



Full wwPDB NMR Structure Validation Report ⓘ

Feb 28, 2026 – 06:52 PM UTC

PDB ID : 2RQF / pdb_00002rqf
Title : Solution structure of juvenile hormone binding protein from silkworm in complex with JH III
Authors : Suzuki, R.; Fujimoto, Z.; Shiotsuki, T.; Momma, M.; Tase, A.; Yamazaki, T.
Deposited on : 2009-04-27

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
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

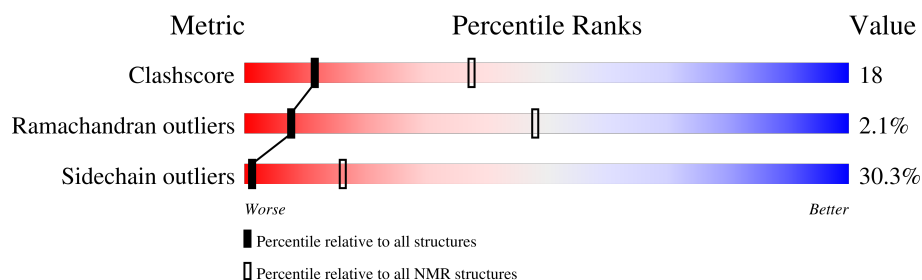
1 Overall quality at a glance

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	227	 54% 35% 7% ..

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 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:5-A:225 (221)	0.38	1

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 4 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 6, 7, 11, 19
2	9, 13, 18, 20
3	5, 12, 17
4	10, 14
Single-model clusters	8; 15; 16

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3521 atoms, of which 1766 are hydrogens and 0 are deuteriums.

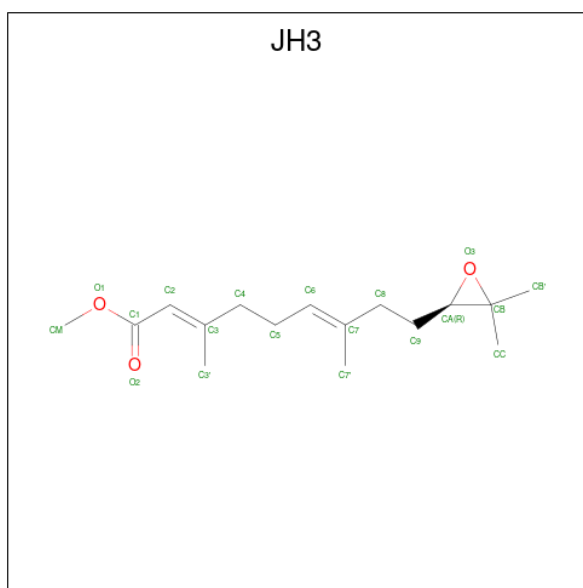
- Molecule 1 is a protein called Hemolymph juvenile hormone binding protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	227	3476	1094	1740	285	349	8	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9U556
A	-1	SER	-	expression tag	UNP Q9U556

- Molecule 2 is methyl (2E,6E)-9-[(2R)-3,3-dimethyloxiran-2-yl]-3,7-dimethylnona-2,6-dienoate (CCD ID: JH3) (formula: C₁₆H₂₆O₃).



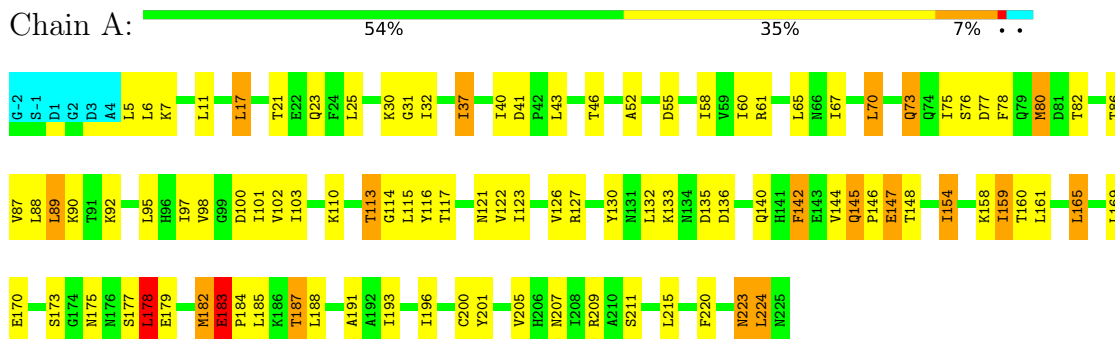
Mol	Chain	Residues	Atoms			
			Total	C	H	O
2	A	1	45	16	26	3

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: Hemolymph juvenile hormone binding protein

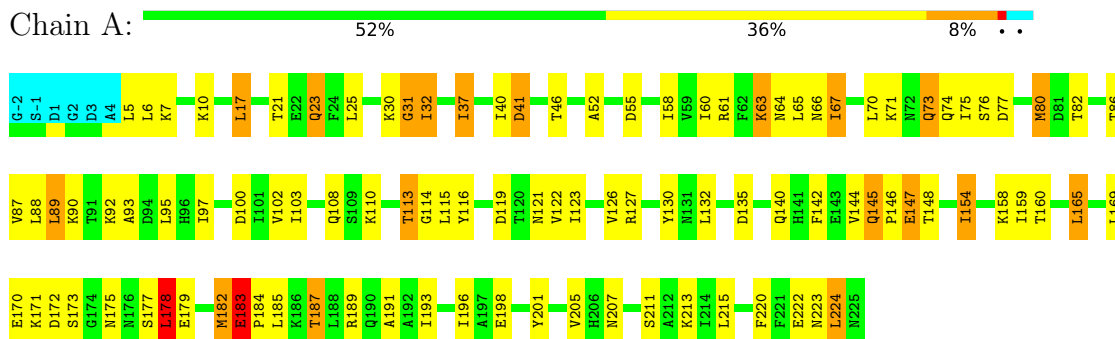


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

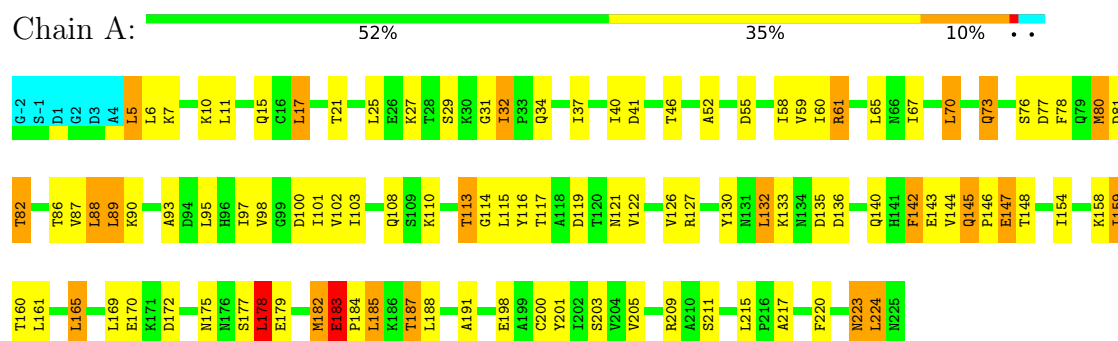
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Hemolymph juvenile hormone binding protein



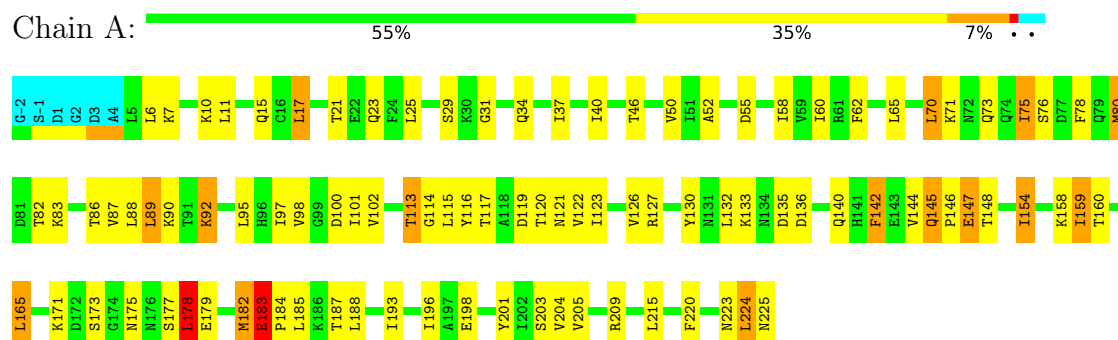
4.2.2 Score per residue for model 2

- Molecule 1: Hemolymph juvenile hormone binding protein



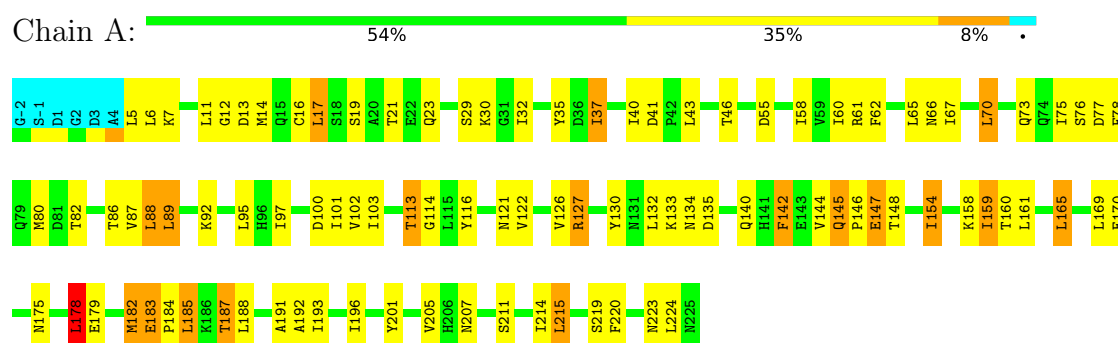
4.2.3 Score per residue for model 3

- Molecule 1: Hemolymph juvenile hormone binding protein



4.2.4 Score per residue for model 4

- Molecule 1: Hemolymph juvenile hormone binding protein



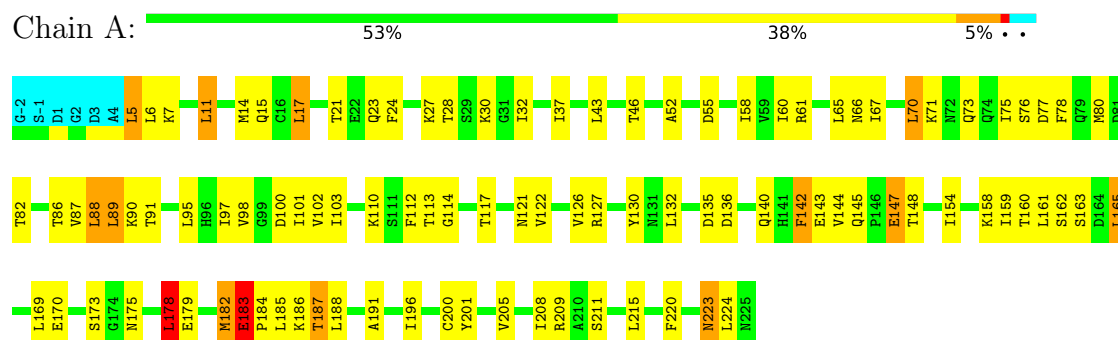
4.2.5 Score per residue for model 5

- Molecule 1: Hemolymph juvenile hormone binding protein



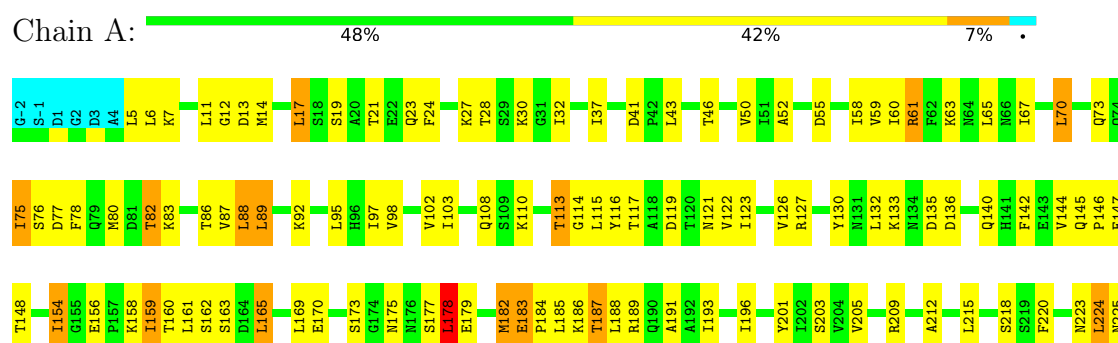
4.2.6 Score per residue for model 6

- Molecule 1: Hemolymph juvenile hormone binding protein



4.2.7 Score per residue for model 7

- Molecule 1: Hemolymph juvenile hormone binding protein



4.2.8 Score per residue for model 8

- Molecule 1: Hemolymph juvenile hormone binding protein



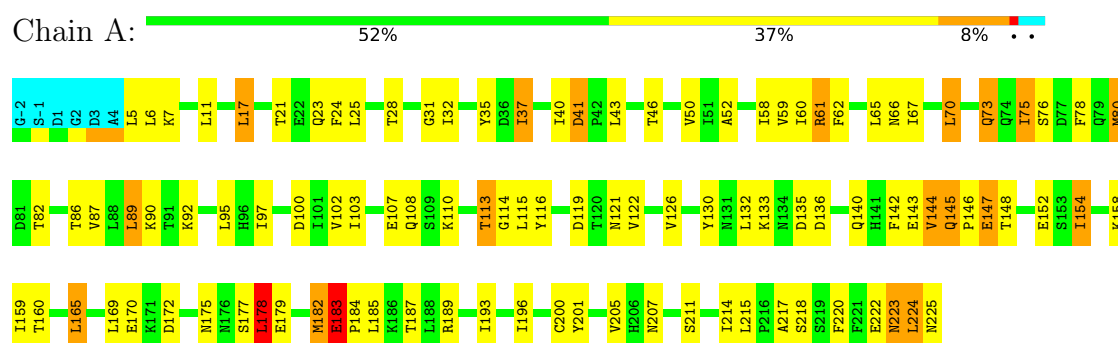
4.2.9 Score per residue for model 9

- Molecule 1: Hemolymph juvenile hormone binding protein



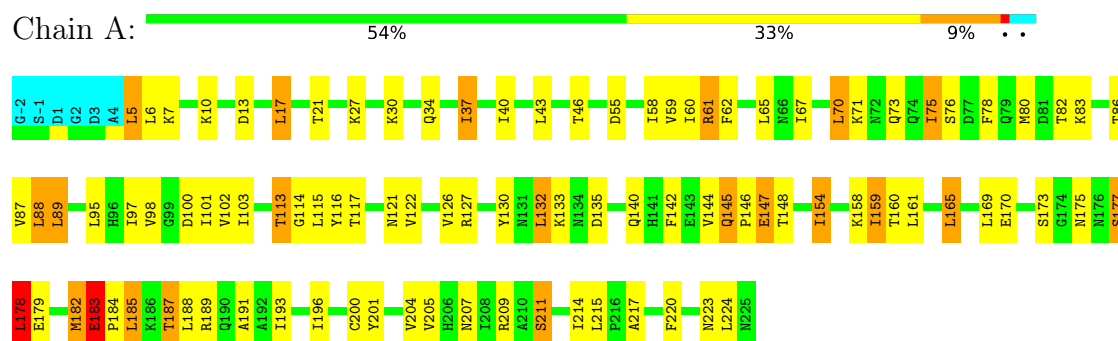
4.2.10 Score per residue for model 10

- Molecule 1: Hemolymph juvenile hormone binding protein



4.2.11 Score per residue for model 11

- Molecule 1: Hemolymph juvenile hormone binding protein



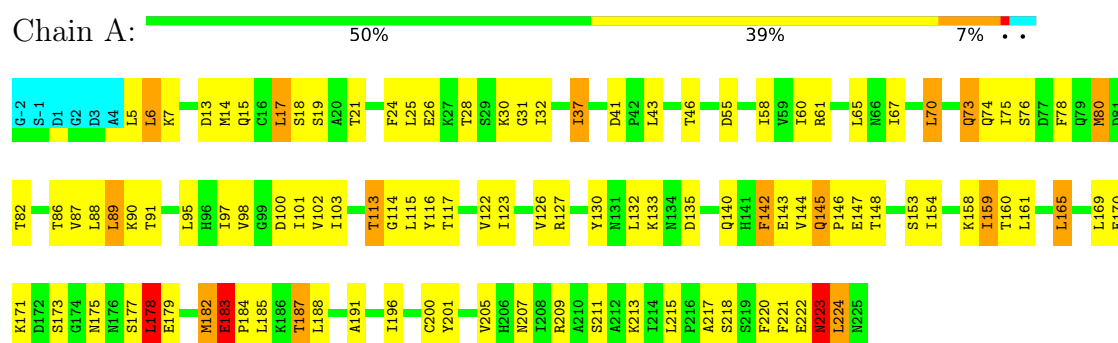
4.2.12 Score per residue for model 12

- Molecule 1: Hemolymph juvenile hormone binding protein



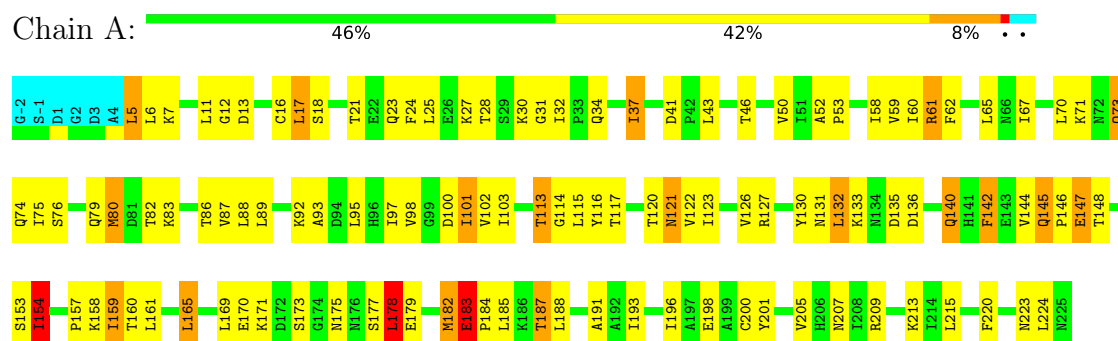
4.2.13 Score per residue for model 13

- Molecule 1: Hemolymph juvenile hormone binding protein



4.2.14 Score per residue for model 14

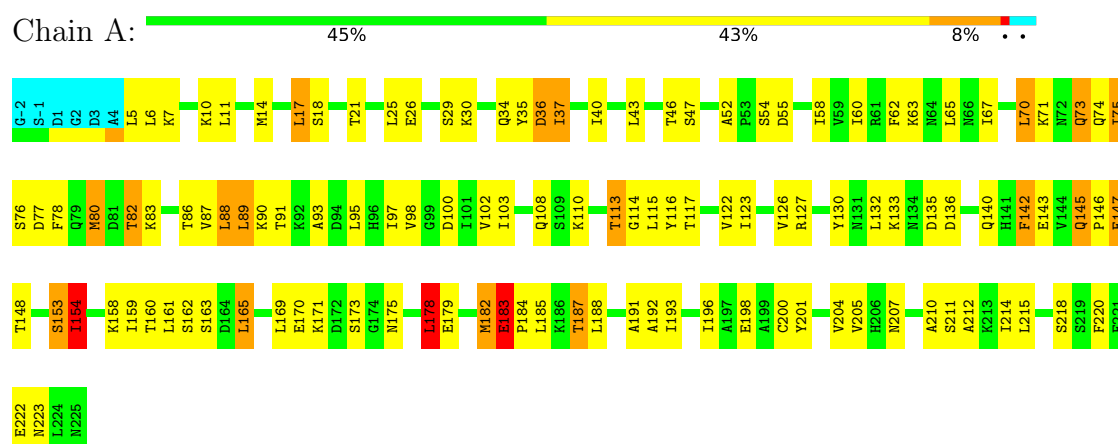
- Molecule 1: Hemolymph juvenile hormone binding protein



- Molecule 1: Hemolymph juvenile hormone binding protein

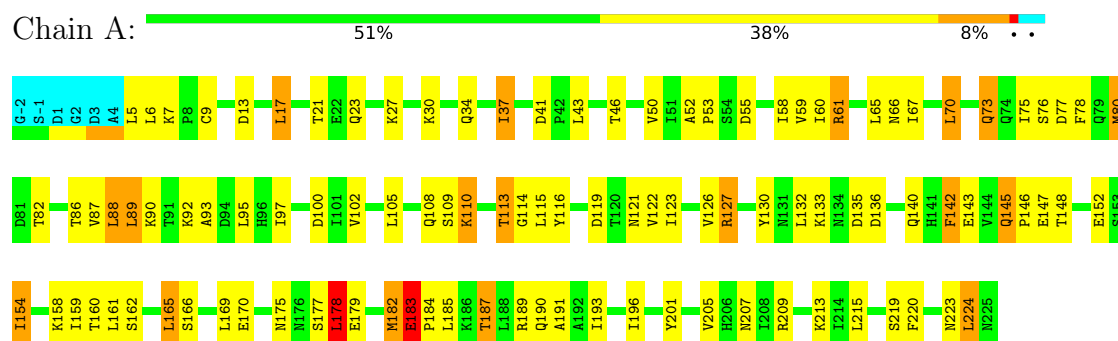


- Molecule 1: Hemolymph juvenile hormone binding protein



4.2.17 Score per residue for model 17

- Molecule 1: Hemolymph juvenile hormone binding protein



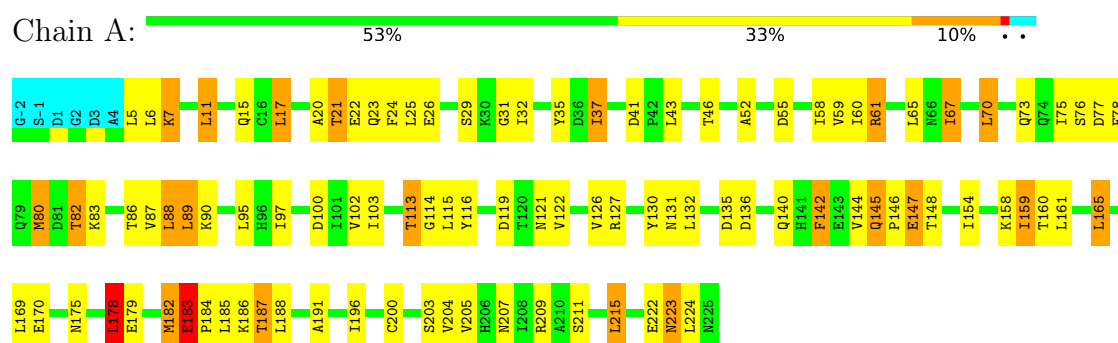
4.2.18 Score per residue for model 18

- Molecule 1: Hemolymph juvenile hormone binding protein



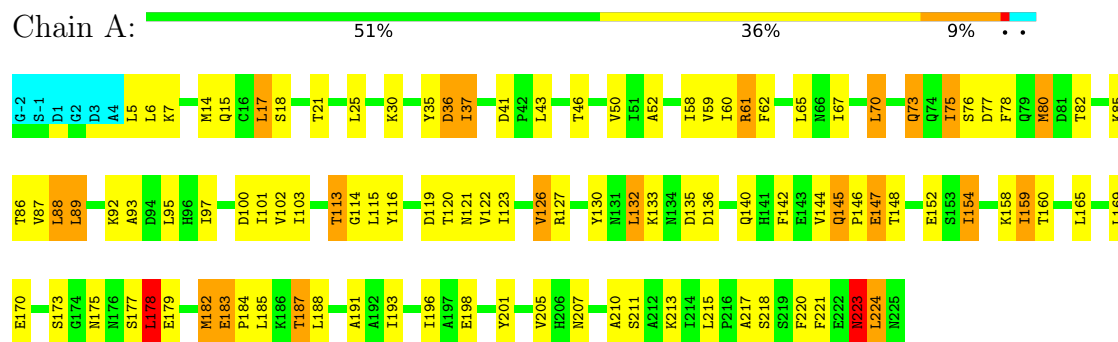
4.2.19 Score per residue for model 19

- Molecule 1: Hemolymph juvenile hormone binding protein



4.2.20 Score per residue for model 20

- Molecule 1: Hemolymph juvenile hormone binding protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

No chemical shift data was provided.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: JH3

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	1701	1716	1716	60±7
2	A	19	26	26	7±2
All	All	34400	34840	34840	1225

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LEU:HD12	1:A:95:LEU:HD21	0.95	1.37	19	19
1:A:144:VAL:HG12	2:A:300:JH3:HB'	0.93	1.37	19	8
1:A:25:LEU:HD21	1:A:204:VAL:HG13	0.92	1.39	12	2
1:A:102:VAL:HG22	1:A:113:THR:HG23	0.91	1.43	13	19
1:A:17:LEU:HD11	2:A:300:JH3:H3'	0.86	1.46	9	18
1:A:95:LEU:HD12	1:A:122:VAL:HG21	0.83	1.47	16	19
1:A:132:LEU:HD21	1:A:224:LEU:HD22	0.83	1.48	11	3
1:A:11:LEU:HD23	1:A:80:MET:HE2	0.81	1.50	2	3
1:A:70:LEU:HD13	1:A:95:LEU:HD21	0.75	1.58	14	1
1:A:75:ILE:HD11	1:A:89:LEU:HD13	0.74	1.58	7	2
1:A:154:ILE:HG22	1:A:193:ILE:HG21	0.74	1.60	18	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:217:ALA:HB1	1:A:224:LEU:HD13	0.73	1.61	11	4
1:A:67:ILE:HG22	1:A:95:LEU:HD22	0.71	1.60	19	12
1:A:89:LEU:HD11	2:A:300:JH3:HMA	0.71	1.62	2	4
1:A:187:THR:HG22	1:A:191:ALA:HB2	0.70	1.64	15	15
1:A:221:PHE:CE2	1:A:224:LEU:HD12	0.69	2.21	18	2
1:A:142:PHE:CD1	2:A:300:JH3:HB'B	0.69	2.23	3	12
1:A:80:MET:HE2	1:A:130:TYR:CZ	0.67	2.25	7	1
1:A:31:GLY:O	1:A:32:ILE:HD13	0.67	1.90	15	2
2:A:300:JH3:C2	2:A:300:JH3:H7'B	0.67	2.20	19	18
1:A:62:PHE:CE2	1:A:101:ILE:HD12	0.66	2.25	14	1
1:A:37:ILE:HG22	1:A:207:ASN:CG	0.66	2.15	4	12
1:A:58:ILE:HG21	1:A:184:PRO:HB3	0.66	1.67	16	10
1:A:11:LEU:HD12	1:A:223:ASN:OD1	0.66	1.91	5	1
1:A:37:ILE:HG22	1:A:207:ASN:CB	0.65	2.21	10	12
1:A:35:TYR:CD1	1:A:214:ILE:HD13	0.65	2.26	18	1
1:A:142:PHE:CE2	1:A:224:LEU:HD11	0.65	2.27	8	3
1:A:95:LEU:HD12	1:A:122:VAL:CG2	0.65	2.21	7	19
1:A:142:PHE:CZ	1:A:224:LEU:HD11	0.64	2.26	11	3
1:A:87:VAL:HG23	1:A:130:TYR:CD1	0.64	2.27	13	19
1:A:35:TYR:CZ	1:A:214:ILE:HG21	0.64	2.28	9	2
1:A:60:ILE:HD12	1:A:103:ILE:CD1	0.64	2.23	12	9
1:A:25:LEU:HD21	1:A:204:VAL:CG1	0.64	2.21	12	1
1:A:17:LEU:CD1	2:A:300:JH3:H3'	0.63	2.22	12	18
1:A:31:GLY:C	1:A:32:ILE:HD13	0.63	2.17	1	2
1:A:65:LEU:HD22	1:A:97:ILE:CG2	0.63	2.24	9	20
1:A:60:ILE:HG23	1:A:103:ILE:HD13	0.63	1.71	2	8
1:A:142:PHE:CD2	2:A:300:JH3:HCA	0.63	2.28	4	1
1:A:161:LEU:HD12	1:A:178:LEU:CD1	0.63	2.24	9	7
1:A:144:VAL:HG11	1:A:209:ARG:HA	0.63	1.70	8	7
1:A:89:LEU:HD11	2:A:300:JH3:CM	0.62	2.24	16	16
1:A:102:VAL:CG2	1:A:113:THR:HG23	0.62	2.22	12	8
1:A:80:MET:HB2	1:A:87:VAL:HG22	0.62	1.70	4	1
1:A:80:MET:HE1	1:A:224:LEU:HD21	0.62	1.70	15	4
1:A:58:ILE:HG22	1:A:60:ILE:HD11	0.62	1.71	19	15
1:A:67:ILE:CG2	1:A:95:LEU:HD22	0.61	2.25	13	11
1:A:217:ALA:HB1	1:A:224:LEU:CD1	0.61	2.25	11	2
1:A:11:LEU:HD11	1:A:223:ASN:O	0.61	1.94	10	6
1:A:70:LEU:CD1	1:A:95:LEU:HD21	0.61	2.21	19	11
1:A:60:ILE:HG21	1:A:188:LEU:HD11	0.61	1.72	12	3
1:A:97:ILE:CD1	1:A:196:ILE:HD13	0.61	2.26	15	19
1:A:187:THR:O	1:A:191:ALA:HB3	0.61	1.95	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:THR:HG22	1:A:191:ALA:CB	0.61	2.25	2	11
1:A:6:LEU:HD11	1:A:220:PHE:CE2	0.61	2.31	12	2
1:A:142:PHE:CG	2:A:300:JH3:HB'B	0.61	2.30	14	6
1:A:98:VAL:HG22	1:A:117:THR:HG23	0.61	1.70	18	11
1:A:11:LEU:HD23	1:A:80:MET:CE	0.60	2.26	8	1
1:A:11:LEU:HD12	1:A:12:GLY:N	0.60	2.11	14	3
1:A:17:LEU:HD13	1:A:78:PHE:CE2	0.60	2.30	7	8
1:A:132:LEU:HD21	1:A:224:LEU:CD1	0.60	2.26	20	1
1:A:6:LEU:HD21	1:A:220:PHE:CD2	0.60	2.31	9	17
1:A:88:LEU:HD13	1:A:127:ARG:HG2	0.60	1.73	6	16
1:A:80:MET:HG3	1:A:87:VAL:HG22	0.60	1.73	10	5
1:A:14:MET:HE3	1:A:78:PHE:CE1	0.59	2.31	5	1
1:A:11:LEU:CD2	1:A:80:MET:HE2	0.59	2.25	2	2
1:A:80:MET:HE3	1:A:130:TYR:CZ	0.59	2.32	5	3
1:A:17:LEU:HD13	1:A:78:PHE:CZ	0.59	2.32	20	9
1:A:120:THR:HG21	1:A:193:ILE:HD11	0.59	1.73	18	6
1:A:25:LEU:HD13	1:A:73:GLN:OE1	0.59	1.98	13	12
1:A:17:LEU:HD22	1:A:78:PHE:CD2	0.59	2.33	16	7
1:A:154:ILE:CG2	1:A:193:ILE:HG21	0.59	2.27	14	16
1:A:132:LEU:HD21	1:A:224:LEU:HD13	0.59	1.73	18	4
1:A:18:SER:HA	1:A:75:ILE:HD12	0.59	1.74	20	3
1:A:102:VAL:HG22	1:A:113:THR:HB	0.59	1.74	6	1
1:A:89:LEU:HD11	2:A:300:JH3:HM	0.59	1.72	12	3
1:A:78:PHE:HB2	1:A:89:LEU:HD12	0.58	1.74	10	1
1:A:147:GLU:HG2	1:A:205:VAL:HG21	0.58	1.75	12	11
1:A:80:MET:CG	1:A:87:VAL:HG22	0.58	2.29	13	9
1:A:147:GLU:HG3	1:A:205:VAL:HG21	0.58	1.76	19	5
1:A:6:LEU:HD21	1:A:220:PHE:CE2	0.57	2.35	16	7
1:A:114:GLY:N	1:A:165:LEU:HD23	0.57	2.14	10	17
1:A:40:ILE:HD13	1:A:204:VAL:CG1	0.57	2.30	16	2
1:A:20:ALA:HB1	1:A:24:PHE:CZ	0.57	2.34	19	1
1:A:6:LEU:HD13	1:A:24:PHE:CZ	0.57	2.34	19	1
1:A:87:VAL:HG23	1:A:130:TYR:CD2	0.57	2.35	7	1
1:A:59:VAL:HG12	1:A:61:ARG:HD2	0.56	1.76	17	9
1:A:208:ILE:HG21	2:A:300:JH3:H7'	0.56	1.78	6	2
1:A:199:ALA:HA	1:A:202:ILE:HD12	0.56	1.76	15	1
1:A:115:LEU:HD23	1:A:116:TYR:N	0.56	2.16	5	16
1:A:208:ILE:HG22	2:A:300:JH3:HCB	0.55	1.76	5	2
1:A:37:ILE:HG22	1:A:207:ASN:HB3	0.55	1.78	17	10
1:A:159:ILE:HD13	1:A:185:LEU:HD13	0.55	1.77	4	4
1:A:32:ILE:HG22	1:A:34:GLN:HG2	0.55	1.77	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:VAL:HG23	1:A:130:TYR:CE1	0.55	2.36	14	2
1:A:144:VAL:HG21	1:A:209:ARG:HB3	0.55	1.77	15	1
1:A:17:LEU:HD13	1:A:78:PHE:CE1	0.55	2.36	18	1
1:A:114:GLY:N	1:A:165:LEU:HD12	0.55	2.17	20	1
1:A:217:ALA:O	1:A:224:LEU:HD12	0.54	2.02	8	1
1:A:24:PHE:CZ	1:A:28:THR:HG21	0.54	2.36	12	1
1:A:17:LEU:HD13	1:A:78:PHE:CD2	0.54	2.38	11	2
1:A:144:VAL:CG1	2:A:300:JH3:HB'	0.54	2.27	2	2
1:A:200:CYS:O	1:A:204:VAL:HG23	0.54	2.02	12	2
1:A:88:LEU:HD22	1:A:127:ARG:NH2	0.54	2.17	9	1
1:A:169:LEU:HD12	1:A:178:LEU:HD11	0.54	1.78	9	19
2:A:300:JH3:H7'	2:A:300:JH3:CC	0.54	2.33	14	2
1:A:114:GLY:HA3	1:A:165:LEU:HD23	0.53	1.79	3	19
1:A:60:ILE:HD12	1:A:103:ILE:HD12	0.53	1.80	2	6
1:A:5:LEU:HD23	1:A:27:LYS:CB	0.53	2.33	17	1
1:A:43:LEU:HD22	1:A:200:CYS:SG	0.53	2.43	15	3
1:A:178:LEU:CD2	1:A:182:MET:HE2	0.53	2.34	9	20
1:A:208:ILE:CG2	2:A:300:JH3:HCB	0.53	2.34	5	1
2:A:300:JH3:H7'B	2:A:300:JH3:H2	0.53	1.79	5	3
1:A:60:ILE:HG21	1:A:188:LEU:CD1	0.53	2.34	14	3
1:A:62:PHE:CD2	1:A:65:LEU:HD11	0.53	2.38	5	3
1:A:183:GLU:HA	1:A:184:PRO:C	0.52	2.30	20	20
1:A:122:VAL:HG22	1:A:193:ILE:HG23	0.52	1.79	18	6
1:A:88:LEU:HD22	1:A:127:ARG:HH11	0.52	1.64	1	1
1:A:43:LEU:HD12	1:A:44:VAL:N	0.52	2.19	8	1
1:A:114:GLY:CA	1:A:165:LEU:HD23	0.52	2.35	3	19
1:A:201:TYR:O	1:A:205:VAL:HG23	0.52	2.05	1	16
1:A:75:ILE:CD1	1:A:89:LEU:HD11	0.52	2.34	3	2
1:A:6:LEU:HD23	1:A:215:LEU:CD1	0.52	2.34	19	1
1:A:88:LEU:HD13	1:A:127:ARG:CG	0.52	2.34	3	3
1:A:43:LEU:O	1:A:67:ILE:HD12	0.52	2.04	11	15
1:A:60:ILE:HD12	1:A:103:ILE:HD13	0.52	1.82	6	3
1:A:80:MET:CE	1:A:224:LEU:HD21	0.52	2.34	12	3
1:A:223:ASN:CG	1:A:223:ASN:O	0.52	2.53	13	2
1:A:142:PHE:HB3	1:A:212:ALA:HB1	0.51	1.81	12	5
1:A:208:ILE:HG21	2:A:300:JH3:H9	0.51	1.81	5	1
1:A:101:ILE:HD11	1:A:103:ILE:HD11	0.51	1.82	18	1
1:A:82:THR:HG23	1:A:130:TYR:OH	0.51	2.04	19	5
1:A:215:LEU:HD12	1:A:219:SER:HB2	0.51	1.80	12	2
1:A:144:VAL:HA	2:A:300:JH3:HB'	0.51	1.82	7	1
1:A:58:ILE:HG23	1:A:105:LEU:CD2	0.51	2.35	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:ILE:HD13	1:A:196:ILE:HD13	0.51	1.81	11	4
1:A:103:ILE:HD13	1:A:165:LEU:HD11	0.51	1.82	1	4
1:A:58:ILE:HG21	1:A:184:PRO:CB	0.51	2.36	13	7
1:A:60:ILE:HD12	1:A:103:ILE:HG13	0.51	1.83	16	1
1:A:92:LYS:HB3	1:A:123:ILE:HG23	0.51	1.83	18	10
1:A:101:ILE:HD11	1:A:188:LEU:HD11	0.51	1.81	6	9
1:A:144:VAL:HG21	1:A:209:ARG:HG2	0.51	1.82	2	5
1:A:142:PHE:CZ	1:A:224:LEU:HD13	0.51	2.40	15	1
1:A:147:GLU:CD	1:A:205:VAL:HG21	0.51	2.31	5	2
1:A:58:ILE:HG22	1:A:60:ILE:CD1	0.50	2.37	17	4
1:A:120:THR:CG2	1:A:121:ASN:N	0.50	2.75	14	1
1:A:11:LEU:HD23	1:A:80:MET:SD	0.50	2.47	3	2
1:A:58:ILE:HG21	1:A:184:PRO:HG3	0.50	1.82	6	3
1:A:113:THR:C	1:A:165:LEU:HD23	0.50	2.32	7	18
1:A:17:LEU:HD11	1:A:78:PHE:CE2	0.49	2.42	4	1
1:A:24:PHE:O	1:A:28:THR:HG23	0.49	2.07	15	7
1:A:5:LEU:HD23	1:A:27:LYS:HB2	0.49	1.83	5	7
1:A:221:PHE:CD1	1:A:224:LEU:HD11	0.49	2.42	15	1
1:A:147:GLU:OE2	1:A:205:VAL:HG11	0.49	2.08	19	1
1:A:144:VAL:HG21	1:A:209:ARG:CG	0.49	2.37	2	6
1:A:144:VAL:HG11	1:A:209:ARG:HG2	0.49	1.85	14	1
1:A:123:ILE:HD12	1:A:153:SER:HB3	0.48	1.85	14	4
1:A:67:ILE:HG23	1:A:97:ILE:HG13	0.48	1.86	12	1
1:A:14:MET:HE3	1:A:78:PHE:CD1	0.48	2.43	5	1
2:A:300:JH3:H7'B	2:A:300:JH3:C2	0.48	2.38	5	2
1:A:52:ALA:HB3	1:A:58:ILE:HB	0.48	1.86	1	16
2:A:300:JH3:H7'	2:A:300:JH3:HCB	0.48	1.85	14	1
1:A:188:LEU:O	1:A:192:ALA:HB3	0.48	2.08	16	2
1:A:70:LEU:HD22	1:A:200:CYS:SG	0.48	2.48	15	4
1:A:159:ILE:HD11	1:A:188:LEU:HB3	0.48	1.84	12	9
1:A:88:LEU:HD13	1:A:127:ARG:HG3	0.48	1.85	4	1
1:A:127:ARG:NH2	1:A:150:THR:HG21	0.48	2.23	5	1
1:A:144:VAL:HG23	1:A:144:VAL:O	0.48	2.07	15	1
1:A:73:GLN:HA	1:A:93:ALA:HB2	0.48	1.84	8	9
1:A:88:LEU:HD22	1:A:127:ARG:NH1	0.48	2.23	1	1
1:A:31:GLY:HA2	1:A:37:ILE:HG22	0.48	1.84	12	3
1:A:35:TYR:HB2	1:A:37:ILE:HD11	0.48	1.86	15	1
1:A:103:ILE:HG22	1:A:103:ILE:O	0.47	2.09	14	1
1:A:142:PHE:CE1	2:A:300:JH3:HB'B	0.47	2.45	11	1
1:A:17:LEU:HD23	1:A:18:SER:N	0.47	2.23	13	1
1:A:120:THR:OG1	1:A:157:PRO:HA	0.47	2.08	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:MET:HE3	1:A:130:TYR:CE2	0.47	2.43	5	2
1:A:35:TYR:C	1:A:36:ASP:CG	0.47	2.82	8	3
1:A:17:LEU:CG	2:A:300:JH3:H3'	0.47	2.39	17	2
1:A:211:SER:HA	1:A:214:ILE:HD12	0.47	1.85	11	1
1:A:35:TYR:CE1	1:A:214:ILE:HG21	0.47	2.45	18	1
1:A:6:LEU:HD21	1:A:220:PHE:CG	0.47	2.45	9	2
1:A:21:THR:HG22	1:A:22:GLU:N	0.47	2.25	19	1
1:A:221:PHE:CD1	1:A:221:PHE:C	0.47	2.93	20	2
1:A:36:ASP:OD2	1:A:210:ALA:HB1	0.47	2.10	20	2
1:A:218:SER:HA	1:A:221:PHE:CE1	0.46	2.45	18	1
1:A:144:VAL:HG12	2:A:300:JH3:CB'	0.46	2.41	6	6
1:A:217:ALA:HB1	1:A:221:PHE:CE2	0.46	2.45	20	2
1:A:58:ILE:HD13	1:A:184:PRO:HB3	0.46	1.88	16	1
1:A:101:ILE:HG23	1:A:165:LEU:HD13	0.46	1.87	20	1
2:A:300:JH3:HCB	2:A:300:JH3:H7'	0.46	1.87	8	3
1:A:6:LEU:HD13	1:A:24:PHE:CE1	0.46	2.46	19	1
1:A:126:VAL:HG22	1:A:201:TYR:CE2	0.46	2.46	20	1
1:A:89:LEU:HD22	2:A:300:JH3:HMA	0.46	1.88	3	1
1:A:122:VAL:CG2	1:A:193:ILE:HG23	0.46	2.40	14	5
1:A:53:PRO:HD2	1:A:187:THR:HG21	0.46	1.88	17	2
1:A:62:PHE:HE2	1:A:101:ILE:HD12	0.46	1.70	14	1
1:A:120:THR:HG22	1:A:121:ASN:N	0.46	2.26	14	1
1:A:58:ILE:CG2	1:A:60:ILE:HD11	0.45	2.41	3	4
1:A:159:ILE:HD13	1:A:185:LEU:CD1	0.45	2.41	4	2
1:A:73:GLN:OE1	1:A:73:GLN:N	0.45	2.49	12	1
1:A:62:PHE:CG	1:A:65:LEU:HD11	0.45	2.46	10	6
1:A:78:PHE:HB3	1:A:89:LEU:HD12	0.45	1.88	3	1
1:A:25:LEU:HD22	1:A:204:VAL:HG12	0.45	1.88	3	1
1:A:101:ILE:CD1	1:A:188:LEU:HD11	0.45	2.40	13	5
1:A:89:LEU:HG	2:A:300:JH3:H3'B	0.45	1.87	15	1
1:A:145:GLN:CB	1:A:146:PRO:HD2	0.45	2.41	15	17
1:A:161:LEU:HD12	1:A:178:LEU:HD11	0.45	1.87	9	1
1:A:144:VAL:HG11	1:A:209:ARG:CG	0.45	2.42	14	1
1:A:60:ILE:HG22	1:A:62:PHE:CE1	0.45	2.47	5	2
1:A:103:ILE:HG22	1:A:105:LEU:HD21	0.45	1.86	18	1
1:A:105:LEU:HD12	1:A:110:LYS:HD2	0.45	1.88	17	2
1:A:161:LEU:HD12	1:A:169:LEU:HD12	0.45	1.88	4	3
1:A:161:LEU:CD1	1:A:169:LEU:HD12	0.45	2.41	12	6
1:A:177:SER:O	1:A:178:LEU:C	0.45	2.59	3	9
1:A:25:LEU:HD22	1:A:204:VAL:CG1	0.44	2.42	3	1
1:A:223:ASN:HD22	1:A:223:ASN:N	0.44	2.10	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:ILE:HG21	1:A:185:LEU:CD1	0.44	2.43	12	3
1:A:24:PHE:CE1	1:A:28:THR:HG21	0.44	2.47	6	2
1:A:40:ILE:C	1:A:40:ILE:HD12	0.44	2.38	1	1
1:A:35:TYR:CD2	1:A:214:ILE:HD13	0.44	2.48	9	2
1:A:87:VAL:HG13	1:A:89:LEU:HD23	0.44	1.90	14	1
1:A:40:ILE:HD12	1:A:41:ASP:HB2	0.43	1.90	10	2
1:A:60:ILE:HG23	1:A:103:ILE:CD1	0.43	2.42	11	5
1:A:80:MET:HE2	1:A:130:TYR:CE2	0.43	2.48	14	1
1:A:40:ILE:HD12	1:A:40:ILE:C	0.43	2.38	10	1
1:A:11:LEU:HD21	1:A:80:MET:CE	0.43	2.43	16	1
1:A:80:MET:CB	1:A:87:VAL:HG22	0.43	2.41	4	1
1:A:208:ILE:CG2	2:A:300:JH3:H7'	0.43	2.44	12	1
1:A:87:VAL:CG1	1:A:89:LEU:HD23	0.43	2.43	15	1
1:A:21:THR:CG2	1:A:22:GLU:N	0.43	2.81	12	1
1:A:59:VAL:HG12	1:A:61:ARG:CD	0.43	2.43	14	2
1:A:102:VAL:C	1:A:103:ILE:HD12	0.43	2.39	14	1
1:A:58:ILE:HG23	1:A:105:LEU:HD23	0.43	1.91	9	1
1:A:187:THR:HG22	1:A:191:ALA:HB3	0.43	1.89	16	1
1:A:116:TYR:CE2	1:A:188:LEU:HD12	0.43	2.49	4	1
1:A:35:TYR:CB	1:A:37:ILE:HD12	0.42	2.44	8	1
1:A:87:VAL:HG12	1:A:89:LEU:HD23	0.42	1.90	13	2
1:A:101:ILE:CD1	1:A:103:ILE:HD11	0.42	2.43	18	1
1:A:6:LEU:HD12	1:A:7:LYS:H	0.42	1.74	19	1
1:A:17:LEU:HD11	2:A:300:JH3:C3'	0.42	2.40	19	1
1:A:132:LEU:HD22	1:A:140:GLN:HE21	0.42	1.75	14	1
1:A:87:VAL:HG23	1:A:130:TYR:HD2	0.42	1.73	7	1
1:A:32:ILE:HG22	1:A:34:GLN:HG3	0.42	1.91	2	1
1:A:35:TYR:CD2	1:A:214:ILE:HD12	0.42	2.49	10	1
1:A:87:VAL:HG23	1:A:130:TYR:HD1	0.42	1.74	19	1
1:A:142:PHE:CG	2:A:300:JH3:HCA	0.42	2.50	19	1
1:A:189:ARG:O	1:A:193:ILE:HD13	0.42	2.15	1	3
1:A:123:ILE:HD12	1:A:153:SER:CB	0.42	2.45	16	1
1:A:103:ILE:O	1:A:103:ILE:HG22	0.42	2.14	16	1
1:A:144:VAL:O	1:A:144:VAL:HG23	0.42	2.14	6	2
1:A:65:LEU:HD22	1:A:97:ILE:HG22	0.42	1.92	16	1
1:A:43:LEU:HD23	1:A:200:CYS:SG	0.42	2.55	16	8
1:A:189:ARG:HA	1:A:193:ILE:HD13	0.41	1.92	8	1
1:A:63:LYS:O	1:A:64:ASN:C	0.41	2.63	1	1
1:A:7:LYS:HE2	1:A:20:ALA:HB2	0.41	1.92	15	1
1:A:40:ILE:HD13	1:A:204:VAL:HG12	0.41	1.92	16	1
1:A:75:ILE:HG12	1:A:89:LEU:HD11	0.41	1.93	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:VAL:O	1:A:144:VAL:HG22	0.41	2.14	10	1
1:A:166:SER:HA	1:A:178:LEU:HD12	0.41	1.92	12	1
1:A:142:PHE:CE2	1:A:224:LEU:HD13	0.41	2.50	15	1
1:A:11:LEU:HD11	1:A:224:LEU:HA	0.41	1.92	5	1
1:A:17:LEU:HD22	1:A:78:PHE:CD1	0.41	2.51	5	1
1:A:36:ASP:OD2	1:A:214:ILE:HD11	0.41	2.15	16	1
1:A:80:MET:HG2	1:A:87:VAL:HG22	0.40	1.93	13	1
1:A:70:LEU:HD12	1:A:95:LEU:CD2	0.40	2.31	3	1
1:A:35:TYR:CE2	1:A:214:ILE:HG21	0.40	2.51	9	1
1:A:222:GLU:C	1:A:223:ASN:CG	0.40	2.89	18	1
1:A:142:PHE:CB	1:A:212:ALA:HB1	0.40	2.47	12	1
1:A:128:TYR:CD1	1:A:128:TYR:C	0.40	3.00	5	1
1:A:70:LEU:HD13	1:A:200:CYS:SG	0.40	2.57	12	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	220/227 (97%)	195±2 (89±1%)	20±2 (9±1%)	5±1 (2±0%)	8	48
All	All	4400/4540 (97%)	3905 (89%)	401 (9%)	94 (2%)	8	48

All 8 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	135	ASP	20
1	A	140	GLN	20
1	A	178	LEU	20
1	A	183	GLU	20
1	A	31	GLY	8
1	A	154	ILE	3
1	A	223	ASN	2
1	A	177	SER	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	195/198 (98%)	136±4 (70±2%)	59±4 (30±2%)	1	16
All	All	3900/3960 (98%)	2717 (70%)	1183 (30%)	1	16

All 120 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	7	LYS	20
1	A	17	LEU	20
1	A	46	THR	20
1	A	76	SER	20
1	A	82	THR	20
1	A	86	THR	20
1	A	126	VAL	20
1	A	148	THR	20
1	A	154	ILE	20
1	A	158	LYS	20
1	A	159	ILE	20
1	A	160	THR	20
1	A	178	LEU	20
1	A	179	GLU	20
1	A	182	MET	20
1	A	185	LEU	20
1	A	187	THR	20
1	A	215	LEU	20
1	A	21	THR	19
1	A	73	GLN	19
1	A	113	THR	19
1	A	145	GLN	19
1	A	165	LEU	19
1	A	175	ASN	19
1	A	223	ASN	19
1	A	80	MET	18
1	A	89	LEU	18
1	A	132	LEU	18
1	A	170	GLU	18

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Mol	Chain	Res	Type	Models (Total)
1	A	100	ASP	17
1	A	121	ASN	17
1	A	224	LEU	17
1	A	70	LEU	17
1	A	30	LYS	16
1	A	37	ILE	16
1	A	61	ARG	16
1	A	75	ILE	16
1	A	183	GLU	16
1	A	133	LYS	16
1	A	55	ASP	15
1	A	147	GLU	14
1	A	173	SER	14
1	A	142	PHE	14
1	A	23	GLN	13
1	A	32	ILE	13
1	A	41	ASP	13
1	A	90	LYS	13
1	A	211	SER	13
1	A	136	ASP	13
1	A	77	ASP	11
1	A	5	LEU	10
1	A	108	GLN	10
1	A	119	ASP	10
1	A	177	SER	10
1	A	198	GLU	10
1	A	29	SER	10
1	A	88	LEU	10
1	A	143	GLU	10
1	A	110	LYS	9
1	A	213	LYS	9
1	A	40	ILE	8
1	A	83	LYS	8
1	A	13	ASP	8
1	A	14	MET	8
1	A	71	LYS	7
1	A	15	GLN	7
1	A	203	SER	7
1	A	34	GLN	7
1	A	50	VAL	7
1	A	163	SER	7
1	A	218	SER	7

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Mol	Chain	Res	Type	Models (Total)
1	A	10	LYS	6
1	A	63	LYS	6
1	A	222	GLU	6
1	A	162	SER	6
1	A	91	THR	6
1	A	66	ASN	5
1	A	171	LYS	5
1	A	92	LYS	5
1	A	19	SER	5
1	A	152	GLU	5
1	A	11	LEU	5
1	A	74	GLN	4
1	A	225	ASN	4
1	A	127	ARG	4
1	A	67	ILE	3
1	A	144	VAL	3
1	A	172	ASP	3
1	A	186	LYS	3
1	A	36	ASP	3
1	A	189	ARG	3
1	A	26	GLU	3
1	A	16	CYS	2
1	A	109	SER	2
1	A	190	GLN	2
1	A	6	LEU	2
1	A	101	ILE	2
1	A	79	GLN	2
1	A	131	ASN	2
1	A	209	ARG	2
1	A	81	ASP	1
1	A	134	ASN	1
1	A	112	PHE	1
1	A	156	GLU	1
1	A	49	ASP	1
1	A	107	GLU	1
1	A	137	ASN	1
1	A	115	LEU	1
1	A	205	VAL	1
1	A	47	SER	1
1	A	54	SER	1
1	A	153	SER	1
1	A	9	CYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	161	LEU	1
1	A	166	SER	1
1	A	219	SER	1
1	A	18	SER	1
1	A	78	PHE	1
1	A	35	TYR	1
1	A	85	LYS	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 oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	JH3	A	300	-	19,19,19	1.10±0.00	2±0 (10±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is

considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	JH3	A	300	-	26,26,26	1.10±0.00	1±0 (5±1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	JH3	A	300	-	-	0±0,17,25,25	0±0,1,1,1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	300	JH3	C2-C1	2.48	1.52	1.46	4	20
2	A	300	JH3	O1-C1	2.09	1.39	1.34	16	20

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	300	JH3	O3-CA-C9	3.31	112.10	117.85	20	20
2	A	300	JH3	CB-O3-CA	2.02	62.68	60.78	6	7

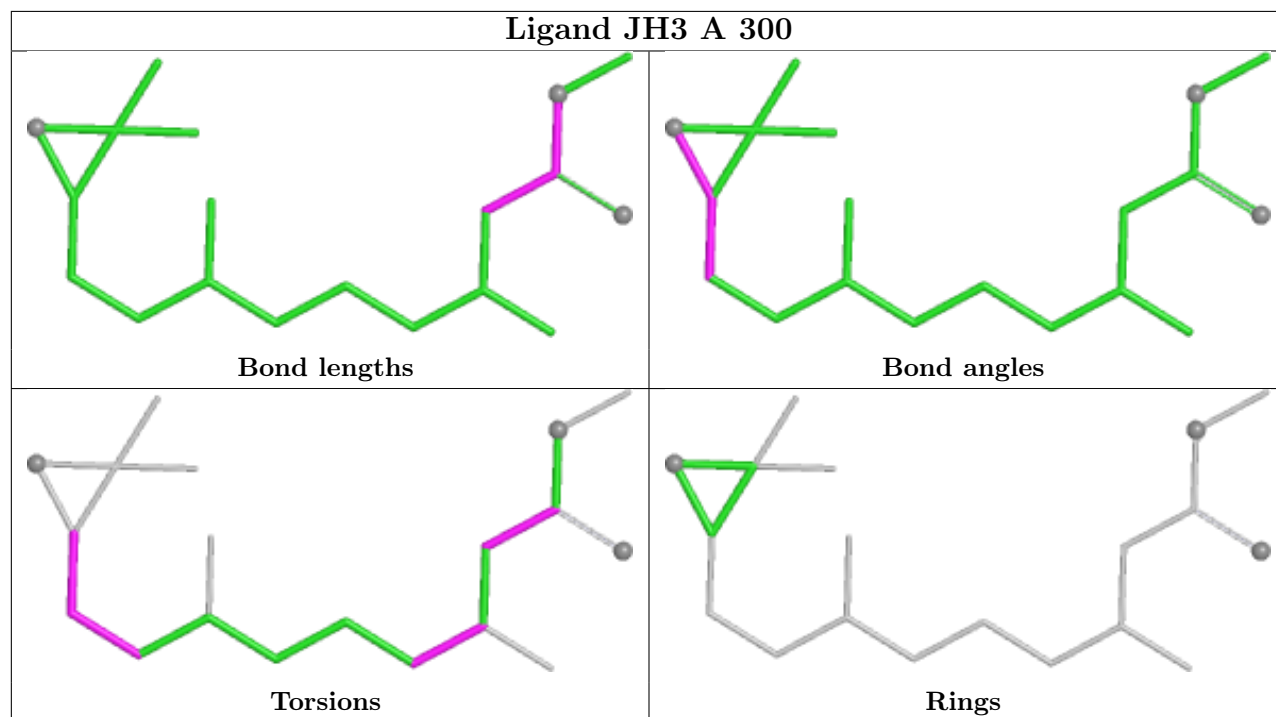
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided