



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 06:06 PM UTC

PDB ID : 2PHG / pdb_00002phg
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

<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

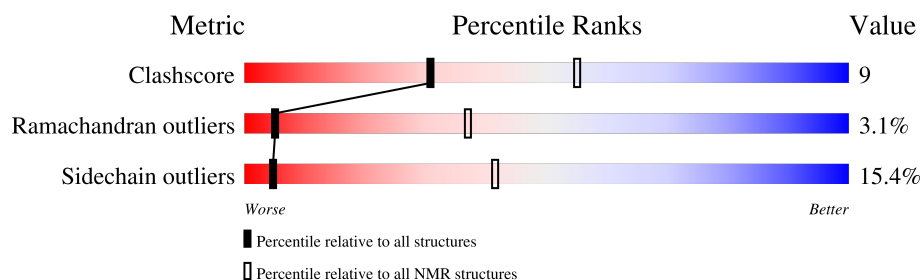
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

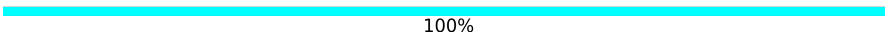
The overall completeness of chemical shifts assignment was not calculated.

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	206	
2	B	26	

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)	1.96	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.

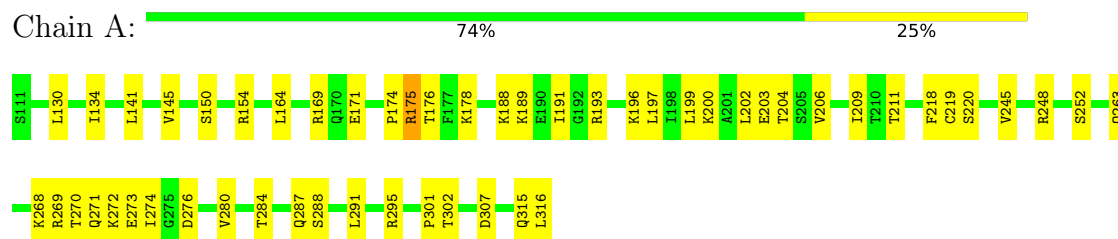
Mol	Chain	Residues	Atoms					Trace
2	B	26	Total	C	N	O	S	0
			204	130	27	45	2	

4 Residue-property plots

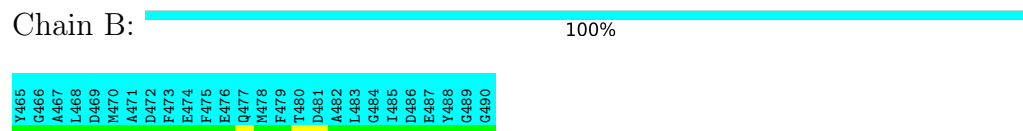
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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: Transcription initiation factor IIB



- Molecule 2: Alpha trans-inducing protein

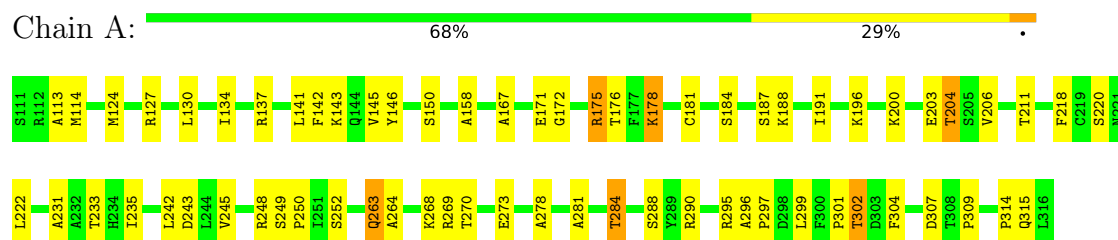


4.2 Scores per residue for each member of the ensemble

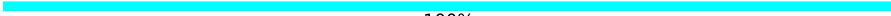
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Transcription initiation factor IIB



- Molecule 2: Alpha trans-inducing protein

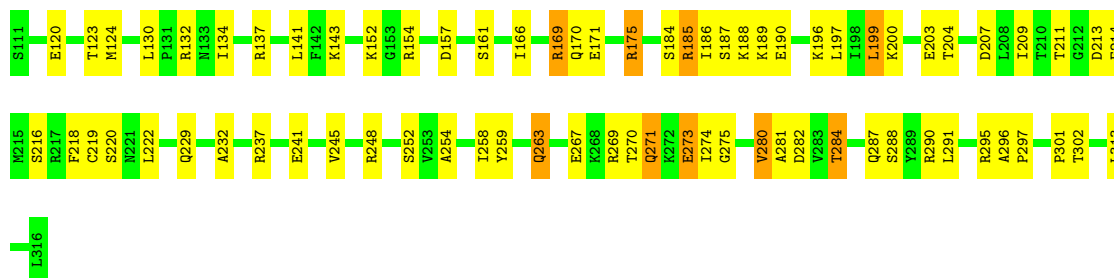
Chain B:  100%



4.2.2 Score per residue for model 2

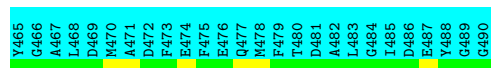
- Molecule 1: Transcription initiation factor IIB

Chain A:  65%  31% •



- Molecule 2: Alpha trans-inducing protein

Chain B:  100%



4.2.3 Score per residue for model 3

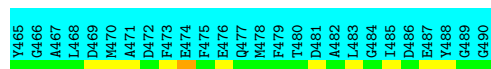
- Molecule 1: Transcription initiation factor IIB

Chain A:  66%  30% •



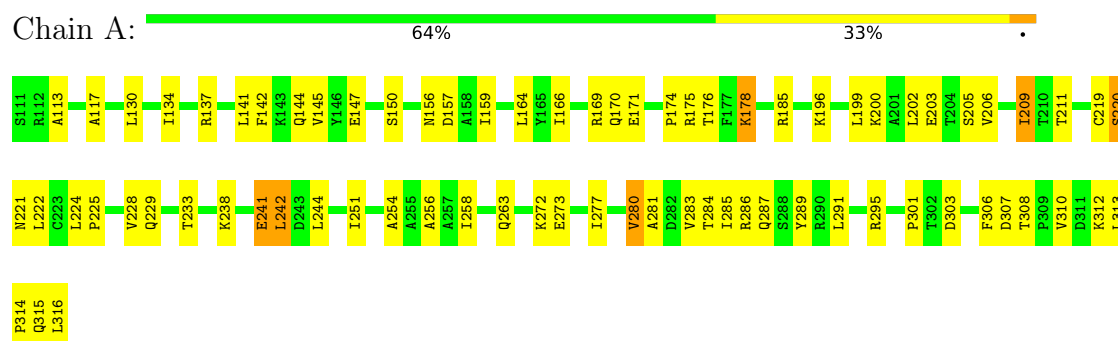
- Molecule 2: Alpha trans-inducing protein

Chain B:  100%

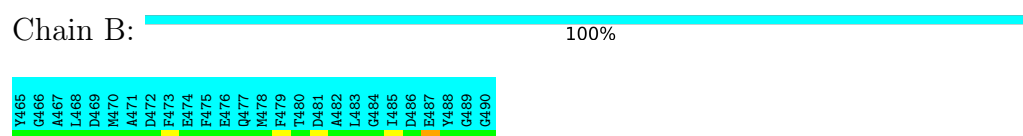


4.2.4 Score per residue for model 4

- Molecule 1: Transcription initiation factor IIB

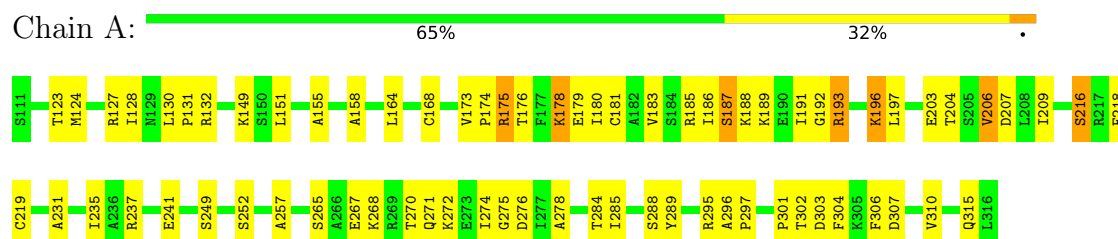


- Molecule 2: Alpha trans-inducing protein

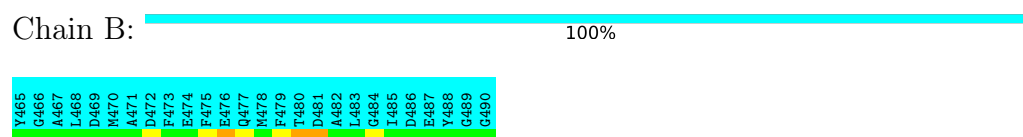


4.2.5 Score per residue for model 5

- Molecule 1: Transcription initiation factor IIB



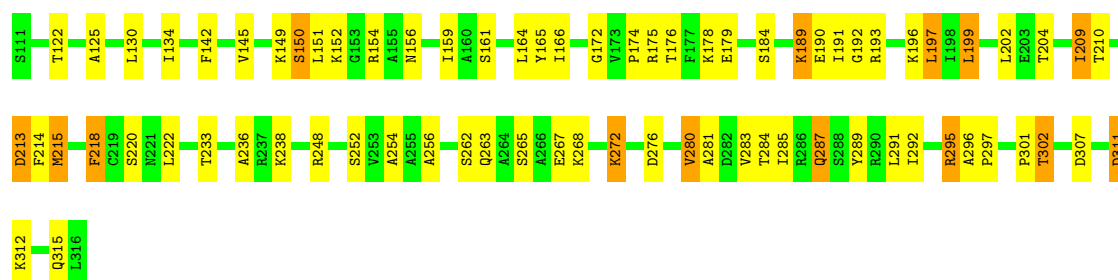
- Molecule 2: Alpha trans-inducing protein



4.2.6 Score per residue for model 6

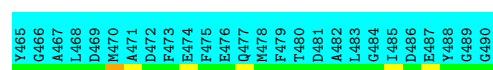
- Molecule 1: Transcription initiation factor IIB





- Molecule 2: Alpha trans-inducing protein

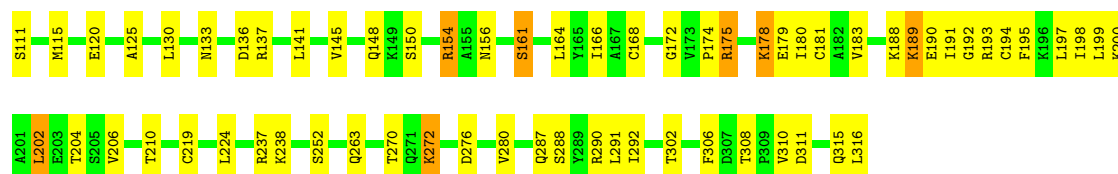
Chain B: 100%



4.2.7 Score per residue for model 7

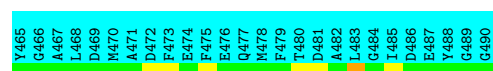
- Molecule 1: Transcription initiation factor IIB

Chain A: 69% 28%



- Molecule 2: Alpha trans-inducing protein

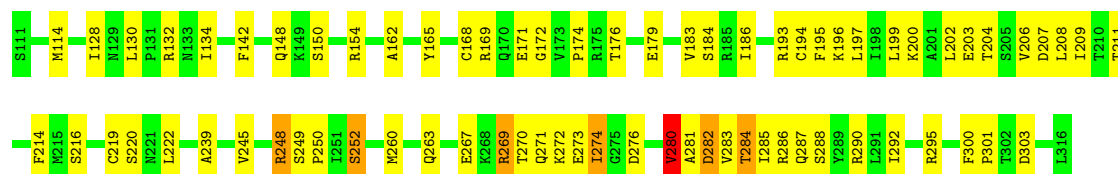
Chain B: 100%



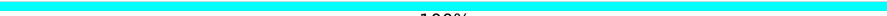
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Transcription initiation factor IIB

Chain A: 65% 32%



- Molecule 2: Alpha trans-inducing protein

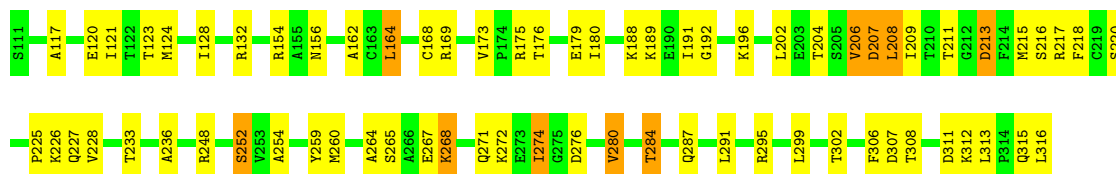
Chain B:  100%



4.2.9 Score per residue for model 9

- Molecule 1: Transcription initiation factor IIB

Chain A:  66%  29%  5%



- Molecule 2: Alpha trans-inducing protein

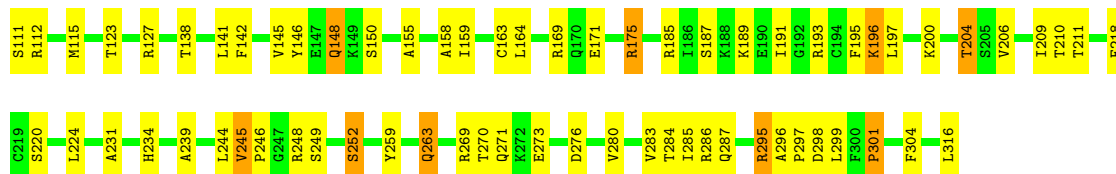
Chain B:  100%



4.2.10 Score per residue for model 10

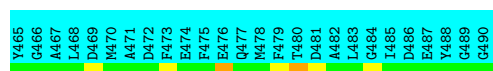
- Molecule 1: Transcription initiation factor IIB

Chain A:  67%  28%  5%



- Molecule 2: Alpha trans-inducing protein

Chain B:  100%



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.

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	290

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: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:124:MET:HE1	1:A:161:SER:HA	0.58	1.74	2	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:111:SER:N	1:A:146:TYR:HH	0.55	1.98	10	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:315:GLN:O	1:A:316:LEU:HB3	0.55	2.02	3	1
1:A:281:ALA:HB3	1:A:284:THR:CB	0.55	2.29	8	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:ARG:HD2	1:A:167:ALA:HA	0.53	1.80	1	1
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:175:ARG:HG2	1:A:316:LEU:HB3	0.51	1.82	4	1
1:A:226:LYS:HA	1:A:226:LYS:HE2	0.51	1.82	9	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:213:ASP:HB2	1:A:280:VAL:HG22	0.50	1.83	2	1
1:A:123:THR:O	1:A:127:ARG:HG2	0.50	2.05	5	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:170:GLN:HA	1:A:282:ASP:HB2	0.49	1.84	2	1
1:A:174:PRO:O	1:A:175:ARG:HB2	0.49	2.07	4	2
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:222:LEU:HB2	1:A:273:GLU:OE1	0.49	2.08	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:165:TYR:O	1:A:169:ARG:HB3	0.49	2.08	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:175:ARG:HB3	1:A:268:LYS:HA	0.48	1.83	1	1
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:145:VAL:HG21	1:A:159:ILE:HG21	0.48	1.85	4	1
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:220:SER:HB3	1:A:224:LEU:HB3	0.48	1.83	4	1
1:A:185:ARG:HD3	1:A:186:ILE:HG22	0.48	1.86	2	1
1:A:128:ILE:HB	1:A:130:LEU:HG	0.48	1.85	8	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:142:PHE:HA	1:A:145:VAL:HG22	0.47	1.86	4	1
1:A:225:PRO:HG2	1:A:228:VAL:HG23	0.47	1.87	4	2
1:A:289:TYR:HE2	1:A:315:GLN:HA	0.47	1.69	5	1
1:A:252:SER:CB	1:A:284:THR:HG23	0.47	2.40	8	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:166:ILE:HD11	1:A:195:PHE:HA	0.46	1.88	7	1
1:A:155:ALA:HB1	1:A:158:ALA:HB3	0.46	1.88	10	1
1:A:120:GLU:HA	1:A:120:GLU:OE1	0.46	2.10	2	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:256:ALA:HA	1:A:285:ILE:HG23	0.45	1.88	4	1
1:A:175:ARG:HG3	1:A:267:GLU:O	0.45	2.10	2	1
1:A:186:ILE:HG12	1:A:187:SER:H	0.45	1.70	5	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:158:ALA:HA	1:A:191:ILE:CG1	0.45	2.41	10	1
1:A:259:TYR:HE2	1:A:316:LEU:HD13	0.45	1.71	10	1
1:A:149:LYS:HB2	1:A:151:LEU:HG	0.45	1.86	5	1
1:A:213:ASP:HA	1:A:218:PHE:CZ	0.45	2.47	9	2
1:A:175:ARG:HD2	1:A:179:GLU:CD	0.45	2.36	7	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: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: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:184:SER:HB3	1:A:188:LYS:HG3	0.44	1.89	2	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: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:260:MET:HE1	1:A:300:PHE:HZ	0.43	1.72	8	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:206:VAL:HG22	1:A:207:ASP:N	0.43	2.27	5	1
1:A:269:ARG:HG2	1:A:274:ILE:HD12	0.43	1.89	8	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:H	1:A:291:LEU:HD23	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:280:VAL:HG12	1:A:284:THR:CG2	0.42	2.45	9	1
1:A:232:ALA:CB	1:A:258:ILE:HA	0.42	2.44	2	1
1:A:113:ALA:HB1	1:A:156:ASN:HB3	0.42	1.90	4	1
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:166:ILE:O	1:A:169:ARG:HG3	0.42	2.14	4	1
1:A:193:ARG:O	1:A:197:LEU:HG	0.42	2.15	10	2
1:A:236:ALA:HB1	1:A:254:ALA:HA	0.42	1.91	9	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:304:PHE:HD1	1:A:306:PHE:H	0.42	1.57	5	1
1:A:189:LYS:O	1:A:193:ARG:HB2	0.42	2.15	6	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:176:THR:HG22	1:A:179:GLU:HG2	0.41	1.91	8	1
1:A:175:ARG:HD3	1:A:179:GLU:OE1	0.41	2.16	9	1
1:A:310:VAL:HG21	1:A:313:LEU:HD22	0.41	1.90	4	1
1:A:124:MET:HE2	1:A:183:VAL:HG21	0.41	1.92	5	1
1:A:235:ILE:HB	1:A:257:ALA:HB1	0.41	1.91	5	1
1:A:262:SER:O	1:A:267:GLU:HB2	0.41	2.15	6	1
1:A:248:ARG:HD2	1:A:287:GLN:OE1	0.41	2.15	8	1
1:A:231:ALA:HB1	1:A:304:PHE:CD1	0.41	2.51	10	1
1:A:207:ASP:HA	1:A:281:ALA:CB	0.41	2.46	2	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:187:SER:O	1:A:191:ILE:HG13	0.41	2.15	1	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:151:LEU:HD21	1:A:191:ILE:HA	0.41	1.92	6	1
1:A:180:ILE:O	1:A:183:VAL:HG12	0.41	2.16	7	1
1:A:178:LYS:HD2	1:A:310:VAL:HG13	0.41	1.92	5	1
1:A:256:ALA:HB2	1:A:285:ILE:HG23	0.41	1.90	6	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:234:HIS:HB3	1:A:301:PRO:HG3	0.41	1.91	10	1
1:A:245:VAL:H	1:A:246:PRO:HD2	0.41	1.76	10	1
1:A:263:GLN:HA	1:A:263:GLN:OE1	0.41	2.15	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:215:MET:SD	1:A:217:ARG:HB2	0.41	2.56	9	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
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:222:LEU:HD22	1:A:273:GLU:CB	0.40	2.47	2	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:259:TYR:CD1	1:A:274:ILE:HG21	0.40	2.51	9	1
1:A:148:GLN:HG3	1:A:150:SER:H	0.40	1.76	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:145:VAL:CG1	1:A:198:ILE:HG12	0.40	2.40	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

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	204/206 (99%)	173±3 (85±2%)	25±3 (12±1%)	6±2 (3±1%)	5	37
2	B	0	-	-	-	-	-
All	All	2040/2320 (88%)	1727 (85%)	249 (12%)	64 (3%)	5	37

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

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Mol	Chain	Res	Type	Models (Total)
1	A	295	ARG	6
1	A	280	VAL	4
1	A	175	ARG	4
1	A	206	VAL	4
1	A	302	THR	3
1	A	154	ARG	3
1	A	208	LEU	3
1	A	311	ASP	3
1	A	183	VAL	2
1	A	274	ILE	2
1	A	176	THR	1
1	A	275	GLY	1
1	A	306	PHE	1
1	A	171	GLU	1
1	A	251	ILE	1
1	A	314	PRO	1
1	A	150	SER	1
1	A	222	LEU	1
1	A	297	PRO	1
1	A	315	GLN	1
1	A	186	ILE	1
1	A	207	ASP	1
1	A	187	SER	1
1	A	245	VAL	1
1	A	248	ARG	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%)	148±5 (85±3%)	27±5 (15±3%)	5 41
2	B	0	-	-	-
All	All	1750/1940 (90%)	1481 (85%)	269 (15%)	5 41

All 103 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	204	THR	7
1	A	211	THR	7
1	A	220	SER	7
1	A	270	THR	6
1	A	287	GLN	6
1	A	164	LEU	6
1	A	150	SER	5
1	A	203	GLU	5
1	A	233	THR	5
1	A	263	GLN	5
1	A	284	THR	5
1	A	295	ARG	5
1	A	302	THR	5
1	A	196	LYS	5
1	A	271	GLN	5
1	A	202	LEU	5
1	A	291	LEU	5
1	A	178	LYS	4
1	A	184	SER	4
1	A	248	ARG	4
1	A	269	ARG	4
1	A	132	ARG	4
1	A	200	LYS	4
1	A	214	PHE	4
1	A	210	THR	4
1	A	303	ASP	4
1	A	171	GLU	3
1	A	175	ARG	3
1	A	290	ARG	3
1	A	185	ARG	3
1	A	218	PHE	3
1	A	161	SER	3
1	A	219	CYS	3
1	A	249	SER	3
1	A	272	LYS	3
1	A	280	VAL	3
1	A	308	THR	3
1	A	267	GLU	3
1	A	268	LYS	3
1	A	143	LYS	2
1	A	242	LEU	2
1	A	123	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	152	LYS	2
1	A	157	ASP	2
1	A	169	ARG	2
1	A	199	LEU	2
1	A	229	GLN	2
1	A	111	SER	2
1	A	145	VAL	2
1	A	193	ARG	2
1	A	260	MET	2
1	A	282	ASP	2
1	A	316	LEU	2
1	A	286	ARG	2
1	A	289	TYR	2
1	A	306	PHE	2
1	A	179	GLU	2
1	A	197	LEU	2
1	A	216	SER	2
1	A	285	ILE	2
1	A	288	SER	2
1	A	154	ARG	2
1	A	189	LYS	2
1	A	213	ASP	2
1	A	238	LYS	2
1	A	292	ILE	2
1	A	115	MET	2
1	A	120	GLU	2
1	A	124	MET	1
1	A	243	ASP	1
1	A	137	ARG	1
1	A	259	TYR	1
1	A	273	GLU	1
1	A	180	ILE	1
1	A	198	ILE	1
1	A	144	GLN	1
1	A	147	GLU	1
1	A	209	ILE	1
1	A	221	ASN	1
1	A	241	GLU	1
1	A	307	ASP	1
1	A	187	SER	1
1	A	122	THR	1
1	A	149	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	165	TYR	1
1	A	190	GLU	1
1	A	215	MET	1
1	A	311	ASP	1
1	A	156	ASN	1
1	A	194	CYS	1
1	A	224	LEU	1
1	A	237	ARG	1
1	A	208	LEU	1
1	A	227	GLN	1
1	A	299	LEU	1
1	A	312	LYS	1
1	A	315	GLN	1
1	A	112	ARG	1
1	A	148	GLN	1
1	A	244	LEU	1
1	A	276	ASP	1
1	A	298	ASP	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 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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided