A:176:TYR:CZ	0.44	3.06	1	1
1:A:105:ALA:HB1	1:A:263:SER:OG	0.44	2.11	10	1
1:A:47:PHE:CE2	1:A:60:ILE:CG2	0.44	3.00	5	1
1:A:198:LEU:HD23	1:A:202:LYS:HG3	0.43	1.89	6	1
1:A:282:ASN:O	1:A:283:TYR:CG	0.43	2.71	1	1
1:A:49:GLN:HG3	1:A:50:VAL:HG13	0.43	1.90	9	3
1:A:193:THR:OG1	1:A:357:VAL:HG21	0.43	2.13	10	1
1:A:366:THR:HG22	1:A:370:LYS:HG2	0.43	1.90	8	1
1:A:149:PHE:CZ	1:A:204:MET:CE	0.43	3.01	2	1
1:A:272:ASN:CG	1:A:275:LEU:HD12	0.43	2.33	1	1
1:A:121:LEU:HD12	1:A:139:LEU:CD2	0.43	2.43	10	1
1:A:90:TYR:CB	1:A:92:PHE:CE2	0.43	3.00	3	1
1:A:117:TYR:CD1	1:A:245:THR:HG22	0.43	2.48	8	1
1:A:307:TYR:CE2	1:A:311:LEU:CD1	0.43	3.01	7	2
1:A:192:LEU:HD13	1:A:192:LEU:C	0.43	2.34	10	1
1:A:10:TRP:CD2	1:A:57:PRO:CG	0.43	3.01	7	1
1:A:107:PRO:O	1:A:285:LEU:HD21	0.43	2.13	7	1
1:A:90:TYR:CE2	1:A:305:LYS:CG	0.43	3.01	7	1
1:A:33:ILE:HG21	1:A:275:LEU:HD13	0.43	1.89	9	1
1:A:217:PHE:CD1	1:A:218:ASN:N	0.43	2.86	2	1
1:A:106:TYR:CE1	1:A:266:ILE:CD1	0.43	3.00	4	1
1:A:20:LEU:HD11	1:A:284:LEU:HD21	0.43	1.90	2	1
1:A:42:LYS:O	1:A:43:LEU:HD23	0.43	2.14	10	4
1:A:258:PHE:CD1	1:A:330:MET:CG	0.43	3.02	7	1
1:A:230:TRP:CD1	1:A:231:ALA:N	0.43	2.86	6	1
1:A:361:LEU:HD23	1:A:361:LEU:N	0.43	2.28	6	1
1:A:125:PRO:CG	1:A:245:THR:HG21	0.43	2.43	3	1
1:A:96:ALA:CB	1:A:261:VAL:HG21	0.43	2.44	5	1
1:A:42:LYS:O	1:A:43:LEU:HG	0.43	2.14	6	1
1:A:10:TRP:CE3	1:A:43:LEU:HD12	0.43	2.49	2	1
1:A:97:VAL:HG21	1:A:107:PRO:HD3	0.42	1.90	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:TYR:CD1	1:A:258:PHE:CD2	0.42	3.07	8	2
1:A:308:GLU:O	1:A:312:ALA:HB2	0.42	2.14	3	1
1:A:364:ALA:O	1:A:368:ILE:HD12	0.42	2.14	3	1
1:A:202:LYS:O	1:A:203:HIS:CG	0.42	2.71	10	2
1:A:108:ILE:HA	1:A:285:LEU:HD21	0.42	1.90	6	1
1:A:79:ILE:HG22	1:A:106:TYR:OH	0.42	2.14	3	2
1:A:59:ILE:HD13	1:A:280:LEU:CD2	0.42	2.42	3	1
1:A:329:ILE:HG22	1:A:330:MET:N	0.42	2.29	8	1
1:A:160:LEU:HD11	1:A:250:PHE:CE1	0.42	2.49	5	1
1:A:283:TYR:N	1:A:283:TYR:CD1	0.42	2.87	5	1
1:A:104:ILE:HD12	1:A:104:ILE:C	0.42	2.35	10	1
1:A:129:TRP:CZ3	1:A:160:LEU:HD13	0.42	2.49	3	1
1:A:85:PHE:CD2	1:A:89:LEU:CD1	0.42	3.02	7	1
1:A:155:TYR:CE2	1:A:258:PHE:CG	0.42	3.07	1	1
1:A:121:LEU:HD12	1:A:122:LEU:HB2	0.42	1.92	4	1
1:A:116:ILE:HG23	1:A:243:GLY:O	0.42	2.14	6	1
1:A:147:LEU:HD21	1:A:226:ILE:HD11	0.42	1.91	8	1
1:A:64:HIS:HE2	1:A:329:ILE:HG22	0.42	1.73	2	1
1:A:176:TYR:CD1	1:A:176:TYR:N	0.42	2.87	1	2
1:A:59:ILE:HG22	1:A:60:ILE:N	0.42	2.29	4	2
1:A:217:PHE:CG	1:A:225:THR:CG2	0.42	3.00	8	1
1:A:246:VAL:CG2	1:A:247:LEU:N	0.42	2.83	10	5
1:A:97:VAL:O	1:A:103:LEU:HD23	0.42	2.13	3	1
1:A:183:VAL:CG1	1:A:184:ASP:N	0.42	2.83	8	3
1:A:178:ILE:HG21	1:A:335:GLN:NE2	0.42	2.30	3	1
1:A:301:ALA:HB2	1:A:320:THR:HB	0.42	1.91	7	1
1:A:86:GLN:HG2	1:A:94:TRP:CZ2	0.42	2.49	7	1
1:A:168:ALA:HB1	1:A:339:PHE:CE1	0.42	2.50	10	1
1:A:118:ASN:HB3	1:A:121:LEU:HD12	0.42	1.90	9	1
1:A:90:TYR:CG	1:A:92:PHE:CZ	0.42	3.08	6	1
1:A:256:LYS:N	1:A:257:PRO:CD	0.42	2.83	7	1
1:A:53:THR:HG23	1:A:55:ASP:HB2	0.42	1.92	8	1
1:A:79:ILE:O	1:A:80:THR:HG23	0.41	2.15	10	1
1:A:311:LEU:HB2	1:A:317:ILE:HG21	0.41	1.92	6	1
1:A:369:THR:HG23	1:A:369:THR:O	0.41	2.14	6	1
1:A:209:ASP:O	1:A:213:ALA:CB	0.41	2.68	3	1
1:A:357:VAL:HG12	1:A:361:LEU:CD1	0.41	2.45	8	1
1:A:10:TRP:CG	1:A:57:PRO:HG2	0.41	2.50	10	1
1:A:79:ILE:HG21	1:A:106:TYR:CZ	0.41	2.51	8	1
1:A:47:PHE:N	1:A:48:PRO:HD2	0.41	2.30	1	1
1:A:78:GLU:OE1	1:A:104:ILE:HG22	0.41	2.15	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:222:THR:HG21	1:A:225:THR:HB	0.41	1.91	10	1
1:A:210:TYR:OH	1:A:230:TRP:CZ2	0.41	2.74	9	1
1:A:2:THR:HG21	1:A:271:PRO:HD2	0.41	1.92	9	1
1:A:88:LYS:O	1:A:304:LEU:HD12	0.41	2.15	8	1
1:A:78:GLU:O	1:A:79:ILE:CG2	0.41	2.69	7	1
1:A:9:ILE:N	1:A:9:ILE:CD1	0.41	2.84	7	1
1:A:122:LEU:HD21	1:A:124:ASN:O	0.41	2.15	1	1
1:A:171:TYR:CD1	1:A:176:TYR:CE2	0.41	3.09	1	1
1:A:122:LEU:HD21	1:A:125:PRO:HA	0.41	1.93	5	1
1:A:172:GLU:CG	1:A:173:ASN:N	0.41	2.83	6	1
1:A:99:TYR:CE1	1:A:332:ASN:OD1	0.41	2.74	6	1
1:A:171:TYR:CD2	1:A:175:LYS:O	0.41	2.74	6	1
1:A:192:LEU:CD2	1:A:357:VAL:HG22	0.41	2.45	3	1
1:A:133:PRO:HB3	1:A:198:LEU:HD21	0.41	1.91	2	1
1:A:97:VAL:CG2	1:A:103:LEU:CD2	0.41	2.99	7	1
1:A:259:VAL:HG23	1:A:328:GLU:C	0.41	2.37	1	1
1:A:150:ASN:OD1	1:A:156:PHE:CD2	0.41	2.74	9	1
1:A:150:ASN:OD1	1:A:156:PHE:CG	0.41	2.74	2	1
1:A:171:TYR:CE1	1:A:174:GLY:O	0.40	2.74	4	1
1:A:246:VAL:HG11	1:A:322:GLU:CD	0.40	2.36	4	1
1:A:336:MET:O	1:A:340:TRP:CD1	0.40	2.74	5	2
1:A:203:HIS:O	1:A:203:HIS:CD2	0.40	2.75	10	1
1:A:155:TYR:CZ	1:A:258:PHE:CZ	0.40	3.10	1	1
1:A:129:TRP:CD1	1:A:248:PRO:O	0.40	2.74	9	1
1:A:117:TYR:CE2	1:A:243:GLY:O	0.40	2.75	3	1
1:A:47:PHE:CZ	1:A:57:PRO:CG	0.40	3.05	3	1
1:A:90:TYR:HB3	1:A:92:PHE:CE2	0.40	2.51	3	1
1:A:230:TRP:O	1:A:230:TRP:CD1	0.40	2.74	1	1
1:A:181:VAL:CG1	1:A:183:VAL:CG2	0.40	2.99	4	1
1:A:149:PHE:CE1	1:A:195:LEU:HD11	0.40	2.51	5	1
1:A:135:LEU:HD23	1:A:139:LEU:CD1	0.40	2.45	10	1
1:A:64:HIS:CG	1:A:261:VAL:HG12	0.40	2.50	9	1
1:A:62:TRP:O	1:A:67:PHE:CE2	0.40	2.74	9	1
1:A:147:LEU:HD12	1:A:224:MET:C	0.40	2.37	3	1
1:A:282:ASN:O	1:A:283:TYR:CD1	0.40	2.75	3	1
1:A:133:PRO:HG3	1:A:198:LEU:HD21	0.40	1.93	7	1
1:A:337:SER:O	1:A:341:TYR:CE2	0.40	2.74	7	1
1:A:282:ASN:N	1:A:282:ASN:ND2	0.40	2.70	1	1
1:A:210:TYR:CD2	1:A:214:GLU:OE2	0.40	2.75	3	1
1:A:10:TRP:CD2	1:A:57:PRO:HG2	0.40	2.50	7	1
1:A:62:TRP:CD1	1:A:66:ARG:CB	0.40	3.04	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:171:TYR:CZ	1:A:174:GLY:O	0.40	2.74	2	1
1:A:60:ILE:HD11	1:A:62:TRP:CZ3	0.40	2.50	7	1
1:A:94:TRP:CH2	1:A:103:LEU:CD1	0.40	3.05	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	368/370 (99%)	328±4 (89±1%)	33±5 (9±1%)	7±2 (2±1%)	14	57
All	All	3680/3700 (99%)	3283 (89%)	329 (9%)	68 (2%)	14	57

All 32 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	284	LEU	8
1	A	236	ASP	6
1	A	104	ILE	6
1	A	257	PRO	4
1	A	56	GLY	4
1	A	285	LEU	3
1	A	107	PRO	3
1	A	331	PRO	3
1	A	41	ASP	3
1	A	208	THR	2
1	A	241	ASN	2
1	A	57	PRO	2
1	A	248	PRO	2
1	A	16	GLY	2
1	A	271	PRO	1
1	A	272	ASN	1
1	A	269	ALA	1
1	A	239	LYS	1
1	A	237	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	203	HIS	1
1	A	165	GLY	1
1	A	15	LYS	1
1	A	220	GLY	1
1	A	354	ARG	1
1	A	4	GLU	1
1	A	14	ASP	1
1	A	3	GLU	1
1	A	97	VAL	1
1	A	166	GLY	1
1	A	255	SER	1
1	A	69	GLY	1
1	A	221	GLU	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	296/297 (100%)	244±5 (82±2%)	53±5 (18±2%)	5	40
All	All	2960/2970 (100%)	2435 (82%)	525 (18%)	5	40

All 172 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	148	MET	10
1	A	212	ILE	10
1	A	211	SER	9
1	A	43	LEU	8
1	A	192	LEU	8
1	A	47	PHE	7
1	A	102	LYS	7
1	A	277	LYS	7
1	A	46	LYS	7
1	A	140	LYS	7
1	A	127	LYS	7
1	A	67	PHE	6

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Mol	Chain	Res	Type	Models (Total)
1	A	263	SER	6
1	A	204	MET	6
1	A	139	LEU	6
1	A	362	LYS	6
1	A	78	GLU	6
1	A	210	TYR	6
1	A	98	ARG	6
1	A	26	LYS	6
1	A	344	ARG	6
1	A	15	LYS	6
1	A	341	TYR	6
1	A	308	GLU	6
1	A	42	LYS	6
1	A	179	LYS	6
1	A	6	LYS	5
1	A	55	ASP	5
1	A	246	VAL	5
1	A	219	LYS	5
1	A	121	LEU	5
1	A	111	GLU	5
1	A	314	ASP	5
1	A	214	GLU	5
1	A	66	ARG	5
1	A	131	GLU	5
1	A	202	LYS	5
1	A	261	VAL	5
1	A	88	LYS	5
1	A	62	TRP	5
1	A	135	LEU	5
1	A	370	LYS	4
1	A	128	THR	4
1	A	255	SER	4
1	A	142	LYS	4
1	A	237	THR	4
1	A	285	LEU	4
1	A	82	ASP	4
1	A	207	ASP	4
1	A	241	ASN	4
1	A	14	ASP	4
1	A	175	LYS	4
1	A	114	SER	4
1	A	359	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	10	TRP	4
1	A	170	LYS	4
1	A	297	LYS	3
1	A	256	LYS	3
1	A	172	GLU	3
1	A	286	THR	3
1	A	236	ASP	3
1	A	58	ASP	3
1	A	336	MET	3
1	A	72	GLN	3
1	A	307	TYR	3
1	A	44	GLU	3
1	A	80	THR	3
1	A	281	GLU	3
1	A	87	ASP	3
1	A	28	GLU	3
1	A	29	LYS	3
1	A	365	GLN	3
1	A	239	LYS	3
1	A	95	ASP	3
1	A	183	VAL	3
1	A	273	LYS	3
1	A	89	LEU	3
1	A	328	GLU	3
1	A	270	SER	3
1	A	189	LYS	3
1	A	31	THR	3
1	A	155	TYR	3
1	A	119	LYS	3
1	A	203	HIS	3
1	A	144	LYS	3
1	A	130	GLU	3
1	A	299	LEU	3
1	A	354	ARG	3
1	A	335	GLN	3
1	A	136	ASP	2
1	A	2	THR	2
1	A	147	LEU	2
1	A	326	LYS	2
1	A	238	SER	2
1	A	251	LYS	2
1	A	208	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	200	LYS	2
1	A	3	GLU	2
1	A	153	GLU	2
1	A	118	ASN	2
1	A	234	ASN	2
1	A	310	GLU	2
1	A	267	ASN	2
1	A	287	ASP	2
1	A	20	LEU	2
1	A	361	LEU	2
1	A	99	TYR	2
1	A	306	SER	2
1	A	49	GLN	2
1	A	83	LYS	2
1	A	296	ASP	2
1	A	86	GLN	2
1	A	73	SER	2
1	A	177	ASP	2
1	A	138	GLU	2
1	A	352	SER	2
1	A	253	GLN	2
1	A	224	MET	2
1	A	120	ASP	2
1	A	290	LEU	2
1	A	93	THR	1
1	A	320	THR	1
1	A	145	SER	1
1	A	64	HIS	1
1	A	30	ASP	1
1	A	22	GLU	1
1	A	85	PHE	1
1	A	366	THR	1
1	A	367	ARG	1
1	A	164	ASP	1
1	A	355	GLN	1
1	A	100	ASN	1
1	A	291	GLU	1
1	A	39	HIS	1
1	A	313	LYS	1
1	A	122	LEU	1
1	A	45	GLU	1
1	A	41	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	274	GLU	1
1	A	65	ASP	1
1	A	198	LEU	1
1	A	272	ASN	1
1	A	323	ASN	1
1	A	349	ASN	1
1	A	358	ASP	1
1	A	227	ASN	1
1	A	157	THR	1
1	A	294	ASN	1
1	A	8	VAL	1
1	A	171	TYR	1
1	A	322	GLU	1
1	A	156	PHE	1
1	A	345	THR	1
1	A	316	ARG	1
1	A	34	LYS	1
1	A	25	LYS	1
1	A	27	PHE	1
1	A	337	SER	1
1	A	321	MET	1
1	A	284	LEU	1
1	A	18	ASN	1
1	A	304	LEU	1
1	A	282	ASN	1
1	A	193	THR	1
1	A	242	TYR	1
1	A	356	THR	1
1	A	233	SER	1
1	A	4	GLU	1
1	A	197	ASP	1
1	A	185	ASN	1
1	A	247	LEU	1
1	A	221	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

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 ⓘ

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 7114

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping ⓘ

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	4389
Number of shifts mapped to atoms	4389
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	15

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	369	-0.18 ± 0.04	None needed (< 0.5 ppm)
$^{13}C_\beta$	337	0.05 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	336	-0.08 ± 0.09	None needed (< 0.5 ppm)
^{15}N	343	1.20 ± 0.29	Should be applied

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 3998 atoms were assigned a chemical shift out of a possible 4432. 50 out of 50 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1756/1803 (97%)	710/717 (99%)	703/738 (95%)	343/348 (99%)
Sidechain	1934/2254 (86%)	1188/1316 (90%)	724/854 (85%)	22/84 (26%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	308/375 (82%)	159/195 (82%)	141/166 (85%)	8/14 (57%)
Overall	3998/4432 (90%)	2057/2228 (92%)	1568/1758 (89%)	373/446 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 4013 atoms were assigned a chemical shift out of a possible 4450. 50 out of 50 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1759/1808 (97%)	711/719 (99%)	705/740 (95%)	343/349 (98%)
Sidechain	1946/2267 (86%)	1196/1324 (90%)	728/858 (85%)	22/85 (26%)
Aromatic	308/375 (82%)	159/195 (82%)	141/166 (85%)	8/14 (57%)
Overall	4013/4450 (90%)	2066/2238 (92%)	1574/1764 (89%)	373/448 (83%)

7.1.4   Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	44	GLU	HB2	-0.22	3.08 − 0.98	-10.7
1	A	229	PRO	HA	1.23	6.05 − 2.75	-9.6
1	A	228	GLY	HA2	1.52	5.87 − 2.07	-6.4
1	A	160	LEU	HD13	-1.02	2.16 − -0.64	-6.4
1	A	160	LEU	HD12	-1.02	2.16 − -0.64	-6.4
1	A	160	LEU	HD11	-1.02	2.16 − -0.64	-6.4
1	A	251	LYS	HG2	-0.28	2.67 − 0.07	-6.3
1	A	182	GLY	HA3	1.50	5.80 − 2.00	-6.3
1	A	281	GLU	HG3	0.97	3.31 − 1.21	-6.1
1	A	40	PRO	HG3	0.06	3.56 − 0.26	-5.6
1	A	248	PRO	HG2	0.24	3.48 − 0.38	-5.5
1	A	44	GLU	HB3	0.83	3.10 − 0.90	-5.3
1	A	40	PRO	HG2	0.33	3.48 − 0.38	-5.2
1	A	305	LYS	HG3	-0.06	2.76 − -0.04	-5.1
1	A	86	GLN	HG2	0.96	3.67 − 0.97	-5.0

7.1.5   Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-

defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A: