wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2ERM
Title	:	Solution structure of a biologically active human FGF-1 monomer, complexed to a hexasaccharide heparin-analogue
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Deposited on	:	2005-10-25

This is a wwPDB NMR Structure Validation Summary 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 (i) symbol.

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

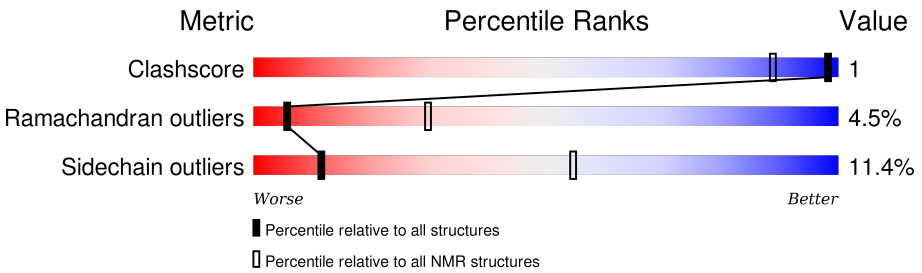
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	139	72% 12% • 11% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	A	GNS	156	12	-
2	A	GNS	160	6	-
2	A	IDR	157	14	-
2	A	IDS	159	9	-

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 20 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:27-A:104, A:108-A:126, A:130-A:150 (118)	0.51	2

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 2 single-model clusters were found.

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2263 atoms, of which 1103 are hydrogens and 0 are deuteriums.

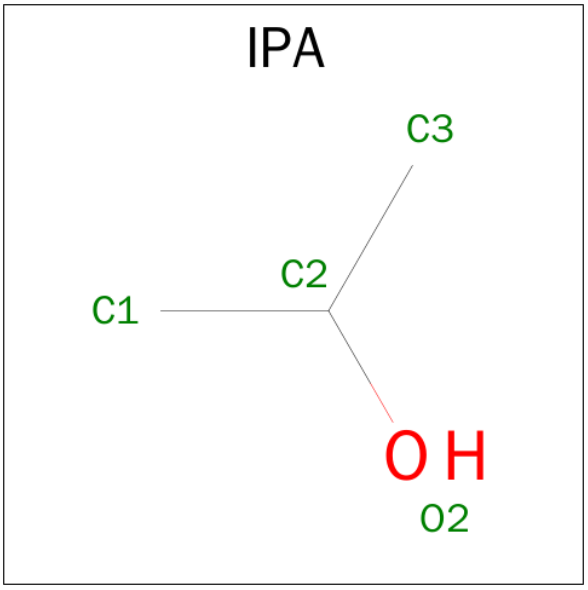
- Molecule 1 is a protein called Heparin-binding growth factor 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	133	2108	671	1044	185	204	4	0

- Molecule 2 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
2	A	6	144	38	52	3	46	5

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			
			Total	C	H	O
3	A	1	11	3	7	1

4 Residue-property plots (i)

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: Heparin-binding growth factor 1

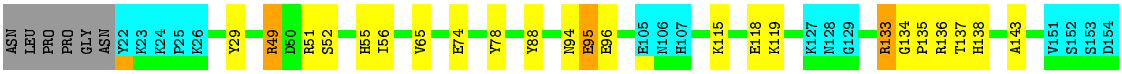
Chain A:

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: Heparin-binding growth factor 1

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Simulated annealing, restrained molecular dynamics.*

Of the 30 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
DYANA	structure solution	1.5
AMBER	refinement	5.0

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 (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GNS, IPA, IDR, IDS, NGY

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	0.58±0.01	0±0/964 (0.0±0.0%)	1.04±0.03	3±1/1304 (0.2±0.1%)
2	A	0.00±0.00	-	0.00±0.00	-
All	All	0.58	0/19280 (0.0%)	1.05	50/26080 (0.2%)

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	A	0.0±0.0	6.0±2.1
2	A	2.0±1.2	0.0±0.0
All	All	41	119

There are no bond-length outliers.

5 of 12 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	136	ARG	NE-CZ-NH2	-9.99	115.31	120.30	8	4
1	A	133	ARG	NE-CZ-NH2	-9.91	115.34	120.30	9	5
1	A	133	ARG	NE-CZ-NH1	9.51	125.05	120.30	4	7
1	A	136	ARG	NE-CZ-NH1	9.13	124.87	120.30	11	12
1	A	49	ARG	NE-CZ-NH1	7.88	124.24	120.30	6	7

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

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	157	IDR	C1	14
2	A	156	GNS	C1	12
2	A	159	IDS	C1	9
2	A	160	GNS	C1	6

5 of 24 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	A	134	GLY	Peptide	19
1	A	88	TYR	Sidechain	11
1	A	111	TYR	Sidechain	10
1	A	133	ARG	Sidechain,Peptide	9
1	A	29	TYR	Sidechain	9

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	942	925	925	1±1
2	A	92	52	46	0±1
All	All	20760	19680	19560	21

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 1.

5 of 13 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:ARG:HH12	2:A:157:IDR:C6	0.45	2.23	5	1
1:A:136:ARG:HH22	2:A:159:IDS:C6	0.44	2.25	20	1
1:A:132:LYS:NZ	2:A:160:GNS:O2S	0.43	2.51	9	1
1:A:118:GLU:OE2	1:A:119:LYS:NZ	0.41	2.52	17	6
1:A:95:GLU:OE2	1:A:115:LYS:NZ	0.41	2.54	2	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	118/139 (85%)	95±3 (81±3%)	17±3 (15±2%)	5±1 (4±1%)	6 30
All	All	2360/2780 (85%)	1908 (81%)	346 (15%)	106 (4%)	6 30

5 of 29 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	65	VAL	20
1	A	143	ALA	16
1	A	140	GLY	11
1	A	137	THR	8
1	A	126	LYS	6

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	103/122 (84%)	91±3 (89±2%)	12±3 (11±2%)	11 54
All	All	2060/2440 (84%)	1825 (89%)	235 (11%)	11 54

5 of 49 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	118	GLU	20
1	A	51	ARG	20
1	A	136	ARG	17
1	A	135	PRO	14
1	A	49	ARG	13

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)

6 carbohydrates are 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	IDS	A	155	2	13,16,17	1.27±0.06	0±0 (0±0%)
2	GNS	A	156	2	14,15,16	1.90±0.20	1±0 (6±2%)
2	IDR	A	157	2	9,12,13	0.83±0.12	0±0 (0±0%)
2	NGY	A	158	2	18,18,19	0.76±0.05	0±0 (0±0%)
2	IDS	A	159	2	13,16,17	1.28±0.11	0±0 (0±0%)
2	GNS	A	160	2	14,15,16	1.76±0.17	1±0 (6±2%)

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	IDS	A	155	2	16,24,26	1.26±0.22	0±0 (0±0%)
2	GNS	A	156	2	19,22,24	2.01±0.21	0±0 (2±2%)
2	IDR	A	157	2	12,17,19	1.17±0.35	0±0 (0±1%)
2	NGY	A	158	2	20,26,28	1.48±0.22	0±0 (0±1%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	IDS	A	159	2	16,24,26	1.22±0.31	0±0 (0±1%)
2	GNS	A	160	2	19,22,24	1.98±0.26	1±1 (3±4%)

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	IDS	A	155	2	-	0±0,5,26,29	0±0,1,1,1
2	GNS	A	156	2	-	0±0,7,24,27	0±0,1,1,1
2	IDR	A	157	2	-	0±0,0,21,24	0±0,1,1,1
2	NGY	A	158	2	-	0±0,10,27,30	0±0,1,1,1
2	IDS	A	159	2	-	0±0,5,26,29	0±0,1,1,1
2	GNS	A	160	2	-	1±0,7,24,27	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	156	GNS	S1-N	6.96	1.67	1.60	18	18
2	A	160	GNS	S1-N	6.85	1.67	1.60	1	17

5 of 10 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	156	GNS	C3-C2-N	6.86	119.57	110.36	14	2
2	A	160	GNS	O3S-S1-N	6.66	99.38	108.63	1	6
2	A	160	GNS	O2S-S1-N	6.57	99.50	108.63	14	3
2	A	159	IDS	C1-C2-C3	6.49	119.18	109.48	12	2
2	A	156	GNS	O3S-S1-N	5.90	100.43	108.63	20	4

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

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	157	IDR	C1	14
2	A	156	GNS	C1	12
2	A	159	IDS	C1	9

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Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	160	GNS	C1	6

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

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	160	GNS	C3-C2-N-S1	2
2	A	156	GNS	C3-C2-N-S1	1
2	A	159	IDS	S-O2-C2-C3	1

There are no ring outliers.

6.6 Ligand geometry (i)

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
3	IPA	A	15	-	3,3,3	0.64±0.01	0±0 (0±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
3	IPA	A	15	-	3,3,3	0.37±0.04	0±0 (0±0%)

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
3	IPA	A	15	-	-	0±0,0,0,0	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided