Full wwPDB NMR Structure Validation Report (i)

Mar 1, 2022 – 02:37 PM EST

PDB ID	:	2EZI
Title	:	SOLUTION NMR STRUCTURE OF THE IGAMMA SUBDOMAIN OF THE MU END DNA BINDING DOMAIN OF MU PHAGE TRANSPOSASE, 30 STRUCTURES
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Deposited on	:	1997-07-25

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 (i) symbol.

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

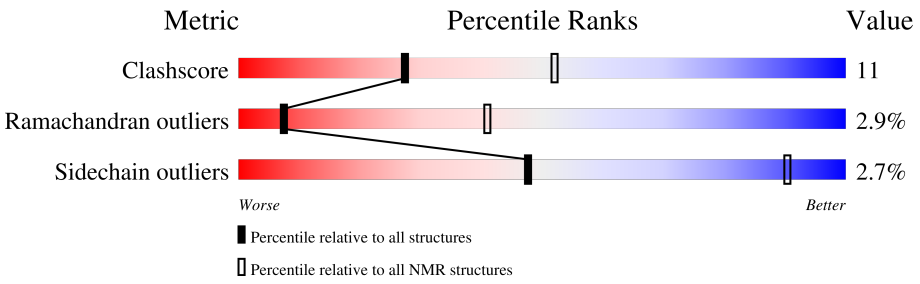
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	75	65% 12% 23%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 15 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:181-A:238 (58)	0.27	15

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 5 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 3, 6, 9, 13, 15, 16, 27
2	4, 7, 14, 17, 19, 20, 21, 24, 26
3	2, 5, 10, 11, 12, 30
4	8, 18, 22
5	28, 29
Single-model clusters	23; 25

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1225 atoms, of which 602 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TRANSPOSASE.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	75	1225	392	602	114	112	5	0

4 Residue-property plots (i)

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: TRANSPOSASE

Chain A: 65% 12% 23%

M173 N174 V175 H176 K177 S178 E179 F180 R194 K197 A211 H214 G215 W216 L231 D232 M235 C239 R240 E241 G242 E243 H244 A245 L246 M247

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: TRANSPOSASE

Chain A: 56% 19% • 23%

M173 N174 V175 H176 K177 S178 E179 F180 A184 W185 I189 E196 A199 C203 A211 G215 W216 Q230 L231 D232 E233 A234 M235 V236 V237 A238 C239 R240 E241 G242 E243 H244 A245 L246 M247

4.2.2 Score per residue for model 2

• Molecule 1: TRANSPOSASE

Chain A: 64% 12% • 23%

M173 N174 V175 H176 K177 S178 E179 F180 E196 K197 P198 A211 H214 G215 W216 R221 L231 D232 M235 C239 R240 E241 G242 E243 H244 A245 L246 M247

4.2.3 Score per residue for model 3

- Molecule 1: TRANSPOSASE

Chain A: 57% 19% • 23%

M173 N174 V175 H176 K177 S178 E179 F180 D181 E182 Q186 R194 P195 E196 K197 A211 H214 G215 W216 L231 D232 E233 A234 M235 V236 V237 A238 C239 R240 E241 G242 E243 H244 A245 L246 M247

4.2.4 Score per residue for model 4

- Molecule 1: TRANSPOSASE

Chain A: 57% 17% • 23%

M173 N174 V175 H176 K177 S178 E179 F180 L193 R194 P195 E196 K197 P198 R201 A211 H214 G215 W216 R227 L231 D232 M235 V236 V237 A238 C239 R240 E241 G242 E243 H244 A245 L246 M247

4.2.5 Score per residue for model 5

- Molecule 1: TRANSPOSASE

Chain A: 60% 15% • 23%

M173 N174 V175 H176 K177 S178 E179 F180 Y192 L193 R194 P195 E196 K197 Y204 A211 H214 G215 W216 S217 I218 L231 M235 C239 R240 E241 G242 E243 H244 A245 L246 M247

4.2.6 Score per residue for model 6

- Molecule 1: TRANSPOSASE

Chain A: 61% 13% • 23%

M173 N174 V175 H176 K177 S178 E179 F180 R194 P198 C203 Y204 A211 G215 R221 L231 D232 E233 A234 M235 V236 V237 A238 C239 R240 E241 G242 E243 H244 A245 L246 M247

4.2.7 Score per residue for model 7

- Molecule 1: TRANSPOSASE

Chain A: 57% 19% • 23%

M173 N174 V175 H176 K177 S178 E179 F180 W185 R194 P198 R201 K202 C203 Y204 A211 H214 G215 W216 P219 S220 R221 R227 D232 M235 C239 R240 E241 G242 E243 H244 A245 L246 M247

4.2.8 Score per residue for model 8

- Molecule 1: TRANSPOSASE

Chain A: 59% 16% • 23%

M173 N174 V175 H176 K177 S178 E179 F180 R194 P195 E196 R206 A211 R212 E213 H214 G215 W216 R227 D232 M235 V236 V237 A238 C239 R240 E241 G242 E243 H244 A245 L246 M247

4.2.9 Score per residue for model 9

- Molecule 1: TRANSPOSASE

Chain A: 51% 23% • 23%

M173 N174 V175 H176 K177 S178 E179 F180 D181 E182 D183 A184 W185 Q186 C203 Y204 E208 L209 A210 A211 R212 E213 H214 G215 W216 S217 I218 R221 L231 D232 M235 V236 C239 R240 E241 G242 E243 H244 A245 L246 M247

4.2.10 Score per residue for model 10

- Molecule 1: TRANSPOSASE

Chain A: 65% 11% • 23%

M173 N174 V175 H176 K177 S178 E179 F180 A199 F200 R201 K202 C203 A211 R212 G215 R221 L231 M235 C239 R240 E241 G242 E243 H244 A245 L246 M247

4.2.11 Score per residue for model 11

- Molecule 1: TRANSPOSASE

Chain A: 57% 19% • 23%

M173 N174 V175 H176 K177 S178 E179 F180 D181 A199 C203 A211 R212 E213 H214 G215 W216 S217 F225 R226 R227 I228 Q229 Q230 L231 M235 V236 V237 A238 C239 R240 E241 G242 E243 H244 A245 L246 M247

4.2.12 Score per residue for model 12

- Molecule 1: TRANSPOSASE

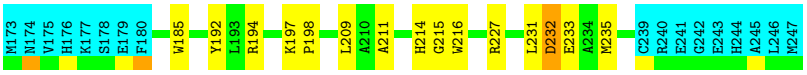
Chain A: 64% 12% • 23%

M173 N174 V175 H176 K177 S178 E179 F180 E196 K197 P198 A211 H214 G215 W216 L231 M235 A238 C239 R240 E241 G242 E243 H244 A245 L246 M247

4.2.13 Score per residue for model 13

- Molecule 1: TRANSPOSASE

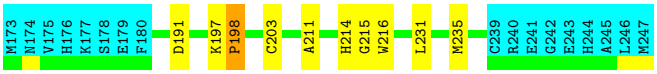
Chain A: 57% 19% • 23%



4.2.14 Score per residue for model 14

- Molecule 1: TRANSPOSASE

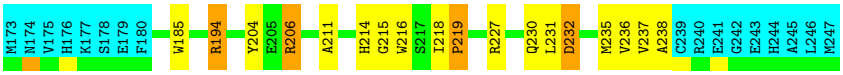
Chain A: 64% 12% • 23%



4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: TRANSPOSASE

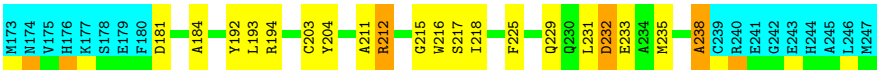
Chain A: 53% 19% 5% 23%



4.2.16 Score per residue for model 16

- Molecule 1: TRANSPOSASE

Chain A: 51% 23% • 23%



4.2.17 Score per residue for model 17

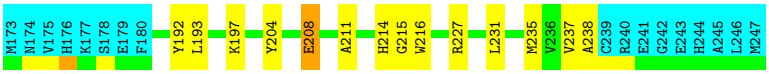
- Molecule 1: TRANSPOSASE

Chain A: 56% 21% 23%

4.2.18 Score per residue for model 18

- Molecule 1: TRANSPOSASE

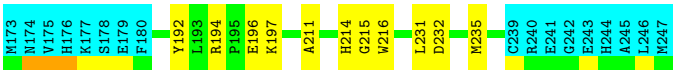
Chain A: 59% 17% • 23%



4.2.19 Score per residue for model 19

- Molecule 1: TRANSPOSASE

Chain A: 63% 15% 23%



4.2.20 Score per residue for model 20

- Molecule 1: TRANSPOSASE

Chain A: 60% 15% • 23%

4.2.21 Score per residue for model 21

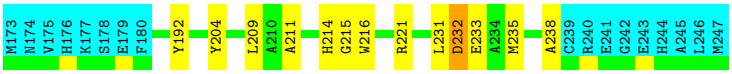
- Molecule 1: TRANSPOSASE

Chain A: 60% 15% • 23%

4.2.22 Score per residue for model 22

- Molecule 1: TRANSPOSASE

Chain A: 60% 16% • 23%



4.2.23 Score per residue for model 23

- Molecule 1: TRANSPOSASE

Chain A: 53% 20% • 23%

4.2.24 Score per residue for model 24

- Molecule 1: TRANSPOSASE

Chain A: 64% 13% 23%

4.2.25 Score per residue for model 25

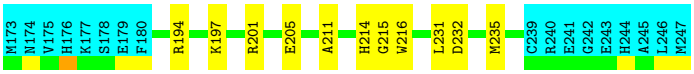
- Molecule 1: TRANSPOSASE

Chain A: 51% 24% • 23%

4.2.26 Score per residue for model 26

- Molecule 1: TRANSPOSASE

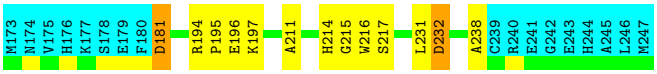
Chain A: 63% 15% 23%



4.2.27 Score per residue for model 27

- Molecule 1: TRANSPOSASE

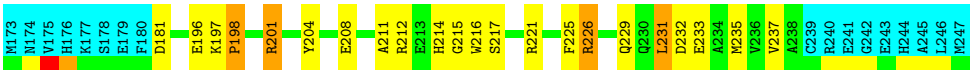
Chain A: 60% 15% • 23%



4.2.28 Score per residue for model 28

- Molecule 1: TRANSPOSASE

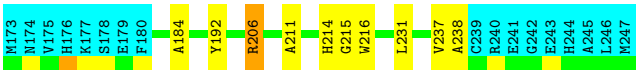
Chain A: 48% 24% 5% 23%



4.2.29 Score per residue for model 29

- Molecule 1: TRANSPOSASE

Chain A: 64% 12% • 23%



4.2.30 Score per residue for model 30

- Molecule 1: TRANSPOSASE

Chain A: 53% 17% 7% 23%

5 Refinement protocol and experimental data overview (i)

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

Of the ? calculated structures, 30 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR (SEE ABOVE)	structure solution	ABOVE)
X-PLOR (SEE ABOVE)	refinement	ABOVE)

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (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	484	471	471	10±4
All	All	14520	14130	14130	308

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:204:TYR:CD1	1:A:221:ARG:NH1	0.65	2.65	6	3
1:A:204:TYR:CE1	1:A:221:ARG:NH1	0.64	2.66	30	4
1:A:211:ALA:O	1:A:215:GLY:N	0.63	2.31	28	30
1:A:185:TRP:CZ3	1:A:227:ARG:NH2	0.63	2.67	23	1
1:A:203:CYS:SG	1:A:204:TYR:N	0.62	2.73	30	7
1:A:214:HIS:CD2	1:A:216:TRP:CH2	0.60	2.90	5	18
1:A:231:LEU:HD12	1:A:235:MET:SD	0.58	2.38	28	8
1:A:225:PHE:CE2	1:A:229:GLN:NE2	0.58	2.72	11	3
1:A:185:TRP:CE3	1:A:227:ARG:NH2	0.57	2.72	23	3
1:A:201:ARG:CG	1:A:201:ARG:HH11	0.57	2.13	23	5
1:A:184:ALA:HB2	1:A:216:TRP:CD2	0.56	2.35	25	7
1:A:231:LEU:O	1:A:232:ASP:CB	0.56	2.53	13	10
1:A:221:ARG:HH11	1:A:221:ARG:CG	0.56	2.14	7	1
1:A:184:ALA:HB2	1:A:216:TRP:CG	0.56	2.36	1	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:201:ARG:CG	1:A:201:ARG:NH1	0.55	2.69	23	2
1:A:192:TYR:CZ	1:A:197:LYS:NZ	0.55	2.75	19	2
1:A:194:ARG:O	1:A:196:GLU:N	0.55	2.40	8	4
1:A:194:ARG:CG	1:A:194:ARG:NH1	0.54	2.70	15	6
1:A:221:ARG:NH1	1:A:221:ARG:CG	0.53	2.68	7	2
1:A:212:ARG:NH1	1:A:212:ARG:CG	0.53	2.72	16	2
1:A:184:ALA:HB2	1:A:216:TRP:CE3	0.53	2.39	23	1
1:A:181:ASP:OD1	1:A:217:SER:N	0.53	2.39	11	5
1:A:194:ARG:O	1:A:197:LYS:N	0.53	2.41	26	3
1:A:186:GLN:NE2	1:A:186:GLN:N	0.53	2.56	30	1
1:A:194:ARG:CG	1:A:194:ARG:HH11	0.52	2.16	15	3
1:A:194:ARG:HH11	1:A:194:ARG:CG	0.52	2.16	8	1
1:A:235:MET:SD	1:A:235:MET:C	0.52	2.88	22	16
1:A:214:HIS:CD2	1:A:216:TRP:CZ2	0.52	2.98	27	1
1:A:218:ILE:CG1	1:A:218:ILE:O	0.51	2.57	25	2
1:A:201:ARG:NH1	1:A:201:ARG:CG	0.51	2.74	17	3
1:A:229:GLN:NE2	1:A:230:GLN:N	0.51	2.58	30	1
1:A:212:ARG:CG	1:A:212:ARG:HH11	0.50	2.17	16	2
1:A:232:ASP:OD1	1:A:233:GLU:N	0.50	2.43	16	7
1:A:235:MET:C	1:A:235:MET:SD	0.50	2.90	16	1
1:A:185:TRP:CZ2	1:A:227:ARG:NE	0.50	2.80	7	1
1:A:192:TYR:CE1	1:A:197:LYS:NZ	0.50	2.79	25	1
1:A:225:PHE:CZ	1:A:229:GLN:CG	0.50	2.94	20	2
1:A:214:HIS:CG	1:A:216:TRP:CZ2	0.49	3.00	27	13
1:A:221:ARG:CG	1:A:221:ARG:HH11	0.49	2.19	22	1
1:A:182:GLU:O	1:A:186:GLN:OE1	0.49	2.30	30	3
1:A:231:LEU:O	1:A:232:ASP:CG	0.49	2.51	2	5
1:A:197:LYS:O	1:A:198:PRO:O	0.49	2.31	14	4
1:A:196:GLU:OE1	1:A:198:PRO:N	0.48	2.46	2	1
1:A:209:LEU:C	1:A:209:LEU:HD23	0.48	2.29	13	1
1:A:213:GLU:OE1	1:A:214:HIS:CD2	0.48	2.66	8	1
1:A:206:ARG:CG	1:A:206:ARG:NH1	0.48	2.76	8	2
1:A:181:ASP:HB3	1:A:184:ALA:HB3	0.48	1.86	23	1
1:A:197:LYS:O	1:A:197:LYS:CG	0.48	2.61	27	1
1:A:185:TRP:CD2	1:A:227:ARG:NH2	0.47	2.82	7	1
1:A:208:GLU:OE1	1:A:218:ILE:CD1	0.47	2.62	24	1
1:A:196:GLU:OE1	1:A:196:GLU:N	0.47	2.47	1	1
1:A:187:PHE:O	1:A:191:ASP:OD2	0.47	2.33	23	1
1:A:235:MET:O	1:A:238:ALA:HB3	0.47	2.10	20	4
1:A:205:GLU:OE1	1:A:205:GLU:N	0.47	2.44	17	1
1:A:233:GLU:N	1:A:233:GLU:CD	0.47	2.67	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:208:GLU:OE2	1:A:221:ARG:NH2	0.47	2.44	28	1
1:A:204:TYR:OH	1:A:218:ILE:CD1	0.47	2.63	16	2
1:A:199:ALA:O	1:A:203:CYS:SG	0.47	2.73	11	1
1:A:235:MET:SD	1:A:235:MET:O	0.46	2.73	6	8
1:A:181:ASP:OD2	1:A:217:SER:O	0.46	2.33	9	2
1:A:204:TYR:O	1:A:208:GLU:OE1	0.46	2.34	18	1
1:A:214:HIS:CB	1:A:216:TRP:CE2	0.46	2.99	14	7
1:A:181:ASP:OD1	1:A:217:SER:O	0.46	2.34	23	3
1:A:201:ARG:O	1:A:205:GLU:OE1	0.46	2.34	26	2
1:A:199:ALA:O	1:A:203:CYS:CB	0.46	2.64	1	2
1:A:181:ASP:CG	1:A:217:SER:O	0.45	2.55	25	2
1:A:206:ARG:CG	1:A:206:ARG:HH11	0.45	2.24	8	1
1:A:196:GLU:O	1:A:197:LYS:C	0.45	2.55	27	8
1:A:181:ASP:OD2	1:A:217:SER:N	0.45	2.40	16	1
1:A:194:ARG:C	1:A:196:GLU:H	0.45	2.15	8	3
1:A:208:GLU:OE1	1:A:218:ILE:HD11	0.45	2.12	9	1
1:A:225:PHE:CD2	1:A:229:GLN:NE2	0.45	2.85	16	1
1:A:226:ARG:NE	1:A:229:GLN:OE1	0.44	2.50	28	1
1:A:194:ARG:C	1:A:196:GLU:N	0.44	2.71	8	2
1:A:194:ARG:NH1	1:A:194:ARG:CG	0.44	2.79	16	2
1:A:204:TYR:CE1	1:A:208:GLU:OE1	0.44	2.70	18	1
1:A:204:TYR:OH	1:A:219:PRO:O	0.44	2.36	7	1
1:A:227:ARG:NH1	1:A:227:ARG:CG	0.44	2.78	30	2
1:A:209:LEU:O	1:A:213:GLU:OE2	0.43	2.35	9	1
1:A:227:ARG:CG	1:A:227:ARG:NH1	0.43	2.79	4	1
1:A:204:TYR:CD1	1:A:221:ARG:NE	0.43	2.87	9	1
1:A:201:ARG:HH21	1:A:221:ARG:NH2	0.43	2.11	10	1
1:A:233:GLU:CD	1:A:233:GLU:H	0.43	2.17	6	2
1:A:204:TYR:CZ	1:A:218:ILE:HD12	0.43	2.49	16	1
1:A:209:LEU:N	1:A:209:LEU:CD2	0.43	2.82	22	1
1:A:237:VAL:O	1:A:237:VAL:HG12	0.42	2.13	18	2
1:A:232:ASP:OD1	1:A:232:ASP:N	0.42	2.53	19	1
1:A:230:GLN:O	1:A:230:GLN:OE1	0.42	2.37	1	1
1:A:185:TRP:CZ2	1:A:189:ILE:HD11	0.42	2.49	1	1
1:A:191:ASP:OD1	1:A:203:CYS:SG	0.42	2.77	14	1
1:A:218:ILE:O	1:A:219:PRO:O	0.42	2.38	15	1
1:A:233:GLU:CD	1:A:233:GLU:N	0.41	2.73	6	1
1:A:197:LYS:NZ	1:A:197:LYS:CB	0.41	2.83	5	1
1:A:206:ARG:NH1	1:A:206:ARG:CG	0.41	2.82	29	1
1:A:186:GLN:N	1:A:186:GLN:CD	0.41	2.74	30	1
1:A:191:ASP:OD1	1:A:192:TYR:N	0.41	2.53	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:231:LEU:CD1	1:A:235:MET:SD	0.41	3.08	23	1
1:A:185:TRP:CZ3	1:A:227:ARG:CZ	0.41	3.04	23	1
1:A:226:ARG:CG	1:A:226:ARG:NH1	0.41	2.82	25	1
1:A:204:TYR:OH	1:A:218:ILE:HD12	0.41	2.16	24	2
1:A:206:ARG:HH11	1:A:206:ARG:HG2	0.41	1.75	15	1
1:A:226:ARG:O	1:A:229:GLN:NE2	0.41	2.50	30	1
1:A:235:MET:O	1:A:238:ALA:CB	0.40	2.69	16	1
1:A:221:ARG:HG2	1:A:221:ARG:HH11	0.40	1.76	30	1
1:A:181:ASP:OD2	1:A:217:SER:C	0.40	2.60	23	1
1:A:194:ARG:N	1:A:194:ARG:CD	0.40	2.83	5	1
1:A:204:TYR:CD1	1:A:204:TYR:C	0.40	2.94	15	1
1:A:221:ARG:CG	1:A:221:ARG:NH1	0.40	2.83	23	1
1:A:227:ARG:CG	1:A:227:ARG:HH11	0.40	2.30	4	1
1:A:197:LYS:N	1:A:198:PRO:CD	0.40	2.84	12	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	58/75 (77%)	55±1 (94±2%)	2±1 (3±2%)	2±1 (3±2%)	7 41
All	All	1740/2250 (77%)	1640 (94%)	49 (3%)	51 (3%)	7 41

All 7 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	231	LEU	16
1	A	232	ASP	10
1	A	198	PRO	9
1	A	238	ALA	6
1	A	195	PRO	4
1	A	181	ASP	4
1	A	219	PRO	2

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	48/63 (76%)	47±1 (97±2%)	1±1 (3±2%)	48 90
All	All	1440/1890 (76%)	1401 (97%)	39 (3%)	48 90

All 13 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	194	ARG	10
1	A	201	ARG	4
1	A	227	ARG	4
1	A	232	ASP	4
1	A	212	ARG	4
1	A	206	ARG	3
1	A	230	GLN	2
1	A	221	ARG	2
1	A	226	ARG	2
1	A	213	GLU	1
1	A	197	LYS	1
1	A	208	GLU	1
1	A	186	GLN	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 monosaccharides 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 (i)

No chemical shift data were provided