



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 02:00 am GMT

PDB ID : 2PHG
Title : Model for VP16 binding to TFIIB
Authors : Jonker, H.R.A.; Wechselberger, R.W.; Boelens, R.; Folkers, G.E.; Kaptein, R.
Deposited on : 2007-04-11

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

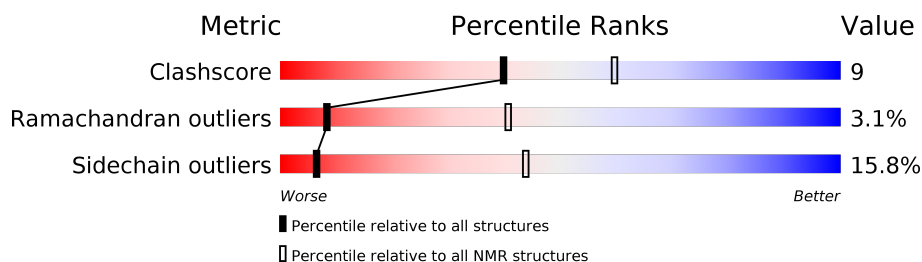
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	206	<div> <div style="width: 64%; background-color: green;"></div> <div style="width: 36%; background-color: yellow;"></div> <div>64% 36%</div> </div>
2	B	26	<div> <div style="width: 100%; background-color: cyan;"></div> <div>100%</div> </div>

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 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:111-A:316 (206)	1.13	8

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 5 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1811 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					Trace
1	A	206	Total	C	N	O	S	0
			1607	1013	287	295	12	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	SER	-	SEE REMARK 999	UNP Q00403

- Molecule 2 is a protein called Alpha trans-inducing protein.

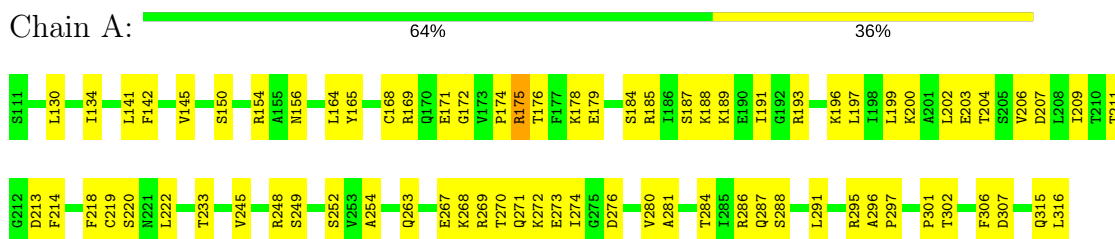
Mol	Chain	Residues	Atoms					Trace
2	B	26	Total	C	N	O	S	0
			204	130	27	45	2	

4 Residue-property plots

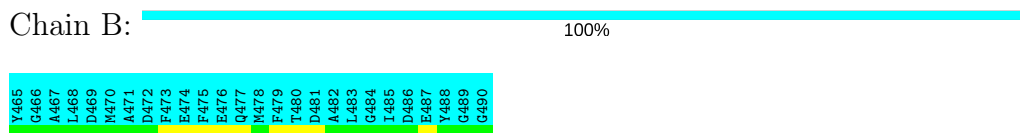
4.1 Average score per residue in the NMR ensemble

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: Transcription initiation factor IIB



- Molecule 2: Alpha trans-inducing protein

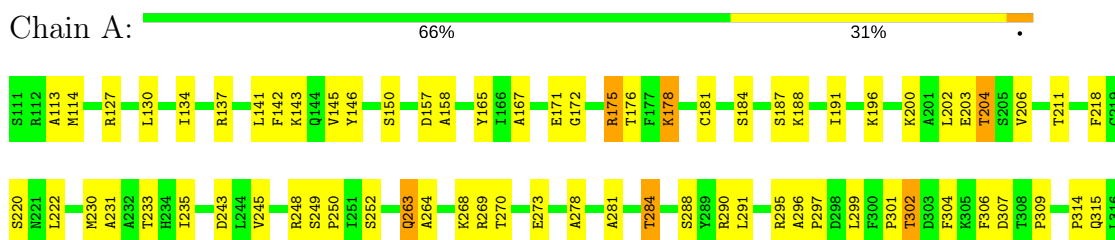


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Transcription initiation factor IIB



- Molecule 2: Alpha trans-inducing protein

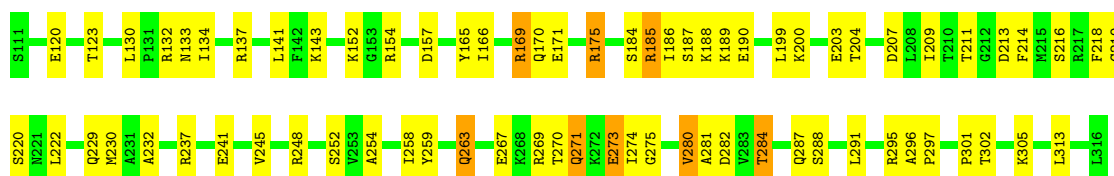
Chain B:  100%



4.2.2 Score per residue for model 2

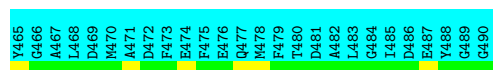
- Molecule 1: Transcription initiation factor IIB

Chain A:  65%  31%  0%



- Molecule 2: Alpha trans-inducing protein

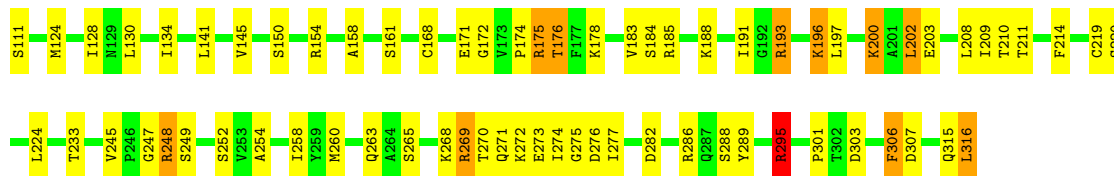
Chain B:  100%



4.2.3 Score per residue for model 3

- Molecule 1: Transcription initiation factor IIB

Chain A:  67%  28%  5%



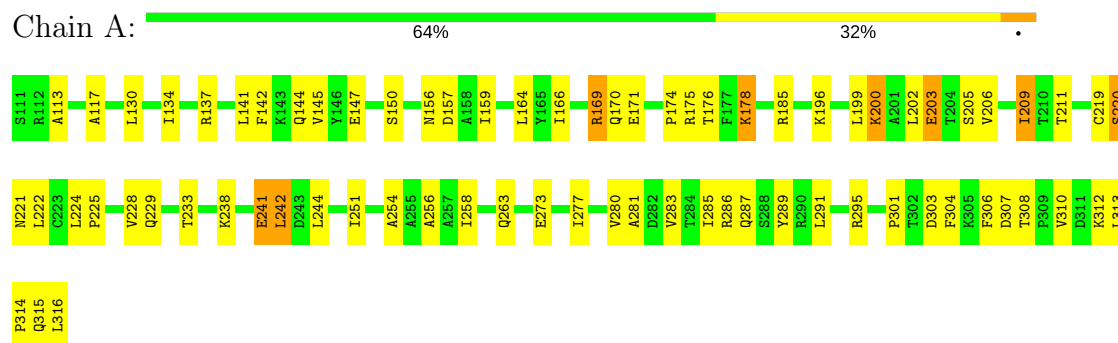
- Molecule 2: Alpha trans-inducing protein

Chain B:  100%

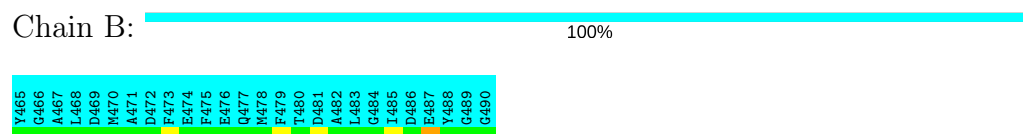


4.2.4 Score per residue for model 4

- Molecule 1: Transcription initiation factor IIB

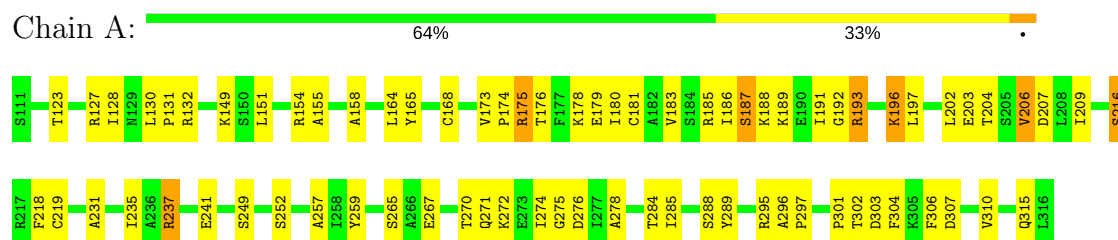


- Molecule 2: Alpha trans-inducing protein

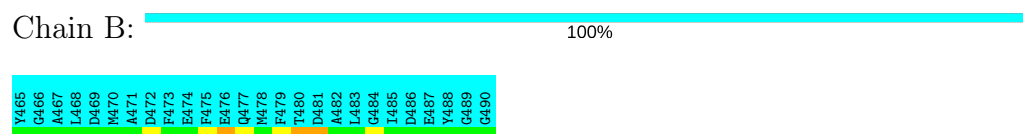


4.2.5 Score per residue for model 5

- Molecule 1: Transcription initiation factor IIB

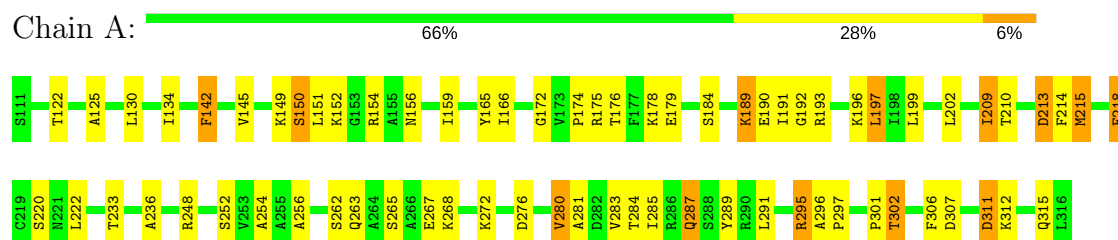


- Molecule 2: Alpha trans-inducing protein



4.2.6 Score per residue for model 6

- Molecule 1: Transcription initiation factor IIB



- Molecule 2: Alpha trans-inducing protein

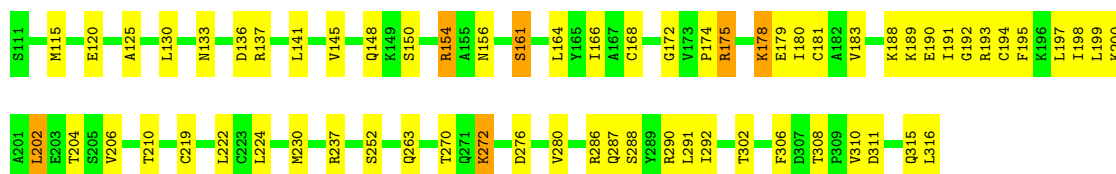
Chain B:  100%



4.2.7 Score per residue for model 7

- Molecule 1: Transcription initiation factor IIB

Chain A:  68% 29% .



- Molecule 2: Alpha trans-inducing protein

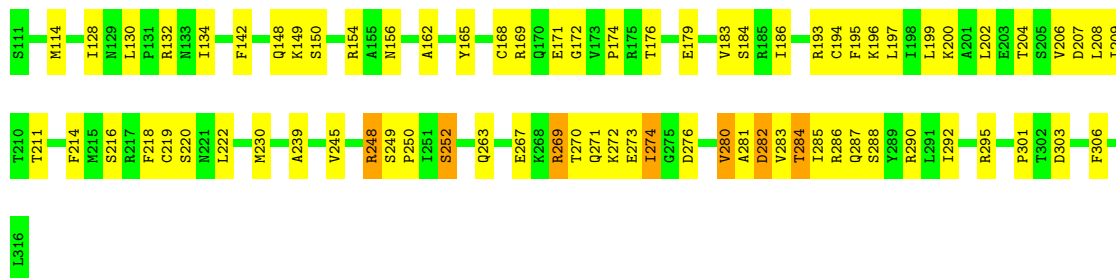
Chain B:  100%



4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Transcription initiation factor IIB

Chain A:  64% 33% .



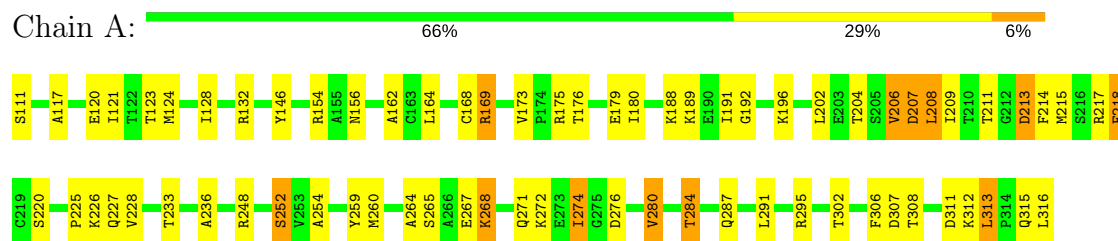
- Molecule 2: Alpha trans-inducing protein

Chain B:  100%

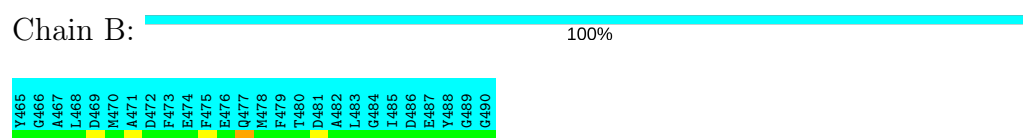


4.2.9 Score per residue for model 9

- Molecule 1: Transcription initiation factor IIB

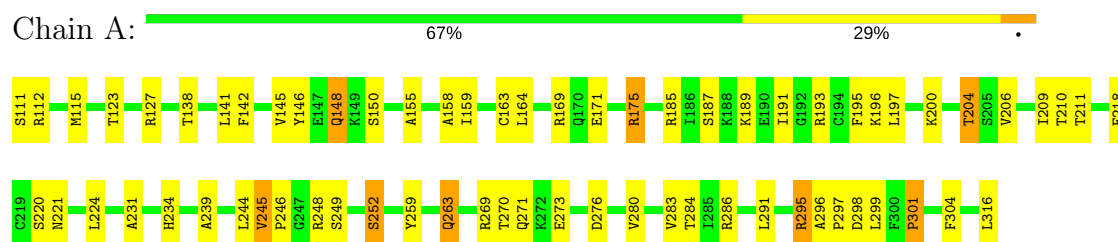


- Molecule 2: Alpha trans-inducing protein

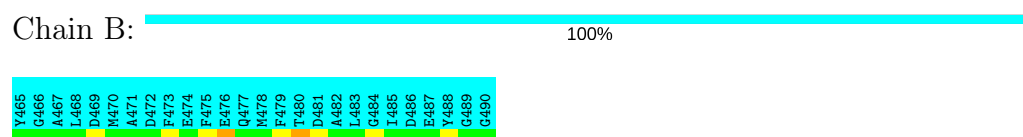


4.2.10 Score per residue for model 10

- Molecule 1: Transcription initiation factor IIB



- Molecule 2: Alpha trans-inducing protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *The model was calculated using HADDOCK.*

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *Top-ranked ensemble, according to the average interaction energy and buried surface area.*

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

Software name	Classification	Version
CNS	structure solution	1.1
HADDOCK	refinement	1.2

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1607	0	1666	29±4
2	B	0	0	0	0±0
All	All	16070	0	16660	288

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:281:ALA:HB3	1:A:284:THR:HB	0.87	1.47	8	3
1:A:222:LEU:HD22	1:A:273:GLU:HB2	0.75	1.58	8	1
1:A:114:MET:HA	1:A:142:PHE:HE2	0.74	1.43	1	2
1:A:145:VAL:HG11	1:A:198:ILE:HG12	0.73	1.59	7	1
1:A:158:ALA:HB1	1:A:191:ILE:HA	0.73	1.59	5	1
1:A:117:ALA:HB2	1:A:156:ASN:HB2	0.72	1.59	4	1
1:A:166:ILE:HD13	1:A:198:ILE:HB	0.71	1.60	7	1
1:A:171:GLU:HB3	1:A:272:LYS:HD2	0.70	1.63	3	1
1:A:265:SER:HA	1:A:307:ASP:HB2	0.70	1.63	9	3
1:A:248:ARG:HD3	1:A:284:THR:HA	0.70	1.64	8	1
1:A:134:ILE:HD11	1:A:172:GLY:HA3	0.69	1.64	3	3
1:A:190:GLU:HG3	1:A:193:ARG:HE	0.68	1.48	7	1
1:A:205:SER:HA	1:A:283:VAL:HG21	0.67	1.64	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:LEU:HD12	1:A:131:PRO:HD2	0.67	1.66	5	1
1:A:272:LYS:HA	1:A:276:ASP:HB3	0.67	1.67	8	5
1:A:154:ARG:HE	1:A:190:GLU:HG2	0.66	1.50	7	1
1:A:245:VAL:HG21	1:A:288:SER:HA	0.66	1.68	3	4
1:A:252:SER:HB2	1:A:284:THR:HG23	0.66	1.66	5	1
1:A:142:PHE:HA	1:A:145:VAL:HG12	0.65	1.67	1	1
1:A:265:SER:HA	1:A:307:ASP:HB3	0.64	1.70	3	1
1:A:206:VAL:HG22	1:A:207:ASP:H	0.64	1.53	9	2
1:A:134:ILE:HD12	1:A:172:GLY:HA2	0.64	1.68	6	1
1:A:252:SER:HB3	1:A:284:THR:HG23	0.64	1.68	8	3
1:A:204:THR:HB	1:A:206:VAL:HG23	0.63	1.70	10	3
1:A:114:MET:HA	1:A:142:PHE:CE2	0.62	2.29	1	1
1:A:216:SER:HA	1:A:219:CYS:SG	0.62	2.34	2	3
1:A:141:LEU:HD13	1:A:202:LEU:HD11	0.62	1.70	3	1
1:A:242:LEU:HB3	1:A:244:LEU:HD22	0.62	1.72	4	1
1:A:248:ARG:HB2	1:A:284:THR:HG23	0.60	1.74	6	1
1:A:176:THR:HB	1:A:263:GLN:HE22	0.60	1.57	1	1
1:A:128:ILE:HG13	1:A:180:ILE:HG23	0.60	1.73	5	1
1:A:187:SER:HB3	1:A:190:GLU:HG2	0.60	1.72	2	1
1:A:197:LEU:HA	1:A:200:LYS:HE2	0.59	1.74	8	2
1:A:111:SER:N	1:A:146:TYR:HH	0.58	1.96	10	2
1:A:239:ALA:HB1	1:A:245:VAL:HG21	0.58	1.75	10	1
1:A:288:SER:O	1:A:292:ILE:HB	0.58	1.97	8	1
1:A:252:SER:HB2	1:A:284:THR:CG2	0.58	2.29	5	1
1:A:248:ARG:HG3	1:A:284:THR:HA	0.58	1.76	6	1
1:A:121:ILE:HA	1:A:164:LEU:HD21	0.57	1.77	9	1
1:A:162:ALA:HA	1:A:191:ILE:HG23	0.57	1.76	9	1
1:A:206:VAL:HB	1:A:282:ASP:HB3	0.56	1.75	8	1
1:A:176:THR:HB	1:A:263:GLN:NE2	0.56	2.16	1	1
1:A:280:VAL:HG12	1:A:281:ALA:H	0.55	1.61	4	1
1:A:263:GLN:HG2	1:A:313:LEU:HD21	0.55	1.77	2	1
1:A:239:ALA:HB1	1:A:292:ILE:HD11	0.55	1.78	8	1
1:A:281:ALA:HB3	1:A:284:THR:CB	0.55	2.29	8	1
1:A:315:GLN:O	1:A:316:LEU:HB3	0.55	2.02	3	1
1:A:175:ARG:HG3	1:A:263:GLN:HA	0.54	1.80	1	1
1:A:188:LYS:HA	1:A:191:ILE:HD12	0.54	1.78	9	4
1:A:191:ILE:O	1:A:195:PHE:HB3	0.54	2.02	10	1
1:A:155:ALA:HA	1:A:186:ILE:HD12	0.54	1.77	5	1
1:A:174:PRO:HB2	1:A:268:LYS:HE3	0.53	1.80	3	1
1:A:130:LEU:HD11	1:A:174:PRO:HG3	0.53	1.80	8	1
1:A:137:ARG:HD2	1:A:167:ALA:HA	0.53	1.80	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:274:ILE:HG23	1:A:275:GLY:H	0.53	1.62	2	2
1:A:151:LEU:HB2	1:A:159:ILE:HD11	0.53	1.79	6	1
1:A:264:ALA:O	1:A:307:ASP:HB3	0.53	2.04	1	1
1:A:176:THR:HG23	1:A:178:LYS:H	0.53	1.62	3	3
1:A:286:ARG:HH22	1:A:316:LEU:HB3	0.52	1.62	3	1
1:A:178:LYS:HE3	1:A:178:LYS:HA	0.52	1.79	1	1
1:A:196:LYS:HA	1:A:199:LEU:HD23	0.52	1.82	6	1
1:A:281:ALA:CB	1:A:284:THR:HB	0.52	2.34	6	2
1:A:171:GLU:HA	1:A:271:GLN:HB3	0.52	1.80	2	1
1:A:158:ALA:HA	1:A:191:ILE:HG12	0.52	1.81	1	1
1:A:125:ALA:HB1	1:A:130:LEU:HB2	0.52	1.81	6	1
1:A:175:ARG:HG3	1:A:268:LYS:HA	0.52	1.82	3	1
1:A:273:GLU:HG3	1:A:277:ILE:HD12	0.52	1.82	3	1
1:A:269:ARG:HG3	1:A:273:GLU:HG3	0.51	1.79	10	1
1:A:280:VAL:HG12	1:A:284:THR:HG21	0.51	1.81	8	2
1:A:178:LYS:HA	1:A:181:CYS:SG	0.51	2.45	5	2
1:A:226:LYS:HA	1:A:226:LYS:HE2	0.51	1.82	9	1
1:A:175:ARG:HG2	1:A:316:LEU:HB3	0.51	1.82	4	1
1:A:123:THR:O	1:A:127:ARG:HG3	0.51	2.06	10	1
1:A:265:SER:HA	1:A:307:ASP:CB	0.51	2.36	3	1
1:A:166:ILE:HG12	1:A:199:LEU:HG	0.51	1.83	7	1
1:A:168:CYS:O	1:A:173:VAL:HB	0.51	2.05	9	1
1:A:123:THR:O	1:A:127:ARG:HG2	0.50	2.05	5	1
1:A:213:ASP:HB2	1:A:280:VAL:HG22	0.50	1.83	2	1
1:A:199:LEU:HD12	1:A:203:GLU:HG2	0.50	1.82	4	1
1:A:296:ALA:HB1	1:A:297:PRO:HD2	0.50	1.83	10	4
1:A:154:ARG:HD2	1:A:190:GLU:OE2	0.50	2.07	2	1
1:A:168:CYS:SG	1:A:174:PRO:HD3	0.50	2.46	8	1
1:A:218:PHE:CE2	1:A:278:ALA:HA	0.50	2.41	5	2
1:A:178:LYS:HD2	1:A:314:PRO:HD2	0.50	1.84	1	1
1:A:186:ILE:HG12	1:A:187:SER:N	0.50	2.22	5	1
1:A:174:PRO:O	1:A:175:ARG:HB2	0.49	2.07	4	2
1:A:170:GLN:HA	1:A:282:ASP:HB2	0.49	1.84	2	1
1:A:207:ASP:HB2	1:A:283:VAL:HG12	0.49	1.83	8	1
1:A:155:ALA:HA	1:A:186:ILE:CD1	0.49	2.38	5	1
1:A:166:ILE:O	1:A:170:GLN:HG2	0.49	2.07	4	1
1:A:272:LYS:HA	1:A:276:ASP:CB	0.49	2.37	9	2
1:A:209:ILE:HB	1:A:280:VAL:O	0.49	2.07	6	2
1:A:222:LEU:HB2	1:A:273:GLU:OE1	0.49	2.08	4	1
1:A:165:TYR:O	1:A:169:ARG:HB3	0.49	2.08	8	1
1:A:175:ARG:HB3	1:A:268:LYS:HA	0.48	1.83	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:238:LYS:HA	1:A:241:GLU:HB3	0.48	1.84	4	1
1:A:124:MET:O	1:A:128:ILE:HG12	0.48	2.07	3	2
1:A:176:THR:HB	1:A:315:GLN:O	0.48	2.08	4	1
1:A:188:LYS:HA	1:A:191:ILE:HG13	0.48	1.84	5	1
1:A:137:ARG:O	1:A:141:LEU:HG	0.48	2.08	7	3
1:A:248:ARG:CB	1:A:284:THR:HG23	0.48	2.38	6	1
1:A:239:ALA:HA	1:A:299:LEU:HD12	0.48	1.84	10	1
1:A:145:VAL:HG21	1:A:159:ILE:HG21	0.48	1.85	4	1
1:A:220:SER:HB3	1:A:224:LEU:HB3	0.48	1.83	4	1
1:A:128:ILE:HB	1:A:130:LEU:HG	0.48	1.85	8	1
1:A:185:ARG:HD3	1:A:186:ILE:HG22	0.48	1.86	2	1
1:A:271:GLN:HE22	1:A:285:ILE:HD11	0.48	1.68	8	1
1:A:158:ALA:HB2	1:A:187:SER:HB2	0.47	1.86	1	1
1:A:264:ALA:HA	1:A:313:LEU:HD11	0.47	1.85	9	1
1:A:125:ALA:HA	1:A:130:LEU:HB2	0.47	1.85	7	1
1:A:225:PRO:HG2	1:A:228:VAL:HG23	0.47	1.87	4	2
1:A:252:SER:CB	1:A:284:THR:HG23	0.47	2.40	8	1
1:A:142:PHE:HA	1:A:145:VAL:HG22	0.47	1.86	4	1
1:A:289:TYR:HE2	1:A:315:GLN:HA	0.47	1.69	5	1
1:A:130:LEU:HB3	1:A:134:ILE:HG13	0.47	1.86	3	2
1:A:249:SER:HB3	1:A:250:PRO:HD2	0.47	1.86	8	2
1:A:213:ASP:HA	1:A:218:PHE:HZ	0.47	1.69	6	2
1:A:142:PHE:CE2	1:A:159:ILE:HB	0.47	2.44	10	1
1:A:175:ARG:HD3	1:A:176:THR:HG22	0.47	1.86	1	1
1:A:263:GLN:HB2	1:A:316:LEU:HG	0.47	1.87	4	1
1:A:174:PRO:HA	1:A:270:THR:HA	0.47	1.85	5	1
1:A:158:ALA:CB	1:A:191:ILE:HA	0.46	2.38	5	1
1:A:218:PHE:HE2	1:A:278:ALA:HA	0.46	1.71	1	1
1:A:272:LYS:HG2	1:A:277:ILE:HG13	0.46	1.87	3	1
1:A:290:ARG:HD3	1:A:315:GLN:OE1	0.46	2.11	7	1
1:A:155:ALA:HB1	1:A:158:ALA:HB3	0.46	1.88	10	1
1:A:166:ILE:HD11	1:A:195:PHE:HA	0.46	1.88	7	1
1:A:166:ILE:HG22	1:A:202:LEU:HD12	0.46	1.88	6	1
1:A:296:ALA:HB2	1:A:312:LYS:HG3	0.46	1.88	6	1
1:A:120:GLU:HA	1:A:120:GLU:OE1	0.46	2.10	2	1
1:A:256:ALA:HA	1:A:285:ILE:HG23	0.45	1.88	4	1
1:A:186:ILE:HG12	1:A:187:SER:H	0.45	1.70	5	1
1:A:175:ARG:HG3	1:A:267:GLU:O	0.45	2.10	2	1
1:A:196:LYS:HB2	1:A:196:LYS:NZ	0.45	2.27	5	1
1:A:113:ALA:HB3	1:A:146:TYR:HE1	0.45	1.72	1	1
1:A:158:ALA:HA	1:A:191:ILE:CG1	0.45	2.41	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:259:TYR:HE2	1:A:316:LEU:HD13	0.45	1.71	10	1
1:A:130:LEU:HD13	1:A:134:ILE:HG21	0.45	1.89	2	2
1:A:161:SER:HB3	1:A:183:VAL:HG13	0.45	1.89	7	1
1:A:213:ASP:HA	1:A:218:PHE:CZ	0.45	2.47	9	2
1:A:149:LYS:HB2	1:A:151:LEU:HG	0.45	1.86	5	1
1:A:175:ARG:HB2	1:A:268:LYS:HA	0.45	1.87	9	1
1:A:307:ASP:O	1:A:309:PRO:HD3	0.45	2.11	1	1
1:A:315:GLN:O	1:A:316:LEU:HB2	0.45	2.10	4	2
1:A:117:ALA:HB2	1:A:156:ASN:HD21	0.44	1.72	9	1
1:A:138:THR:HG23	1:A:163:CYS:HB2	0.44	1.88	10	1
1:A:194:CYS:HA	1:A:197:LEU:HD12	0.44	1.90	8	1
1:A:196:LYS:HD3	1:A:199:LEU:HD12	0.44	1.90	8	1
1:A:158:ALA:HB1	1:A:191:ILE:HG12	0.44	1.89	3	1
1:A:196:LYS:O	1:A:200:LYS:HB2	0.44	2.11	4	1
1:A:141:LEU:HD22	1:A:202:LEU:HD22	0.44	1.88	7	1
1:A:174:PRO:O	1:A:175:ARG:HB3	0.44	2.13	6	1
1:A:283:VAL:HA	1:A:286:ARG:HB3	0.44	1.87	10	1
1:A:295:ARG:HG3	1:A:296:ALA:H	0.44	1.71	10	1
1:A:184:SER:HB3	1:A:188:LYS:HG3	0.44	1.89	2	1
1:A:222:LEU:HD22	1:A:273:GLU:HB3	0.44	1.89	2	1
1:A:175:ARG:CB	1:A:268:LYS:HA	0.44	2.43	1	1
1:A:168:CYS:HB2	1:A:173:VAL:HG22	0.44	1.89	5	1
1:A:174:PRO:O	1:A:179:GLU:HG3	0.43	2.12	7	1
1:A:306:PHE:CZ	1:A:310:VAL:HG22	0.43	2.48	7	1
1:A:176:THR:CG2	1:A:178:LYS:HG2	0.43	2.43	6	1
1:A:222:LEU:HD22	1:A:273:GLU:HG2	0.43	1.90	1	1
1:A:169:ARG:HD3	1:A:199:LEU:HD21	0.43	1.89	2	1
1:A:190:GLU:HA	1:A:193:ARG:HG3	0.43	1.90	7	1
1:A:269:ARG:HG2	1:A:274:ILE:HD12	0.43	1.89	8	1
1:A:206:VAL:HG22	1:A:207:ASP:N	0.43	2.27	5	1
1:A:231:ALA:O	1:A:235:ILE:HG13	0.43	2.14	5	1
1:A:141:LEU:HD13	1:A:166:ILE:HD12	0.43	1.88	2	1
1:A:291:LEU:HD23	1:A:291:LEU:H	0.43	1.74	2	1
1:A:237:ARG:O	1:A:241:GLU:HG3	0.43	2.13	5	2
1:A:306:PHE:HZ	1:A:310:VAL:HG22	0.43	1.74	7	1
1:A:175:ARG:O	1:A:176:THR:HB	0.43	2.14	3	2
1:A:254:ALA:O	1:A:258:ILE:HG13	0.43	2.13	3	3
1:A:215:MET:HB3	1:A:218:PHE:CE2	0.43	2.49	6	1
1:A:280:VAL:HG12	1:A:284:THR:CG2	0.42	2.45	9	1
1:A:113:ALA:HB1	1:A:156:ASN:HB3	0.42	1.90	4	1
1:A:232:ALA:CB	1:A:258:ILE:HA	0.42	2.44	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:272:LYS:HG2	1:A:276:ASP:HB3	0.42	1.89	7	1
1:A:141:LEU:O	1:A:145:VAL:HG22	0.42	2.14	10	1
1:A:273:GLU:HA	1:A:277:ILE:HB	0.42	1.90	4	1
1:A:224:LEU:HD13	1:A:269:ARG:HD2	0.42	1.91	3	1
1:A:236:ALA:HB1	1:A:254:ALA:HA	0.42	1.91	9	1
1:A:193:ARG:O	1:A:197:LEU:HG	0.42	2.15	10	2
1:A:166:ILE:O	1:A:169:ARG:HG3	0.42	2.14	4	1
1:A:127:ARG:NE	1:A:127:ARG:HA	0.42	2.30	1	1
1:A:133:ASN:HA	1:A:136:ASP:HB3	0.42	1.90	7	1
1:A:113:ALA:HB3	1:A:146:TYR:CE1	0.42	2.50	1	1
1:A:154:ARG:NE	1:A:190:GLU:HG2	0.42	2.26	7	1
1:A:189:LYS:O	1:A:193:ARG:HB2	0.42	2.15	6	1
1:A:304:PHE:HD1	1:A:306:PHE:H	0.42	1.57	5	1
1:A:176:THR:HG21	1:A:263:GLN:NE2	0.42	2.29	8	1
1:A:151:LEU:HD23	1:A:159:ILE:HG12	0.41	1.91	6	1
1:A:175:ARG:HD3	1:A:179:GLU:OE1	0.41	2.16	9	1
1:A:176:THR:HG22	1:A:179:GLU:HG2	0.41	1.91	8	1
1:A:248:ARG:HD2	1:A:287:GLN:OE1	0.41	2.15	8	1
1:A:262:SER:O	1:A:267:GLU:HB2	0.41	2.15	6	1
1:A:231:ALA:HB1	1:A:304:PHE:CD1	0.41	2.51	10	1
1:A:310:VAL:HG21	1:A:313:LEU:HD22	0.41	1.90	4	1
1:A:235:ILE:HB	1:A:257:ALA:HB1	0.41	1.91	5	1
1:A:169:ARG:HA	1:A:173:VAL:HB	0.41	1.92	9	1
1:A:175:ARG:CG	1:A:263:GLN:HB2	0.41	2.46	10	1
1:A:207:ASP:HA	1:A:281:ALA:CB	0.41	2.46	2	1
1:A:187:SER:O	1:A:191:ILE:HG13	0.41	2.15	1	1
1:A:151:LEU:HD21	1:A:191:ILE:HA	0.41	1.92	6	1
1:A:183:VAL:O	1:A:185:ARG:HG2	0.41	2.16	5	1
1:A:206:VAL:HG13	1:A:207:ASP:N	0.41	2.30	5	1
1:A:180:ILE:O	1:A:183:VAL:HG12	0.41	2.16	7	1
1:A:256:ALA:HB2	1:A:285:ILE:HG23	0.41	1.90	6	1
1:A:178:LYS:HD2	1:A:310:VAL:HG13	0.41	1.92	5	1
1:A:175:ARG:HD3	1:A:263:GLN:OE1	0.41	2.15	7	1
1:A:236:ALA:CB	1:A:254:ALA:HA	0.41	2.46	6	1
1:A:245:VAL:H	1:A:246:PRO:HD2	0.41	1.76	10	1
1:A:234:HIS:HB3	1:A:301:PRO:HG3	0.41	1.91	10	1
1:A:215:MET:SD	1:A:217:ARG:HB2	0.41	2.56	9	1
1:A:263:GLN:HA	1:A:263:GLN:OE1	0.41	2.15	4	1
1:A:142:PHE:HE1	1:A:156:ASN:O	0.41	1.99	6	1
1:A:196:LYS:O	1:A:199:LEU:HB2	0.41	2.16	6	1
1:A:231:ALA:HB1	1:A:304:PHE:CE2	0.40	2.51	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:CYS:SG	1:A:172:GLY:HA3	0.40	2.56	7	1
1:A:258:ILE:HG22	1:A:274:ILE:HD11	0.40	1.93	3	1
1:A:178:LYS:HE3	1:A:181:CYS:SG	0.40	2.56	1	1
1:A:235:ILE:HG23	1:A:299:LEU:HB3	0.40	1.94	1	1
1:A:259:TYR:CD1	1:A:274:ILE:HG21	0.40	2.51	9	1
1:A:134:ILE:HD12	1:A:168:CYS:CB	0.40	2.47	3	1
1:A:247:GLY:O	1:A:248:ARG:HD2	0.40	2.16	3	1
1:A:283:VAL:O	1:A:287:GLN:HB2	0.40	2.17	6	1
1:A:222:LEU:HD22	1:A:273:GLU:CB	0.40	2.47	2	1
1:A:175:ARG:HD2	1:A:179:GLU:CD	0.40	2.36	7	1
1:A:162:ALA:HB1	1:A:195:PHE:HA	0.40	1.92	8	1
1:A:220:SER:HA	1:A:224:LEU:HB3	0.40	1.93	10	1
1:A:148:GLN:HG3	1:A:150:SER:H	0.40	1.76	7	1
1:A:128:ILE:HD11	1:A:180:ILE:HG23	0.40	1.94	9	1
1:A:148:GLN:OE1	1:A:150:SER:HB2	0.40	2.17	10	1
1:A:145:VAL:CG1	1:A:198:ILE:HG12	0.40	2.40	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	204/206 (99%)	173±3 (85±2%)	25±3 (12±1%)	6±2 (3±1%)	8	41
2	B	0	-	-	-	-	-
All	All	2040/2320 (88%)	1727 (85%)	249 (12%)	64 (3%)	8	41

All 27 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	301	PRO	8
1	A	209	ILE	7
1	A	295	ARG	6
1	A	206	VAL	4
1	A	175	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	280	VAL	4
1	A	311	ASP	3
1	A	208	LEU	3
1	A	154	ARG	3
1	A	302	THR	3
1	A	274	ILE	2
1	A	183	VAL	2
1	A	275	GLY	1
1	A	297	PRO	1
1	A	171	GLU	1
1	A	245	VAL	1
1	A	207	ASP	1
1	A	248	ARG	1
1	A	176	THR	1
1	A	251	ILE	1
1	A	187	SER	1
1	A	314	PRO	1
1	A	150	SER	1
1	A	306	PHE	1
1	A	186	ILE	1
1	A	315	GLN	1
1	A	222	LEU	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	175/175 (100%)	147±4 (84±2%)	28±4 (16±2%)	6 44
2	B	0	-	-	-
All	All	1750/1940 (90%)	1473 (84%)	277 (16%)	6 44

All 104 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	252	SER	8
1	A	220	SER	7

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Mol	Chain	Res	Type	Models (Total)
1	A	211	THR	7
1	A	202	LEU	7
1	A	306	PHE	6
1	A	291	LEU	6
1	A	204	THR	6
1	A	270	THR	6
1	A	271	GLN	5
1	A	200	LYS	5
1	A	295	ARG	5
1	A	214	PHE	5
1	A	218	PHE	5
1	A	233	THR	5
1	A	263	GLN	5
1	A	287	GLN	5
1	A	203	GLU	5
1	A	150	SER	5
1	A	248	ARG	5
1	A	302	THR	5
1	A	210	THR	4
1	A	303	ASP	4
1	A	284	THR	4
1	A	165	TYR	4
1	A	184	SER	4
1	A	185	ARG	4
1	A	132	ARG	4
1	A	164	LEU	4
1	A	169	ARG	4
1	A	269	ARG	4
1	A	230	MET	4
1	A	286	ARG	3
1	A	171	GLU	3
1	A	175	ARG	3
1	A	219	CYS	3
1	A	249	SER	3
1	A	178	LYS	3
1	A	154	ARG	3
1	A	196	LYS	3
1	A	289	TYR	3
1	A	267	GLU	3
1	A	308	THR	3
1	A	157	ASP	3
1	A	213	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	179	GLU	2
1	A	143	LYS	2
1	A	156	ASN	2
1	A	149	LYS	2
1	A	259	TYR	2
1	A	145	VAL	2
1	A	193	ARG	2
1	A	152	LYS	2
1	A	290	ARG	2
1	A	268	LYS	2
1	A	115	MET	2
1	A	237	ARG	2
1	A	221	ASN	2
1	A	161	SER	2
1	A	229	GLN	2
1	A	282	ASP	2
1	A	120	GLU	2
1	A	123	THR	2
1	A	288	SER	2
1	A	260	MET	2
1	A	316	LEU	2
1	A	197	LEU	2
1	A	276	ASP	1
1	A	311	ASP	1
1	A	227	GLN	1
1	A	208	LEU	1
1	A	285	ILE	1
1	A	312	LYS	1
1	A	241	GLU	1
1	A	292	ILE	1
1	A	122	THR	1
1	A	133	ASN	1
1	A	304	PHE	1
1	A	313	LEU	1
1	A	224	LEU	1
1	A	137	ARG	1
1	A	194	CYS	1
1	A	147	GLU	1
1	A	244	LEU	1
1	A	305	LYS	1
1	A	187	SER	1
1	A	144	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	190	GLU	1
1	A	148	GLN	1
1	A	243	ASP	1
1	A	189	LYS	1
1	A	242	LEU	1
1	A	209	ILE	1
1	A	112	ARG	1
1	A	111	SER	1
1	A	272	LYS	1
1	A	216	SER	1
1	A	307	ASP	1
1	A	142	PHE	1
1	A	280	VAL	1
1	A	298	ASP	1
1	A	315	GLN	1
1	A	273	GLU	1
1	A	215	MET	1
1	A	222	LEU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided