



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 04:43 AM BST

PDB ID : 2NLU
Title : Domain-Swapped Dimer of the PWWP Module of Human Hepatoma-derived Growth Factor
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Deposited on : 2006-10-20

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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

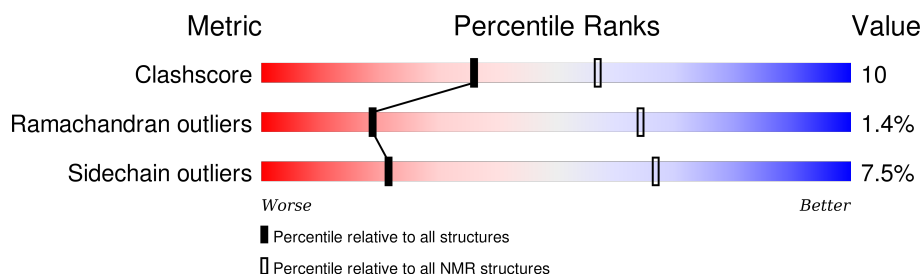
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	100	
1	B	100	

2 Ensemble composition and analysis

This entry contains 16 models. Model 13 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:10-A:32, B:144-B:191 (71)	0.67	15
2	A:43-A:91, B:109-B:132 (73)	0.81	13

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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	3, 6, 8, 9, 10, 11, 14
2	1, 4, 5, 12, 13
3	2, 7, 15, 16

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3219 atoms, of which 1587 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hepatoma-derived growth factor.

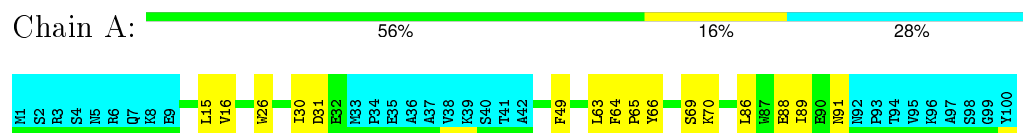
Mol	Chain	Residues	Atoms						Trace
1	A	100	Total	C	H	N	O	S	0
			1610	525	794	138	149	4	
1	B	100	Total	C	H	N	O	S	0
			1609	525	793	138	149	4	

4 Residue-property plots

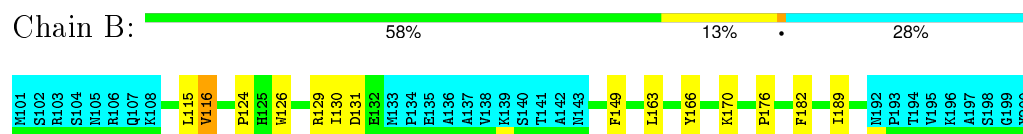
4.1 Average score per residue in the NMR ensemble

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: Hepatoma-derived growth factor



- Molecule 1: Hepatoma-derived growth factor

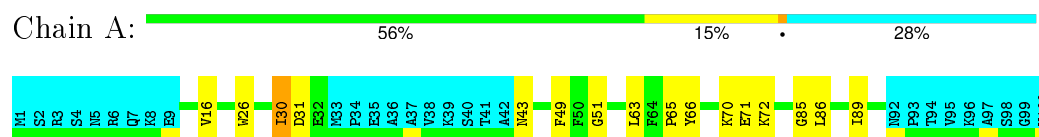


4.2 Scores per residue for each member of the ensemble

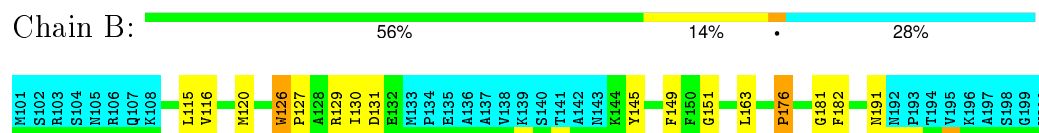
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Hepatoma-derived growth factor



- Molecule 1: Hepatoma-derived growth factor

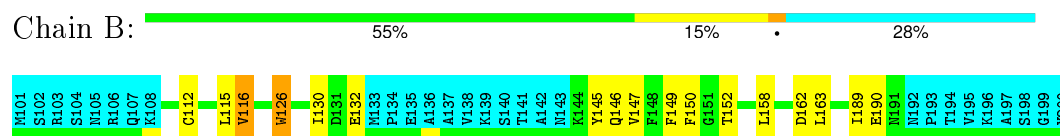


4.2.2 Score per residue for model 2

- Molecule 1: Hepatoma-derived growth factor

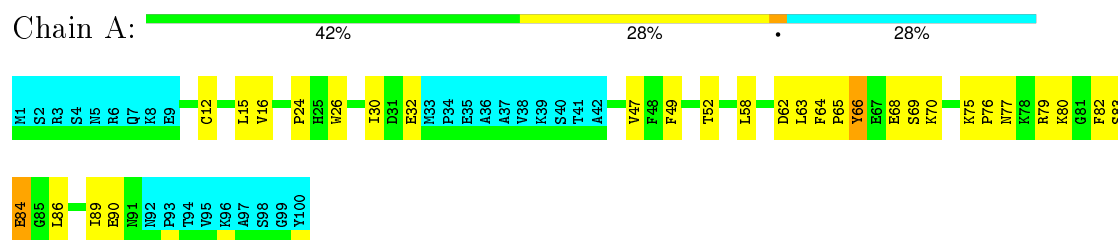


- Molecule 1: Hepatoma-derived growth factor

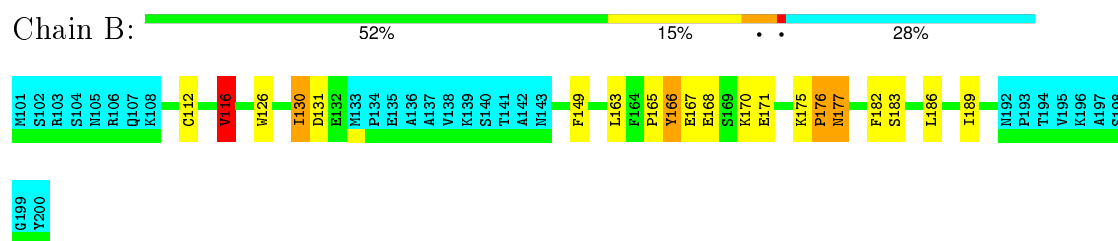


4.2.3 Score per residue for model 3

- Molecule 1: Hepatoma-derived growth factor



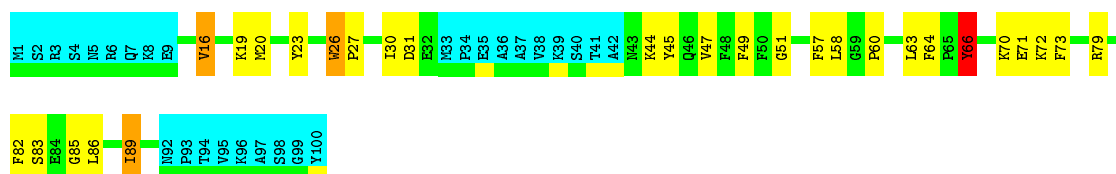
- Molecule 1: Hepatoma-derived growth factor



4.2.4 Score per residue for model 4

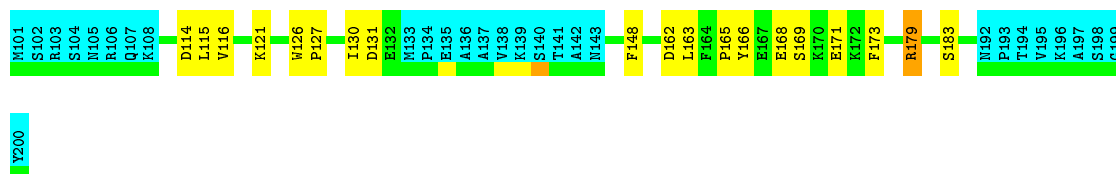
- Molecule 1: Hepatoma-derived growth factor





- Molecule 1: Hepatoma-derived growth factor

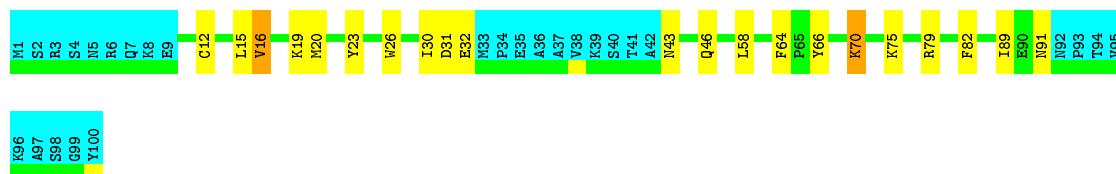
Chain B: 53% 18% 28%



4.2.5 Score per residue for model 5

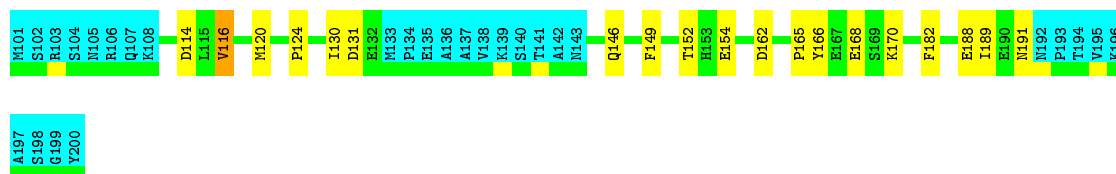
- Molecule 1: Hepatoma-derived growth factor

Chain A: 51% 19% 28%



- Molecule 1: Hepatoma-derived growth factor

Chain B: 53% 18% 28%



4.2.6 Score per residue for model 6

- Molecule 1: Hepatoma-derived growth factor

Chain A: 51% 19% 28%



699
Y100

- Molecule 1: Hepatoma-derived growth factor

Chain B: 

W101 S102 R103 S104 M105 R106 Q107 R108 E109 Y110 L115 V116 P124 H125 W126 I130 M133 P134 E135 A136 A137 V138 K139 S140 T141 A142 M143 K144 Y145 Q146 V147 F148 F149 F150 G151 F157 L158 L163 F164 K170 E184 G185 I189 M191 M192 P193 T194 V195 K196 A197

S198 G199 Y200

4.2.7 Score per residue for model 7

- Molecule 1: Hepatoma-derived growth factor

Chain A: 

M1 S2 R3 S4 N5 R6 Q7 R8 E9 C12 V16 W26 P27 I30 D31 E32 M33 P34 E35 A36 A37 V38 K39 S40 T41 A42 F49 F50 Q51 T52 L63 P64 P65 Y66 S69 K70 F73 R79 K80 G85 T89 N92 P93 T94 V95 K96 A97 S98

699
Y100

- Molecule 1: Hepatoma-derived growth factor

Chain B: 

W101 S102 R103 S104 M105 R106 Q107 R108 E109 L115 V116 P124 H125 W126 R129 I130 M133 P134 E135 A136 A137 V138 K139 S140 T141 A142 M143 L163 F164 P165 Y166 P176 F182 G185 L186 T189 M192 P193 T194 V195 K196 S198 G199 Y200

4.2.8 Score per residue for model 8

- Molecule 1: Hepatoma-derived growth factor

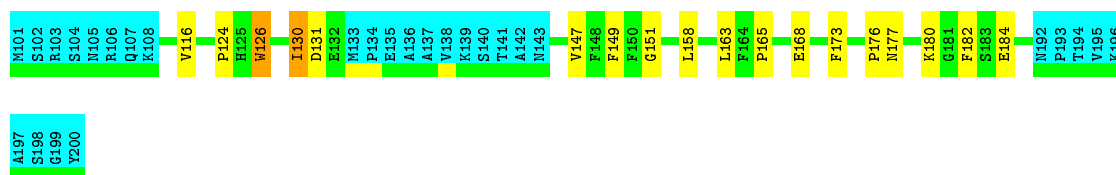
Chain A: 

M1 S2 R3 S4 N5 R6 Q7 R8 E9 C12 V16 W26 P27 I30 D31 E32 M33 P34 E35 A36 A37 V38 K39 S40 T41 A42 V47 F48 F49 E54 L58 P65 Y66 P76 F82 G85 L86 W87 E88 N91 P93 T94 V95 K96 A97 S98 G99

Y100

- Molecule 1: Hepatoma-derived growth factor

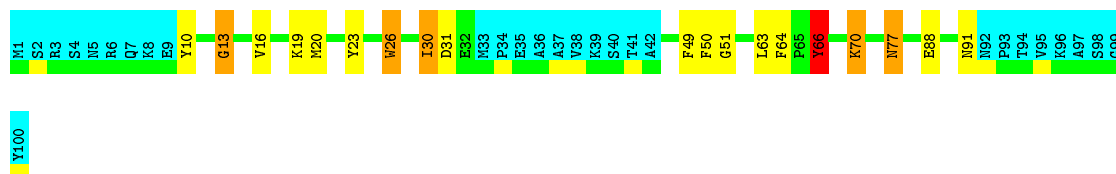
Chain B: 



4.2.9 Score per residue for model 9

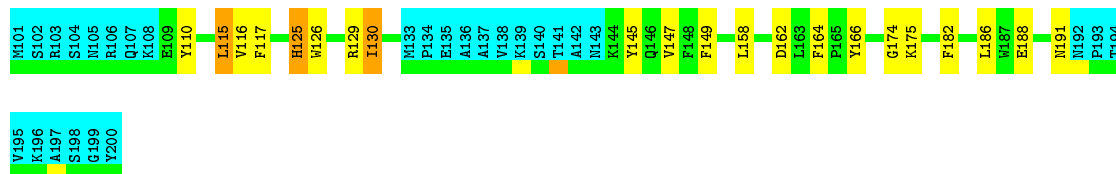
- Molecule 1: Hepatoma-derived growth factor

Chain A: 53% 13% 5% 28%



- Molecule 1: Hepatoma-derived growth factor

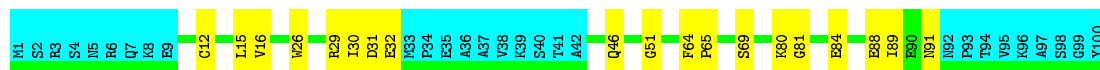
Chain B: 51% 18% 28%



4.2.10 Score per residue for model 10

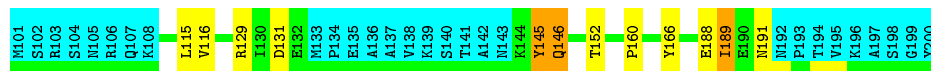
- Molecule 1: Hepatoma-derived growth factor

Chain A: 53% 19% 28%



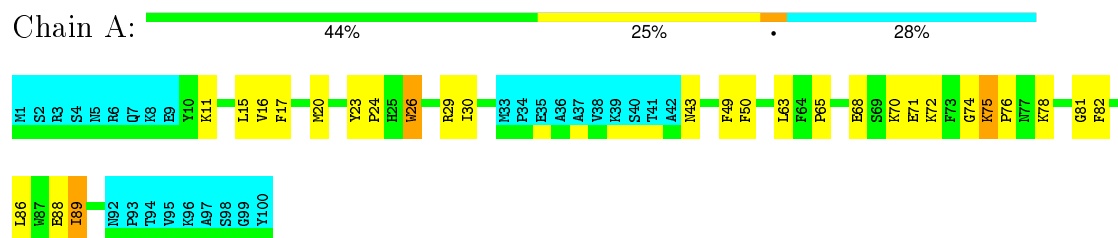
- Molecule 1: Hepatoma-derived growth factor

Chain B: 60% 9% 28%

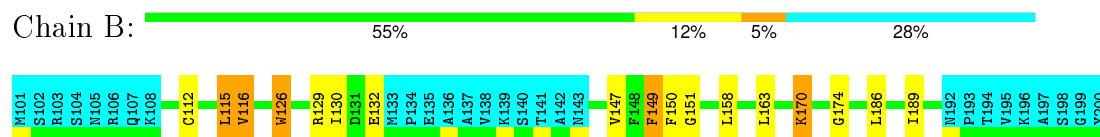


4.2.11 Score per residue for model 11

- Molecule 1: Hepatoma-derived growth factor

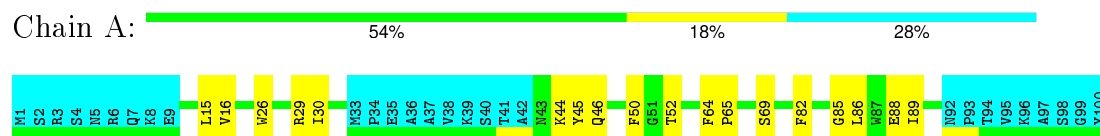


- Molecule 1: Hepatoma-derived growth factor

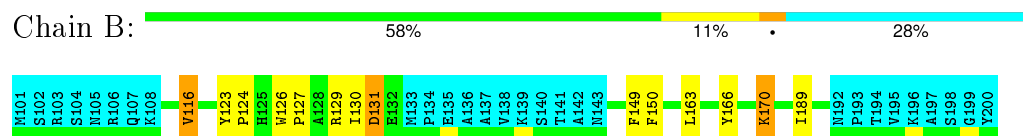


4.2.12 Score per residue for model 12

- Molecule 1: Hepatoma-derived growth factor

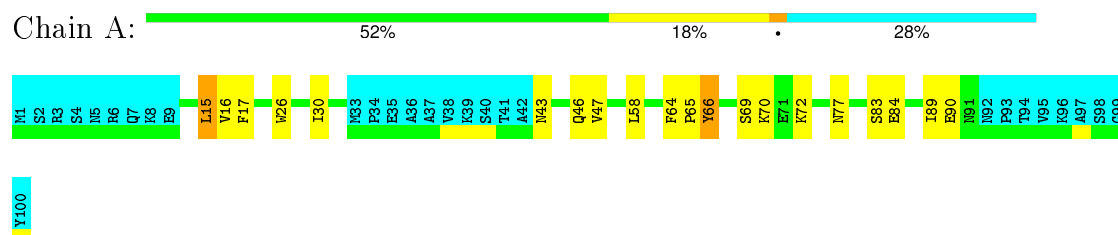


- Molecule 1: Hepatoma-derived growth factor



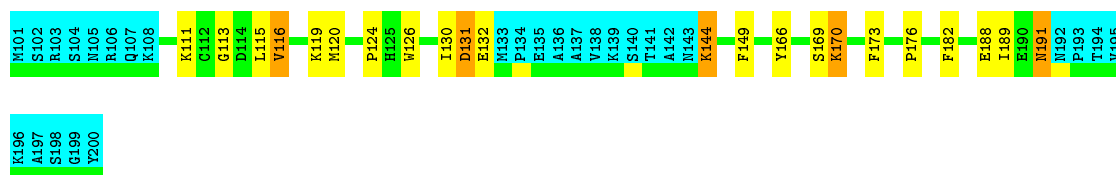
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Hepatoma-derived growth factor



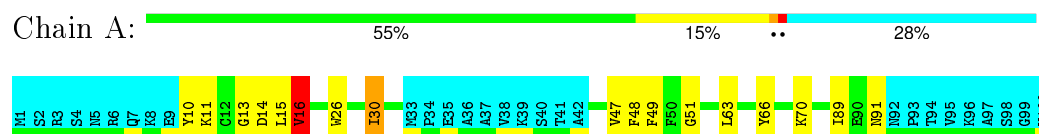
- Molecule 1: Hepatoma-derived growth factor



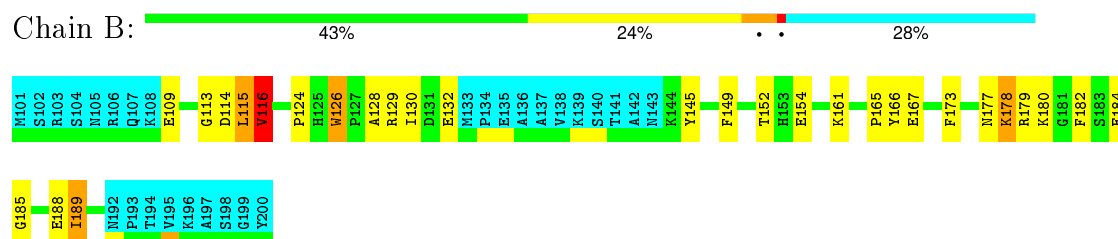


4.2.14 Score per residue for model 14

- Molecule 1: Hepatoma-derived growth factor

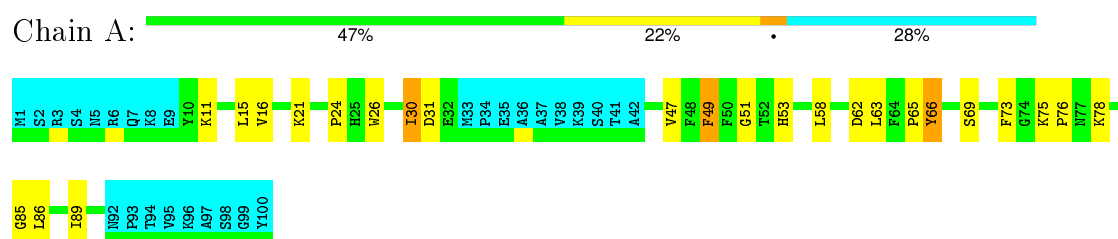


- Molecule 1: Hepatoma-derived growth factor

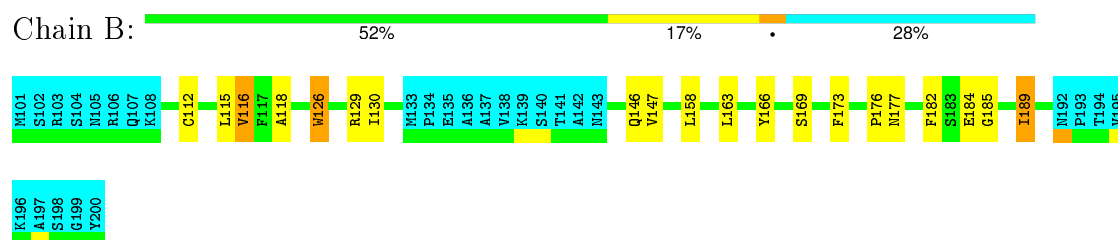


4.2.15 Score per residue for model 15

- Molecule 1: Hepatoma-derived growth factor



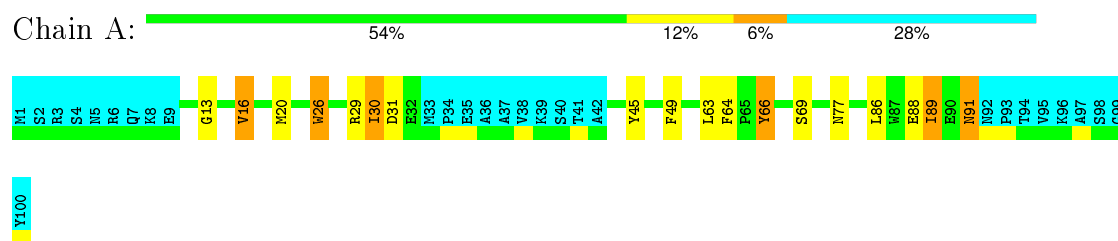
- Molecule 1: Hepatoma-derived growth factor



4.2.16 Score per residue for model 16

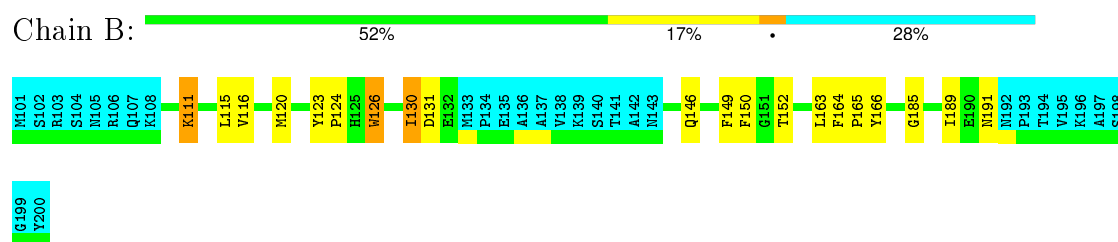
- Molecule 1: Hepatoma-derived growth factor

Chain A:



- Molecule 1: Hepatoma-derived growth factor

Chain B:



5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 16 were deposited, based on the following criterion: *The submitted structures are the 16 structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	1.2
ARIA	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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.41±0.08	0±1/628 (0.0±0.1%)	0.41±0.02	0±0/844 (0.0±0.0%)
1	B	0.39±0.04	0±0/629 (0.0±0.0%)	0.41±0.02	0±0/845 (0.0±0.0%)
All	All	0.41	4/20112 (0.0%)	0.41	0/27024 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	B	0.0±0.0	0.1±0.2
1	A	0.0±0.0	0.1±0.2
All	All	0	2

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
1	A	66	TYR	CE2-CZ	-9.67	1.25	1.38	4	2
1	A	66	TYR	CE1-CZ	9.36	1.50	1.38	4	2

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	B	145	TYR	Sidechain	1
1	A	66	TYR	Sidechain	1

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	605	579	577	18±4
1	B	606	579	577	16±4
All	All	19376	18528	18464	387

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ILE:HD11	1:B:145:TYR:HB3	0.96	1.38	14	2
1:A:65:PRO:HA	1:B:116:VAL:HG12	0.82	1.51	15	4
1:A:79:ARG:HA	1:A:83:SER:HB3	0.75	1.56	4	1
1:B:166:TYR:HE1	1:B:189:ILE:HG13	0.74	1.42	5	1
1:A:63:LEU:HB3	1:B:116:VAL:HG21	0.74	1.58	1	1
1:A:12:CYS:HB3	1:A:32:GLU:HB3	0.73	1.59	10	1
1:A:63:LEU:HG	1:B:116:VAL:CG2	0.72	2.14	9	5
1:A:75:LYS:HB3	1:A:86:LEU:HD13	0.72	1.59	6	1
1:A:63:LEU:HD21	1:B:116:VAL:HG21	0.71	1.62	14	4
1:A:19:LYS:HE2	1:B:162:ASP:HA	0.70	1.62	9	2
1:A:12:CYS:HB3	1:A:32:GLU:HG2	0.70	1.64	7	2
1:A:75:LYS:HD2	1:A:86:LEU:HD11	0.69	1.64	15	1
1:A:49:PHE:HE2	1:B:126:TRP:HB3	0.68	1.48	11	4
1:A:51:GLY:HA2	1:A:85:GLY:HA3	0.68	1.65	2	1
1:A:82:PHE:HA	1:B:126:TRP:NE1	0.68	2.03	12	1
1:A:48:PHE:HB2	1:B:129:ARG:HB2	0.67	1.66	14	1
1:A:15:LEU:HG	1:B:189:ILE:HG12	0.66	1.67	3	1
1:A:69:SER:HB2	1:A:73:PHE:CE1	0.66	2.26	15	1
1:A:27:PRO:HB2	1:B:189:ILE:HG13	0.65	1.67	7	1
1:A:20:MET:HB3	1:A:23:TYR:HB2	0.65	1.69	4	3
1:A:64:PHE:O	1:B:116:VAL:HB	0.64	1.92	5	9
1:A:85:GLY:O	1:A:89:ILE:HG22	0.64	1.93	4	2
1:A:66:TYR:HA	1:A:69:SER:OG	0.64	1.93	15	2
1:A:66:TYR:HB3	1:B:116:VAL:HA	0.63	1.69	16	1
1:A:16:VAL:HG21	1:B:163:LEU:HB3	0.62	1.71	12	3
1:A:66:TYR:HB2	1:A:70:LYS:HB3	0.61	1.70	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:GLY:HA3	1:B:126:TRP:CD1	0.61	2.30	14	1
1:B:177:ASN:HA	1:B:182:PHE:CD1	0.61	2.30	3	1
1:A:20:MET:HB2	1:B:149:PHE:CZ	0.61	2.30	16	3
1:A:51:GLY:HA3	1:B:126:TRP:HE1	0.61	1.56	4	2
1:A:51:GLY:HA3	1:B:126:TRP:NE1	0.61	2.10	4	1
1:A:89:ILE:HG13	1:B:115:LEU:HG	0.61	1.71	7	2
1:A:66:TYR:CE1	1:A:89:ILE:HG13	0.61	2.31	5	1
1:A:11:LYS:O	1:A:30:ILE:HG21	0.61	1.95	15	1
1:A:49:PHE:CE2	1:B:126:TRP:HB3	0.60	2.31	11	9
1:A:70:LYS:HA	1:A:74:GLY:HA3	0.60	1.73	11	1
1:A:88:GLU:HA	1:A:91:ASN:ND2	0.60	2.11	6	3
1:A:46:GLN:HB3	1:B:131:ASP:O	0.60	1.96	12	1
1:A:26:TRP:HB3	1:B:149:PHE:HE2	0.60	1.57	16	5
1:A:16:VAL:HB	1:B:164:PHE:O	0.60	1.97	7	4
1:A:12:CYS:HB2	1:A:32:GLU:HB3	0.59	1.75	8	1
1:B:188:GLU:HA	1:B:191:ASN:HD21	0.59	1.58	10	4
1:A:46:GLN:HB3	1:B:131:ASP:HB3	0.59	1.75	10	2
1:A:16:VAL:HG21	1:B:163:LEU:HD13	0.59	1.74	3	1
1:A:26:TRP:HE1	1:B:151:GLY:HA3	0.59	1.57	8	1
1:A:71:GLU:HG3	1:A:72:LYS:HG3	0.58	1.76	4	2
1:B:115:LEU:HD23	1:B:129:ARG:HA	0.58	1.75	15	1
1:A:88:GLU:HA	1:A:91:ASN:HD21	0.58	1.58	6	5
1:A:85:GLY:HA3	1:B:126:TRP:CH2	0.58	2.34	1	3
1:B:151:GLY:HA2	1:B:185:GLY:HA3	0.57	1.76	6	1
1:A:66:TYR:HB2	1:B:116:VAL:HG12	0.57	1.75	5	1
1:A:31:ASP:HA	1:B:145:TYR:HB3	0.57	1.75	2	1
1:A:86:LEU:HG	1:B:127:PRO:HG3	0.57	1.75	4	2
1:B:151:GLY:HA2	1:B:181:GLY:HA3	0.57	1.74	1	1
1:A:16:VAL:HG21	1:B:163:LEU:HG	0.57	1.75	6	1
1:A:66:TYR:O	1:A:70:LYS:HB2	0.57	2.00	14	4
1:A:76:PRO:HB2	1:A:78:LYS:HG3	0.57	1.75	15	1
1:A:89:ILE:HD11	1:B:115:LEU:HG	0.56	1.77	16	1
1:A:30:ILE:HD13	1:A:31:ASP:N	0.56	2.15	1	5
1:A:79:ARG:HB2	1:A:82:PHE:HB3	0.56	1.77	5	2
1:B:167:GLU:HA	1:B:170:LYS:HE3	0.56	1.76	3	1
1:A:50:PHE:CE2	1:B:129:ARG:HB2	0.56	2.35	11	2
1:A:29:ARG:HB2	1:B:150:PHE:CZ	0.56	2.36	16	2
1:B:188:GLU:HA	1:B:191:ASN:ND2	0.56	2.16	9	3
1:B:169:SER:HB2	1:B:173:PHE:CD2	0.55	2.37	15	1
1:A:66:TYR:O	1:A:70:LYS:HB3	0.55	2.02	5	3
1:B:111:LYS:HA	1:B:130:ILE:HG21	0.55	1.78	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:GLY:HA3	1:A:81:GLY:O	0.55	2.01	10	1
1:B:180:LYS:O	1:B:184:GLU:HG2	0.55	2.01	8	1
1:A:51:GLY:HA3	1:B:126:TRP:CH2	0.55	2.36	1	1
1:A:26:TRP:HB3	1:B:149:PHE:CE2	0.55	2.35	16	10
1:A:47:VAL:HG21	1:A:58:LEU:HB2	0.55	1.78	3	5
1:A:12:CYS:HB2	1:A:32:GLU:CB	0.55	2.32	8	1
1:B:112:CYS:HB2	1:B:132:GLU:HB3	0.55	1.78	2	1
1:B:169:SER:HB2	1:B:173:PHE:CE2	0.54	2.36	15	2
1:B:166:TYR:O	1:B:170:LYS:HB3	0.54	2.03	12	2
1:A:66:TYR:HD1	1:A:66:TYR:H	0.54	1.45	3	1
1:A:26:TRP:HB2	1:B:149:PHE:CE2	0.54	2.38	11	1
1:A:26:TRP:CH2	1:B:185:GLY:HA3	0.54	2.37	7	2
1:B:130:ILE:HD13	1:B:131:ASP:N	0.54	2.18	8	3
1:B:112:CYS:SG	1:B:132:GLU:HB3	0.54	2.43	11	1
1:A:80:LYS:HG3	1:A:84:GLU:OE2	0.54	2.03	3	1
1:A:17:PHE:HE2	1:B:170:LYS:HA	0.53	1.64	11	2
1:A:15:LEU:HD23	1:A:29:ARG:HG3	0.53	1.79	10	1
1:A:16:VAL:HA	1:B:166:TYR:HD2	0.52	1.64	16	1
1:A:16:VAL:HG12	1:B:165:PRO:HA	0.52	1.79	8	2
1:B:175:LYS:HD3	1:B:186:LEU:HD11	0.52	1.81	3	1
1:A:77:ASN:HA	1:A:83:SER:OG	0.52	2.05	3	1
1:A:10:TYR:O	1:A:14:ASP:HB2	0.52	2.04	14	1
1:A:76:PRO:HD2	1:A:82:PHE:CE2	0.52	2.40	8	1
1:A:10:TYR:O	1:A:30:ILE:HG21	0.52	2.05	14	1
1:B:176:PRO:HD2	1:B:182:PHE:CZ	0.52	2.40	3	1
1:B:115:LEU:HD23	1:B:116:VAL:N	0.51	2.20	13	3
1:B:149:PHE:HB2	1:B:154:GLU:HB2	0.51	1.82	5	2
1:A:16:VAL:HG21	1:B:163:LEU:HD21	0.51	1.80	4	3
1:A:15:LEU:HG	1:B:189:ILE:CG1	0.51	2.35	3	1
1:B:151:GLY:HA2	1:B:181:GLY:CA	0.51	2.35	1	1
1:B:147:VAL:HG21	1:B:158:LEU:HB2	0.51	1.81	15	5
1:B:185:GLY:O	1:B:189:ILE:HG22	0.51	2.04	15	2
1:B:120:MET:HB3	1:B:123:TYR:HB2	0.51	1.81	16	1
1:A:31:ASP:HB3	1:B:146:GLN:HB2	0.51	1.81	10	1
1:B:145:TYR:HB2	1:B:158:LEU:O	0.51	2.06	6	1
1:A:15:LEU:HD23	1:A:16:VAL:N	0.51	2.21	5	3
1:B:189:ILE:HD12	1:B:190:GLU:N	0.50	2.20	2	2
1:B:176:PRO:HA	1:B:182:PHE:HE2	0.50	1.66	15	1
1:A:66:TYR:HE1	1:A:89:ILE:HG13	0.50	1.66	5	1
1:B:168:GLU:O	1:B:171:GLU:HG2	0.50	2.07	3	1
1:B:176:PRO:HA	1:B:182:PHE:CE2	0.50	2.42	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:144:LYS:NZ	1:B:144:LYS:HB3	0.50	2.21	13	1
1:A:49:PHE:CB	1:A:54:GLU:HB2	0.50	2.36	8	1
1:A:15:LEU:HD11	1:B:189:ILE:HB	0.50	1.84	6	1
1:B:112:CYS:HB3	1:B:130:ILE:HD12	0.50	1.84	3	1
1:A:50:PHE:CD2	1:A:89:ILE:HG22	0.50	2.42	11	1
1:A:16:VAL:CG2	1:B:163:LEU:HG	0.50	2.37	16	3
1:B:110:TYR:HB2	1:B:130:ILE:HD12	0.49	1.84	6	1
1:A:69:SER:HA	1:A:72:LYS:HD3	0.49	1.84	13	1
1:A:49:PHE:HB2	1:A:54:GLU:HB2	0.49	1.84	8	1
1:A:16:VAL:HG12	1:B:166:TYR:CD1	0.49	2.43	7	1
1:A:89:ILE:HD12	1:A:90:GLU:N	0.49	2.22	13	1
1:A:76:PRO:HB3	1:A:83:SER:HA	0.49	1.83	2	1
1:A:45:TYR:HB3	1:B:131:ASP:HA	0.49	1.83	12	1
1:B:113:GLY:HA2	1:B:130:ILE:O	0.49	2.06	13	1
1:A:13:GLY:HA3	1:A:30:ILE:HG13	0.49	1.84	6	2
1:B:174:GLY:HA2	1:B:186:LEU:HD11	0.49	1.85	11	2
1:A:10:TYR:HB3	1:A:30:ILE:HG13	0.49	1.84	9	1
1:A:49:PHE:O	1:A:53:HIS:HA	0.49	2.08	15	1
1:A:16:VAL:HG11	1:B:163:LEU:HD13	0.49	1.84	12	1
1:A:16:VAL:HA	1:B:166:TYR:HB2	0.48	1.84	5	2
1:A:12:CYS:SG	1:A:32:GLU:HB3	0.48	2.48	5	1
1:B:178:LYS:HB3	1:B:182:PHE:CD2	0.48	2.43	14	1
1:B:115:LEU:HD22	1:B:115:LEU:C	0.48	2.28	9	1
1:A:65:PRO:O	1:A:69:SER:HB2	0.48	2.09	10	4
1:A:12:CYS:HA	1:A:30:ILE:HG22	0.48	1.86	10	2
1:A:77:ASN:HA	1:A:83:SER:HB3	0.48	1.86	13	1
1:A:58:LEU:HD22	1:B:118:ALA:HB1	0.48	1.86	15	1
1:A:72:LYS:HB2	1:A:72:LYS:NZ	0.47	2.24	1	1
1:B:147:VAL:HB	1:B:158:LEU:HD13	0.47	1.86	6	1
1:A:76:PRO:HD2	1:A:82:PHE:CE1	0.47	2.43	11	1
1:A:80:LYS:O	1:A:84:GLU:HG2	0.47	2.09	10	1
1:A:11:LYS:HD3	1:A:11:LYS:N	0.47	2.25	11	1
1:A:45:TYR:CE2	1:A:60:PRO:HG3	0.47	2.45	4	1
1:A:89:ILE:CD1	1:B:115:LEU:HG	0.47	2.40	10	1
1:B:167:GLU:HA	1:B:167:GLU:OE1	0.47	2.09	14	1
1:A:84:GLU:O	1:A:88:GLU:HG3	0.47	2.09	2	1
1:A:16:VAL:HG11	1:B:163:LEU:HD21	0.47	1.87	11	1
1:B:166:TYR:CE1	1:B:189:ILE:HG13	0.46	2.34	5	1
1:A:75:LYS:O	1:A:75:LYS:HG3	0.46	2.09	3	1
1:B:114:ASP:O	1:B:129:ARG:HA	0.46	2.10	14	1
1:A:13:GLY:HA2	1:A:30:ILE:O	0.46	2.11	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:PHE:HB3	1:A:88:GLU:HG2	0.46	1.86	12	2
1:A:81:GLY:HA3	1:B:126:TRP:HZ2	0.46	1.69	11	1
1:A:20:MET:HB3	1:A:23:TYR:HD2	0.46	1.71	5	1
1:A:76:PRO:HA	1:A:82:PHE:HE2	0.46	1.71	3	1
1:A:69:SER:HB2	1:A:73:PHE:HE1	0.46	1.67	15	1
1:A:63:LEU:HG	1:B:116:VAL:HG21	0.46	1.88	4	2
1:A:66:TYR:CD2	1:A:70:LYS:HD3	0.46	2.45	4	1
1:A:86:LEU:O	1:A:90:GLU:HB2	0.46	2.10	3	1
1:A:66:TYR:HA	1:A:69:SER:HB2	0.46	1.86	16	1
1:A:29:ARG:HB2	1:B:150:PHE:CE2	0.46	2.46	12	1
1:A:76:PRO:HB2	1:A:78:LYS:HE2	0.46	1.88	11	1
1:B:188:GLU:OE1	1:B:188:GLU:HA	0.46	2.11	10	1
1:B:115:LEU:HB3	1:B:129:ARG:HG3	0.46	1.87	9	1
1:A:89:ILE:HD13	1:A:89:ILE:O	0.46	2.11	2	1
1:B:169:SER:HB3	1:B:173:PHE:CE2	0.45	2.46	13	1
1:A:47:VAL:HB	1:A:58:LEU:HD13	0.45	1.88	15	3
1:B:165:PRO:HG2	1:B:168:GLU:HB3	0.45	1.87	4	1
1:A:49:PHE:CZ	1:B:120:MET:HB2	0.45	2.46	16	2
1:A:65:PRO:HA	1:B:116:VAL:CG1	0.45	2.42	6	1
1:A:79:ARG:HA	1:A:83:SER:CB	0.45	2.36	4	1
1:B:145:TYR:HE1	1:B:160:PRO:HD3	0.45	1.72	10	1
1:B:116:VAL:O	1:B:127:PRO:HA	0.45	2.12	12	1
1:A:63:LEU:HG	1:B:116:VAL:HG22	0.44	1.87	9	1
1:A:31:ASP:HB3	1:B:146:GLN:HB3	0.44	1.87	15	1
1:A:58:LEU:HB3	1:A:62:ASP:HB2	0.44	1.89	3	1
1:A:70:LYS:HG2	1:A:71:GLU:OE2	0.44	2.12	6	1
1:B:112:CYS:HA	1:B:130:ILE:HG22	0.44	1.87	2	1
1:A:26:TRP:CD1	1:B:151:GLY:HA3	0.44	2.46	11	1
1:A:66:TYR:CD1	1:B:116:VAL:HG12	0.44	2.47	9	1
1:B:184:GLU:O	1:B:188:GLU:HG2	0.44	2.12	14	1
1:B:176:PRO:HA	1:B:182:PHE:CD2	0.44	2.47	1	1
1:B:144:LYS:HD3	1:B:157:PHE:HB2	0.44	1.90	6	1
1:A:16:VAL:CG2	1:B:163:LEU:HD22	0.44	2.42	3	1
1:B:117:PHE:HB3	1:B:125:HIS:CD2	0.44	2.47	9	1
1:A:73:PHE:CD1	1:A:73:PHE:N	0.44	2.86	4	1
1:A:17:PHE:CE2	1:B:170:LYS:HA	0.44	2.47	13	2
1:A:12:CYS:SG	1:A:30:ILE:HD12	0.44	2.53	6	1
1:A:65:PRO:HB2	1:A:68:GLU:HB3	0.44	1.89	11	1
1:A:75:LYS:HD2	1:A:75:LYS:N	0.44	2.27	11	1
1:B:166:TYR:N	1:B:166:TYR:CD1	0.44	2.86	3	1
1:A:16:VAL:CG1	1:B:165:PRO:HA	0.44	2.43	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:VAL:HG13	1:B:163:LEU:HD22	0.43	1.89	12	1
1:B:179:ARG:HA	1:B:183:SER:HB3	0.43	1.88	4	1
1:A:86:LEU:HD23	1:A:86:LEU:O	0.43	2.13	8	1
1:A:31:ASP:O	1:B:146:GLN:HB3	0.43	2.13	16	2
1:B:111:LYS:CA	1:B:130:ILE:HG21	0.43	2.43	13	1
1:A:82:PHE:HB2	1:B:126:TRP:CZ2	0.43	2.49	2	2
1:A:52:THR:HG21	1:B:123:TYR:CE1	0.43	2.48	12	1
1:B:176:PRO:HA	1:B:182:PHE:HE1	0.43	1.73	7	1
1:B:112:CYS:CB	1:B:132:GLU:HB3	0.43	2.43	2	1
1:A:46:GLN:HB2	1:B:131:ASP:O	0.42	2.14	13	1
1:A:91:ASN:HD22	1:A:91:ASN:N	0.42	2.12	2	1
1:A:69:SER:HB3	1:A:73:PHE:CD2	0.42	2.48	7	1
1:A:47:VAL:CG1	1:B:128:ALA:HB1	0.42	2.44	14	1
1:A:65:PRO:HA	1:B:116:VAL:HG11	0.42	1.90	6	2
1:A:15:LEU:HD23	1:B:150:PHE:HE2	0.42	1.74	11	2
1:A:86:LEU:O	1:A:86:LEU:HD23	0.42	2.15	12	1
1:A:85:GLY:HA3	1:B:126:TRP:HH2	0.42	1.72	1	1
1:A:26:TRP:CZ2	1:B:182:PHE:HB2	0.42	2.49	5	2
1:A:86:LEU:O	1:A:89:ILE:HD13	0.42	2.14	11	1
1:A:26:TRP:CD1	1:A:27:PRO:HD2	0.42	2.49	4	1
1:A:15:LEU:HD13	1:A:16:VAL:N	0.42	2.29	12	1
1:A:58:LEU:HD21	1:B:120:MET:SD	0.42	2.54	5	1
1:B:173:PHE:N	1:B:173:PHE:CD1	0.42	2.87	8	2
1:B:179:ARG:HA	1:B:183:SER:CB	0.42	2.45	4	1
1:A:50:PHE:CZ	1:B:129:ARG:HB2	0.42	2.50	12	1
1:A:15:LEU:HG	1:B:189:ILE:HD11	0.42	1.91	13	1
1:A:15:LEU:HG	1:B:189:ILE:CD1	0.42	2.45	11	1
1:A:44:LYS:HG3	1:A:57:PHE:HB2	0.42	1.90	4	1
1:B:146:GLN:OE1	1:B:146:GLN:HA	0.42	2.15	15	1
1:A:66:TYR:O	1:A:70:LYS:HG2	0.41	2.15	4	1
1:A:31:ASP:HB3	1:B:148:PHE:HE1	0.41	1.75	4	1
1:B:115:LEU:HG	1:B:129:ARG:HA	0.41	1.92	1	1
1:B:111:LYS:N	1:B:111:LYS:HD2	0.41	2.31	16	1
1:B:115:LEU:HD13	1:B:115:LEU:O	0.41	2.16	9	1
1:A:85:GLY:HA3	1:B:126:TRP:CZ3	0.41	2.50	12	1
1:A:76:PRO:CB	1:A:83:SER:HA	0.41	2.45	2	1
1:B:110:TYR:CB	1:B:130:ILE:HG13	0.41	2.46	9	1
1:A:31:ASP:O	1:B:146:GLN:HB2	0.41	2.15	2	1
1:A:47:VAL:CG2	1:A:58:LEU:HB2	0.41	2.44	3	1
1:B:179:ARG:O	1:B:182:PHE:HB3	0.41	2.16	14	1
1:A:15:LEU:O	1:A:16:VAL:HG13	0.41	2.15	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:177:ASN:O	1:B:178:LYS:HB2	0.41	2.16	14	1
1:B:129:ARG:HH21	1:B:131:ASP:HB2	0.41	1.76	10	1
1:B:113:GLY:O	1:B:114:ASP:HB2	0.41	2.15	14	1
1:A:17:PHE:CE1	1:B:170:LYS:HA	0.41	2.51	6	1
1:B:165:PRO:HB3	1:B:168:GLU:HB2	0.41	1.93	5	1
1:B:177:ASN:HA	1:B:182:PHE:HD1	0.41	1.73	3	1
1:A:19:LYS:HB3	1:B:162:ASP:HB3	0.41	1.93	2	1
1:A:29:ARG:HD3	1:A:32:GLU:OE2	0.41	2.15	2	1
1:A:78:LYS:H	1:A:82:PHE:CB	0.41	2.29	11	1
1:B:115:LEU:HD13	1:B:115:LEU:HA	0.41	1.77	11	1
1:A:89:ILE:HG12	1:B:115:LEU:HD21	0.41	1.92	14	1
1:A:19:LYS:CE	1:B:162:ASP:HA	0.40	2.42	9	1
1:A:50:PHE:HE2	1:A:88:GLU:HB2	0.40	1.76	9	1
1:B:161:LYS:HD2	1:B:161:LYS:HA	0.40	1.76	14	1
1:A:75:LYS:HD3	1:A:86:LEU:HD22	0.40	1.93	6	1
1:B:177:ASN:OD1	1:B:183:SER:HA	0.40	2.16	3	1
1:A:77:ASN:N	1:A:77:ASN:HD22	0.40	2.14	9	1
1:B:119:LYS:HG3	1:B:124:PRO:O	0.40	2.16	13	1
1:B:175:LYS:HG2	1:B:186:LEU:HD21	0.40	1.93	3	1
1:A:87:TRP:O	1:A:91:ASN:ND2	0.40	2.54	2	1
1:A:19:LYS:HE3	1:B:162:ASP:HA	0.40	1.94	4	1
1:A:66:TYR:HD1	1:B:116:VAL:HG12	0.40	1.76	16	1
1:B:176:PRO:HA	1:B:182:PHE:CE1	0.40	2.51	13	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	72/100 (72%)	65±2 (90±3%)	6±2 (9±3%)	1±1 (1±1%)	24	71
1	B	72/100 (72%)	65±2 (90±3%)	6±2 (8±3%)	1±1 (2±2%)	15	58
All	All	2304/3200 (72%)	2076 (90%)	195 (8%)	33 (1%)	19	64

All 18 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	124	PRO	7
1	B	116	VAL	4
1	A	24	PRO	3
1	A	43	ASN	2
1	A	16	VAL	2
1	A	13	GLY	2
1	B	176	PRO	2
1	B	114	ASP	1
1	B	109	GLU	1
1	B	131	ASP	1
1	A	80	LYS	1
1	B	179	ARG	1
1	A	11	LYS	1
1	B	132	GLU	1
1	A	51	GLY	1
1	B	178	LYS	1
1	B	177	ASN	1
1	B	112	CYS	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	62/85 (73%)	58±2 (93±3%)	4±2 (7±3%)	23	68
1	B	62/85 (73%)	57±2 (92±3%)	5±2 (8±3%)	20	66
All	All	1984/2720 (73%)	1836 (93%)	148 (7%)	21	67

All 47 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	30	ILE	14
1	B	130	ILE	12
1	B	126	TRP	9
1	A	89	ILE	8
1	A	26	TRP	8
1	B	166	TYR	7
1	A	66	TYR	7

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Mol	Chain	Res	Type	Models (Total)
1	B	116	VAL	7
1	B	189	ILE	5
1	B	152	THR	5
1	A	16	VAL	5
1	B	115	LEU	4
1	A	91	ASN	4
1	B	131	ASP	3
1	B	170	LYS	3
1	A	52	THR	3
1	A	49	PHE	3
1	A	75	LYS	3
1	B	191	ASN	3
1	B	184	GLU	2
1	B	149	PHE	2
1	A	43	ASN	2
1	A	84	GLU	2
1	A	77	ASN	2
1	A	70	LYS	2
1	B	177	ASN	2
1	B	146	GLN	1
1	B	109	GLU	1
1	B	186	LEU	1
1	A	79	ARG	1
1	B	144	LYS	1
1	B	175	LYS	1
1	A	62	ASP	1
1	B	120	MET	1
1	A	86	LEU	1
1	A	21	LYS	1
1	B	121	LYS	1
1	A	68	GLU	1
1	A	25	HIS	1
1	B	180	LYS	1
1	B	171	GLU	1
1	A	15	LEU	1
1	B	111	LYS	1
1	B	132	GLU	1
1	B	114	ASP	1
1	A	71	GLU	1
1	B	125	HIS	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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided